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WATER-MODERATED U(2.35)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(2.35)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 2.032 cm or 1.684 cm. Some of these experiments were performed without absorber plates, reflecting walls, or dissolved poison (LEU-COMP-THERM-001 and LEU-COMP-THERM-003). Others added absorber plates of various materials between clusters (LEU-COMP-THERM-017). Some circular, triangular-pitched lattices, with pitches of 1.598 cm or 1.895 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, or steel on two opposite sides of the cluster array. A total of 29 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. Primary references are 3, 5, and 6. References 11 - 15 provide supplementary information. Details which are from specific references are so noted.

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 The control blade, the safety blade, and any control or safety rods were withdrawn above the top water reflector for the reported configurations.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 below), no other apparatus was in the tank.[a] (See Figures 1 and 2.)

[a] Tank dimensions were from References 1 - 10. Other information was from private communication, Sid Bierman, July, 1993.

Figure 1. Experiment Tank.

Figure 2. Arranging Fuel Rods.

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

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. The acrylic support plate was supported by two

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

15.3 x 5.08 x 0.635 cm 6061 aluminum channels oriented so that the bottom surface of the support plate was 15.3 cm above the bottom of the tank.[a]

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

The top lattice plates were approximately 77 cm[c] above the fuel rod support plate. They were attached by half-inch-dimeter rods 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, these aluminum lattice supports were doubled, with no effect on the critical separation between clusters (Reference 1, pp. 26 and 28). The bottom lattice plates rested on the fuel rod support plate. The lattice plates were acrylic for the 2.032-cm-pitch experiments reported in References 3 and 5 and were polypropylene for the 1.684-cm-pitch experiments reported in References 5 and 6. The plates were 1.27 cm thick.[d]

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 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.[e]

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.[f]

1.2.5 Water Reflector - The top water surface was always at least 15 centimeters above the

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[a] 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)

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

[c] Reference 4, pp. 11 and 20. Also estimated from figures in Reference 1, pp. 4 and 6.

[d] Reference 4 (p. 20) gives the uncertainty in the thickness of the polypropylene plates as ± 0.4 cm.

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

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

top of the fuel region of the rods. (Reference 14, p. 132)[a] The bottom water reflector also was at least 15 centimeters thick, since the aluminum angle supporting the fuel-rod support plate above the bottom of the tank was 15.3 cm high. The minimum side-reflector thickness including reflecting walls, with the experiment centered in the tank and the longer side of the experiment parallel to the longer side of the tank, was 59 centimeters (Reference 4).

1.2.6 Reflecting Walls

Lead Walls. The lead walls (see Figure 3) are described in Appendix B of Reference 3: "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 Reference 3, Appendix A. The tongues were about 1¼ inches long and the grooves were about 1⅛ inches deep. The dimensions, weights, and enrichments of the slabs varied slightly. Major characteristics of each slab are shown in Table 1.

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

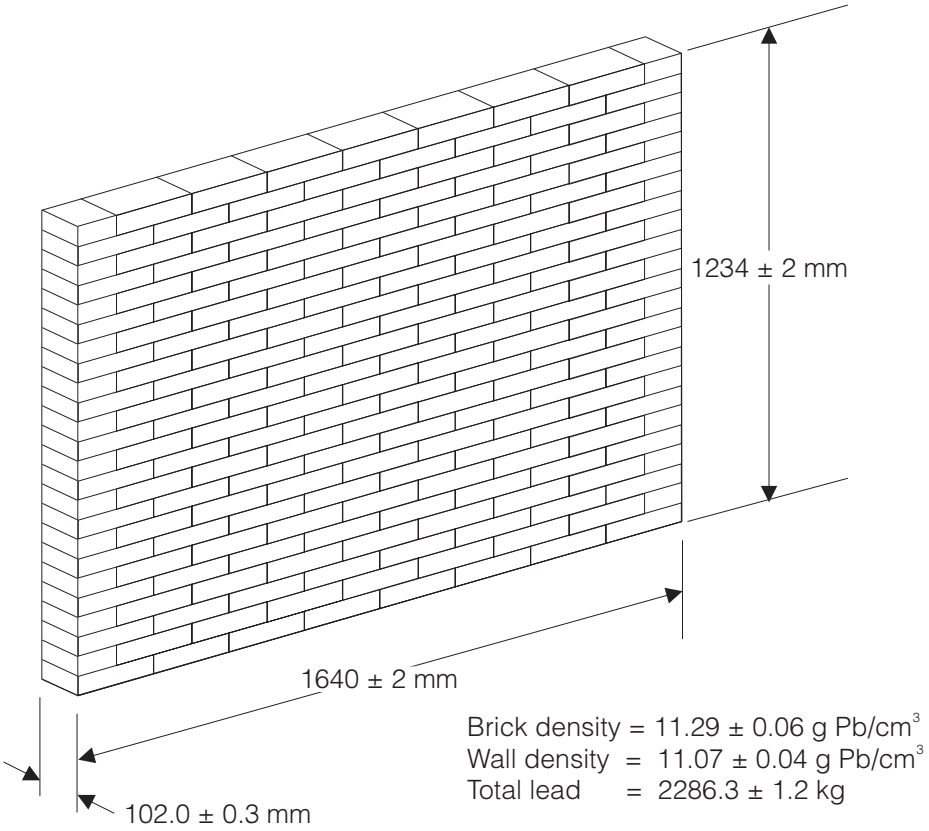


Figure 3. Assembled Lead Wall (Reference 3, Figure 6).

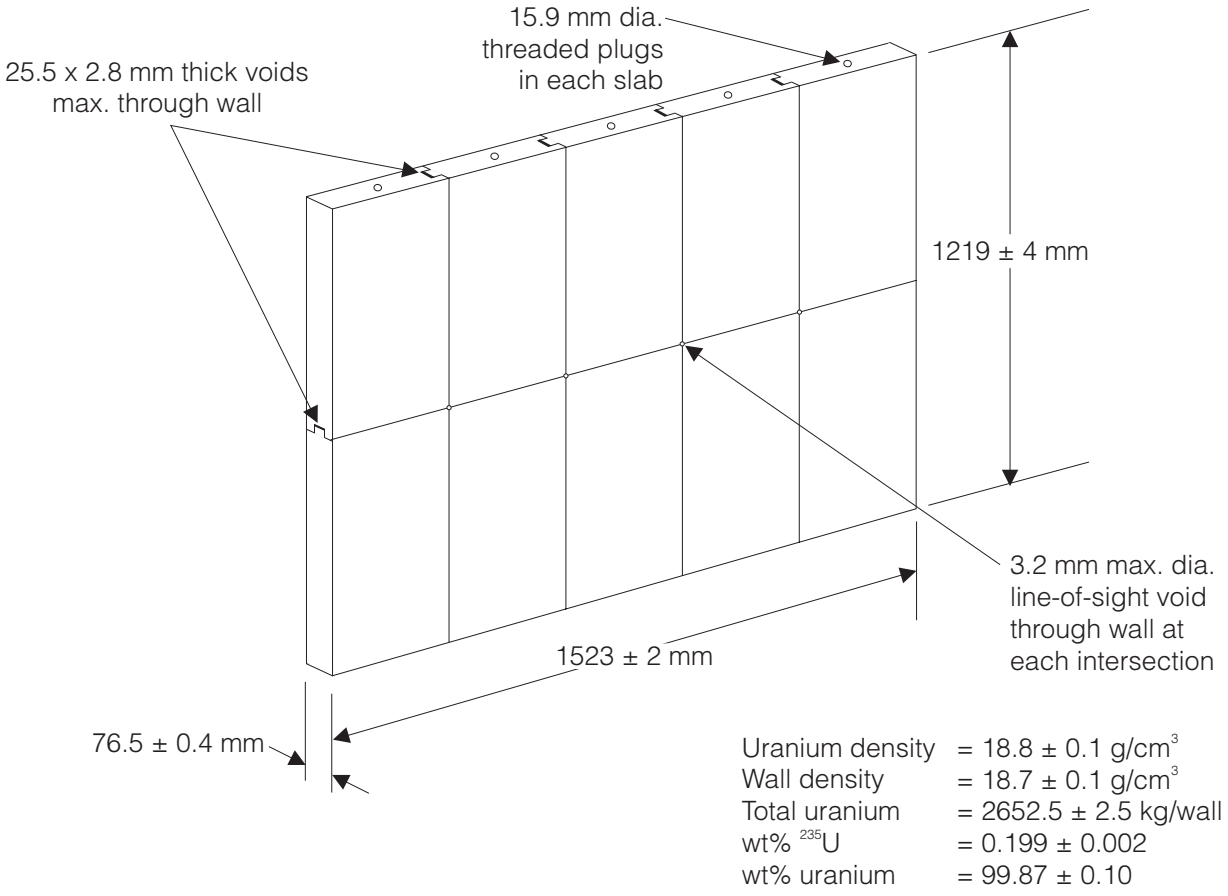


Figure 4. Assembled Depleted Uranium Wall (Reference 3, Figure 5).

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).

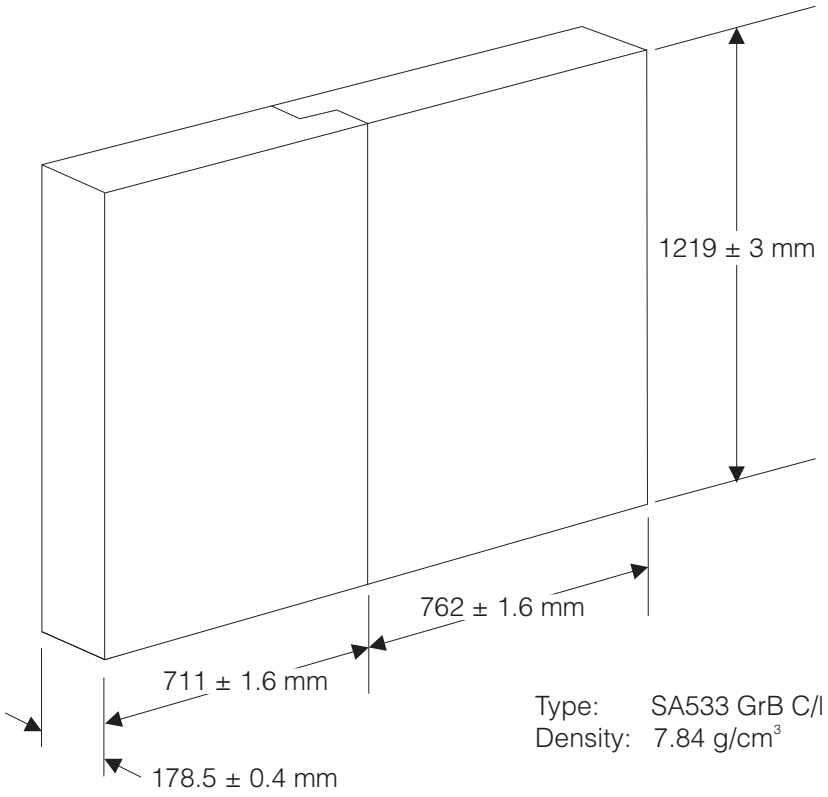


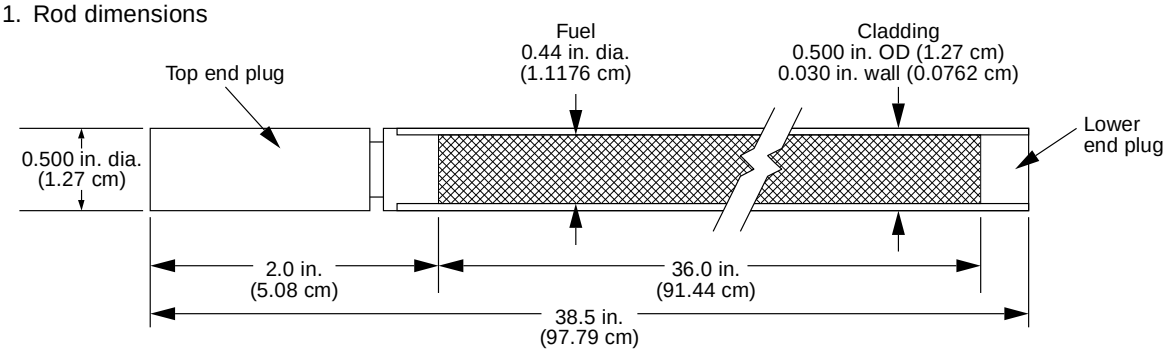
Figure 5. Steel Reflecting Walls (Reference 5, p. 10).

1.2.7 Fuel Rods - Fuel rod dimensions are given in diagrams in References 1, 3-6, and 8. These diagrams are the same as Figure 6, which is a reproduction of an annotated diagram from Reference 13 (Vol 1, p. 29). Reference 13 is cited by Reference 8, p. 2.7, as the source of fuel rod data.

Fuel specifications: 2.35% enriched UO_2

Fuel rods

1. Rod dimensions



2. Cladding: 6061 Aluminum tubing seal welded with a lower end plug of 5052-H32 Aluminum and a top plug of 1100 Aluminum.
3. Total weight of loaded fuel rods: 917 g (average)

Fuel loading
1. Fuel mixture vibrationally compacted.
2. 825 g of UO_2 powder/rod, 726 g of U/rod, 17.08 g of U-235/rod.
3. Enrichment - 2.35 ± 0.05 w/o U-235.
4. Fuel density - 9.20 g/cm (84% theoretical density).

Figure 6. $U(2.35)O_2$ Fuel Rod.

Dimensions of the U(2.35)O_2 fuel rods are summarized in Table 2.

Table 2. 2.35 Wt.% Enriched UO_2 Fuel Rod Dimensions.

Component	Length (cm)	Diameter (cm)
UO_2 fuel	91.44	1.1176
Top end plug (1100 Al)	5.08	1.27
Lower end plug (5052-H32 Al)	1.27	1.1176
Clad (6061 Al)	~93.19[(a)]	1.270 OD (.0762 cm thick)

(a) This length is an approximation based on measuring Figure B-1 in Reference 13 (Vol 1, p. 29). Total rod length is 97.79 cm. The clad envelops the lower end plug, fuel, and ~0.48 cm of the top end plug. Dimensions of the notch shown in the top end plug are not known.

1.2.8 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. All guides were 3.8 cm wide and were either 2.54 cm thick (Reference 3, p. 5) or 1.27 cm thick (Reference 4, p. 27), with a slot for the blades that was either 0.96 cm wide or 0.64 cm wide.[b] During one experiment from the first set of experiments, 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)

[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)

1.2.9 Experimental Method for Determining Critical Configuration[a] **-** The critical configuration was determined by measuring neutron detector count rates (above background) produced by subcritical configurations and extrapolating to the critical condition. In particular, the averages of several (usually four, five, or six) 80-second counts from each of two or three detectors were recorded for each configuration. Generally, the most reactive configuration measured was at least 99% of critical ($M > 100$).

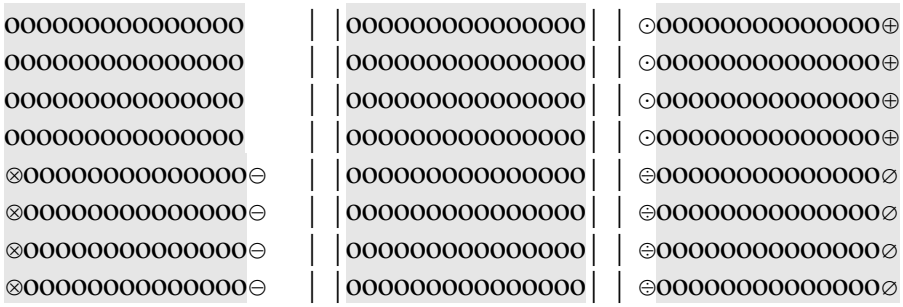
These experiments were with three clusters of predetermined sizes with predetermined separation from the reflecting walls. Separation distance between clusters was varied. The variables plotted were [separation distance]/[count rate] vs. [cluster separation] and [1]/[count rate] vs. [cluster separation]. At least two loadings close to critical were measured. The final result was the average cluster separation distance.[b]

To vary the number of fuel rods or cluster separation, fuel rods were moved in half-row or whole-row increments. An example of half-row increment moves for varying cluster separation is shown in Figure 7 for three 15-by-8-rod clusters. For the four configurations represented in this example, the numbers of empty rows between clusters are 2, 1¾, 1½, and 1¼. The initial configuration is shaded. The separation distance resulting from each of the three moves is determined by multiplying the number of empty rows between clusters by the pitch and adding the constant separation distance between lattice plates, required for the control and safety blade guides.[c]

[a] This information is from study of the logbooks (see Appendix B), which are stored at the Los Alamos National Laboratory Archives.

[b] Plots of both [separation]/[count rate] vs. [separation] and 1/[count rate] vs. [separation]) were used because one tended to overestimate the critical number of rods and the other to underestimate it. The lower critical number prediction was used in applying the operational safety rule that no more than 85% of the difference between latest loading and predicted critical loading could be added. As criticality was approached, both curves tended to predict the same critical number of rods. (Private communication, Duane Clayton, August, 1993.)

[c] Final rod additions were in half- or whole-row increments, so that the average rod worth of the addition was equal to the average rod worth of an entire row.



| | are safety and control blade guide widths
Initial load is shaded.
⊕ → ⊙ first move (1¾)[a]
⊗ → ⊖ second move (1½)[a]
⌀ → ⊜ third move (1¼)[a]

(a) This refers to the resulting average rows of separation between lateral clusters and central cluster after the stated move. Separation distance is then {[average rows of separation] x [pitch]} + [width of safety and control blade guides].

Figure 7. Method of Varying Separation Distances Between Clusters.

1.2.10 Critical Cluster Dimensions and Separations - Cluster sizes and separations for the 29 critical configurations are listed in Table 3. Each configuration consists of three fuel clusters. Typical arrangements of fuel clusters and reflecting walls are shown in Figures 8 and 9.

Table 3. $U(2.35)O_2$ Fuel Rod Critical Configurations. (See Figures 8 and 9.)

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	2.032	19 x 16	13.1[d] ± 0.01	0.0	lead	3 (14)
2	2.032	19 x 16	12.98[d] ± .01	0.66 ± 0.102	lead	3 (14)
3	2.032	19 x 16	10.51[d] ± .08	2.616 ± 0.076	lead	3 (14)
4	2.032	19 x 16	11.09[d] ± .02	0.0	uranium	3 (14)
5	2.032	19 x 16	13.19[d] ± .01	1.321 ± 0.076	uranium	3 (14)
6	2.032	19 x 16	13.37[d] ± .01	1.956 ± 0.102	uranium	3 (14)
7	2.032	19 x 16	12.96[d] ± .02	2.616 ± 0.076	uranium	3 (14)
8	2.032	19 x 16	9.95[d] ± .02	5.405 ± 0.102	uranium	3 (14)
9	2.032	19 x 16	7.82[d] ± .02	10.676 ± 0.152	uranium	3 (14)
10	2.032	19 x 16	9.888 ± .03	0.0	steel	5 (15)
11	2.032	19 x 16	10.438 ± .03	0.66 ± 0.102	steel	5 (15)
12	2.032	19 x 16	10.438 ± .02	1.321 ± 0.076	steel	5 (15)
13	2.032	19 x 16	9.598 ± .02	2.616 ± 0.107	steel	5 (15)
14	2.032	19 x 16	8.748 ± .05	3.912 ± 0.132	steel	5 (15)
15	1.684	25 x 18 (center) 20 x 18 (two outer)	8.566 ± .01	0.0	steel	5 (15)
16	1.684	25 x 18 (center) 20 x 18 (two outer)	9.166 ± .07	0.66 ± 0.102	steel	5 (15)
17	1.684	25 x 18 (center) 20 x 18 (two outer)	9.096 ± .02	1.321 ± 0.076	steel	5 (15)
18	1.684	25 x 18 (center) 20 x 18 (two outer)	9.246 ± .08	1.684 ± 0.013	steel	5 (15)

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)
19	1.684	25 x 18 (center) 20 x 18 (two outer)	8.866 ± .03	2.344 ± 0.103	steel	5 (15)
20	1.684	25 x 18 (center) 20 x 18 (two outer)	8.646 ± .02	3.005 ± 0.077	steel	5 (15)
21	1.684	25 x 18 (center) 20 x 18 (two outer)	8.126 ± .02	3.912 ± 0.132	steel	5 (15)
22	1.684	25 x 18 (center) 20 x 18 (two outer)	7.256 ± .06	6.726 ± 0.127	steel	5 (15)
23	1.684	23 x 18 (center) 20 x 18 (two outer)	9.646 ± .03	0.0	lead	6 (13)
24	1.684	23 x 18 (center) 20 x 18 (two outer)	9.696 ± .02	0.66 ± 0.102	lead	6 (13)
25	1.684	23 x 18 (center) 20 x 18 (two outer)	8.086 ± .02	3.276 ± 0.148	lead	6 (13)
26	1.684	23 x 18 (center) 20 x 18 (two outer)	7.646 ± .02	0.0	uranium	6 (13)
27	1.684	23 x 18 (center) 20 x 18 (two outer)	9.086 ± .03	1.321 ± 0.076	uranium	6 (13)

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)
28	1.684	23 x 18 (center) 20 x 18 (two outer)	9.416 ± .02	2.616 ± 0.107	uranium	6 (13)
29	1.684	23 x 18 (center) 20 x 18 (two outer)	8.776 ± .03	3.912 ± 0.132	uranium	6 (13)

(a) The first dimension is along the direction of cluster placement. Second dimension is the width of facing sides, as shown in Figures 8 and 9.
(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) Reported separations between clusters for this experiment were rod-surface-to-rod-surface (Sid Bierman, private communication, July, 1993), and not between cell boundaries, as was stated in Reference 3 (footnote d, Table II, p. 14). However, the reported separations are actually separations between edges of the holes of the lattice plates (Sid Bierman, private communication, February, 1994). The diameter of the holes was slightly larger than the fuel rod diameter, so that the hole-edge-to-hole-edge separation is 0.74 cm rather than 0.762 cm, which is the average rod-surface-to-rod-surface separation (0.762 cm = pitch – rod diameter). Therefore the cell boundary separations are 0.74 cm less than the separations reported in Reference 3 for the 2.032-cm pitch experiments. This is indicated by footnote (g) of Table II, p 14, Reference 3, which compares table values to previous experimental results from Reference 1. Values in this table have been corrected and are the distance between fuel-rod cell boundaries.

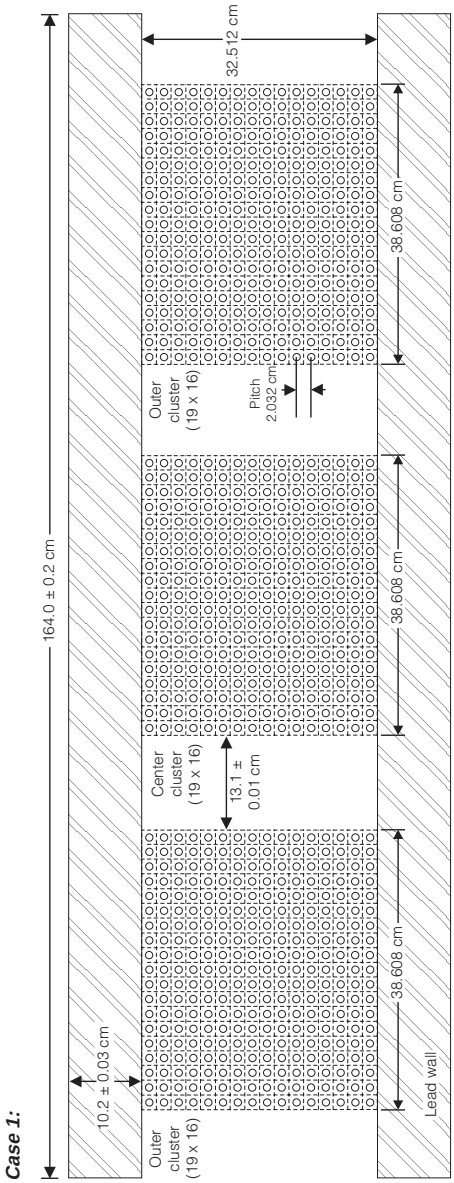


Figure 8. Critical Configuration of Case 1.

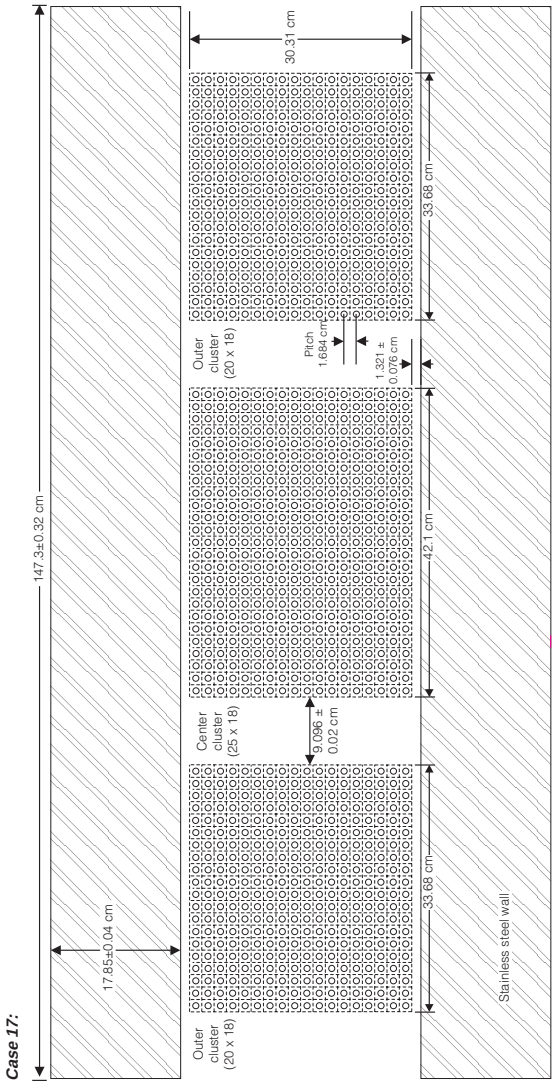


Figure 9. Critical Configuration of Case 17.

1.3 Description of Material Data

1.3.1 UO_2 Fuel - Figure 6 (from Reference 13, Vol. 1, p. 29) and results of a fuel rod sample analysis (Reference 13, Vol. 2, p. 3) are the basis for the fuel material characterization. A fuel rod contains 825 g of UO_2 powder, 726 g of 2.35 wt.% enriched uranium, and 17.08 g of ^{235}U, at an oxide density of 9.20 g/cm^3.[a] The isotopic content of the uranium is given in Table 4.

Table 4. Isotopic Composition of Uranium in 2.35% Enriched UO_2 Fuel Rods (Reference 8, pp. 2.7 and 2.8).

Uranium Isotope	Wt.%[(a)]
^{234}U	0.0137 ± .0007
^{235}U	2.350 ± .01
^{236}U	0.0171 ± .0007
^{238}U	97.62

(a) Values are originally from Reference 13, Vol 2, p. 3. Uncertainties are 3σ. Note that the total of all weight percents is 100.008.

Aluminum Alloys. Aluminum components of the fuel rods are the top (longer) end plug of 1100 aluminum, the lower end plug of 5052 aluminum, and the clad of 6061 aluminum. Measured densities and ASTM Standard chemical compositions of these three types of aluminum are given in Table 5.[b] The ASTM Standard for these three aluminum alloys includes limits on impurities to maximums of 0.05 wt.% each and 0.15 wt.% total.

Experiment support structures, including lattice plate supports and spacer rods, control/safety blade guides, tubes housing the proportional counters, and sleeves for gadolinium control rods, were 6061 aluminum alloy. The experimenters noted that doubling the amount of the aluminum angles supporting the grid plates in one experiment (Reference 1, p. 26) and the control and safety blade guides in another (Reference 1, p. 13) "resulted in no change in the predicted critical separation between fuel rod clusters." (Reference 1, p. 28)

[a] These values are not self-consistent. See discussion in Section 2.1.

[b] From Reference 8, pp. A.2-A.4, and from *Alcoa Aluminum Handbook*, Aluminum Company of America, 1967, pp. 46-50.

Table 5. Measured Densities and Standard Compositions of Aluminum Alloys.

Element	Wt.%
1100 Aluminum (density - 2.70 g/cm^3)	
Si	1.0 (combined maximum)
Fe	
Cu	0.05-0.20 (0.12 nominal)
Mn	0.05 (maximum)
Zn	0.10 (maximum)
Al	99.00 (minimum)
5052 Aluminum (density - 2.69 g/cm^3)	
Si	0.45 (combined maximum)
Fe	
Cu	0.10 (maximum)
Mn	0.10 (maximum)
Mg	2.2-2.8 (2.5 nominal)
Cr	0.15-0.35 (0.25 nominal)
Zn	0.10 (maximum)
Al	remainder (96.10-97.65)
6061 Aluminum (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)

1.3.2 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 Compositions 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)

1.3.3 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.

1.3.4 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

1.3.5 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]

1.3.6 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 14, 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 4, pp. 11 and 20; Reference 6, p. 3; Reference 14, p. 133)

1.3.7 Tank - 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.

[a] Estimated from occasional logbook values.

[b] Interpolated between 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, 1987, p. E-114.

2.0 EVALUATION OF EXPERIMENTAL DATA

Experiments were well documented and carefully performed. There were no significant omissions of data.

2.1 Fuel Rod Data

Some uncertainty exists in the characterization of the fuel rods. Dimensions and masses are stated in the source document (Reference 13, Vol. 1, p. 29) with no mention of measurement techniques or uncertainties. The 3σ-uncertainty in enrichment is stated as 0.01 wt.% without further discussion (Reference 13, Vol. 2, p. 3).

As was mentioned in Section 1.3.1, quantities characterizing the mass of fuel are not self-consistent. Table 8 gives the mass of ^{235}U derived in different ways from the given quantities. The highest and lowest masses represent a difference in uranium mass of less than 0.2% (726 g vs. 727.22 g).

Table 8. Mass of ^{235}U Per $U(2.35)O_2$ Fuel Rod Derived from Different Sets of Given Quantities.

U-235 mass derived from the following given quantities:	U-235 Mass (g)
U-235 mass[(a)]	17.08
Mass of U (726 g)[(b)] and 2.35 wt.% ^{235}U	17.0610
Mass of UO_2 (825 g)[(c)] and 2.07 wt.% ^{235}U in UO_2 [(d)]	17.0775[(e)]
UO_2 density (9.20 g/cm^3)[(c)], volume of fuel[(f)], and 2.07 wt.% ^{235}U in UO_2 [(d)]	17.0827
Mass of UO_2 (825 g)[(c)], 2.35 wt.% ^{235}U, and 2-to-1 ratio of O atoms to U atoms in UO_2	17.0896
Total rod mass (917 g)[(a)], volume[(f)] and density of aluminum, and 2.07 wt.% ^{235}U in UO_2 [(d)]	17.0775

(a) Given only in Reference 1.
(b) Given in References 1 and 8.
(c) Given in all reports on experiments with 2.35 wt.% enriched rods. (References 1, 3-6, and 8.)
(d) Reference 13, Vol. 2, p. 3.
(e) Using this mass and the given wt.%'s of the uranium isotopes gives a formula for uranium dioxide of $UO_{2.012}$. This is within the typical range for UO_2 powders of $UO_{2.005}$ and $UO_{2.129}$.[a]
(f) Calculated from reported dimensions.

The magnitudes of other uncertainties in fuel rod data are taken as half the value of the least significant digit, when the uncertainty is not given. The effects on k_{eff} of the uncertainties in enrichment, fuel diameter, fuel length, clad thickness, pitch, and uranium mass for a near-critical configuration are summarized in Table 9.[b] The last two entries are the calculated

[a] C.R. Tipton, Jr., ed., *Reactor Handbook, Second Edition*, Interscience Publishers, Inc., N.Y., vol. I, p. 292.

[b] Sensitivity studies described in this section used ONEDANT models, with ENDF/B-IV 27-group cross sections, of a homogeneous mixture representing an infinite slab of fuel rods. The

results from two models that contain a combination of individual changes. Results indicate that effects on k_{eff} due to uncertainties in fuel rod characterization and pitch could be as great as 0.30%. Note that this is for the case of all rods having all changes that affect k_{eff} positively, which is unlikely. However, uncertainties of ± 0.30% for 2.032-cm pitch and ± 0.25% for 1.684-cm pitch due to uncertainties in fuel rod characterization may be included in the benchmark-model k_{eff}.

Table 9. 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 →	2.032 cm	1.684 cm	2.032 cm	1.684 cm
Enrichment (± 0.01 wt.%[(b)])	+0.10	+0.08	-0.09	-0.13
Fuel Diameter (± 0.0127 cm)	+0.10	+0.03	-0.08	-0.02
Fuel Length (± 0.127 cm)	-0.07	+0.02	0.00	-0.02
Clad Diameter (± 0.00127 cm)	-0.00	+0.01	+0.01	+0.02
Pitch (± 0.0076 cm[(c)])	-0.14	+0.08	+0.21	-0.09
Uranium Mass (-0.81 g and +0.41 g)	+0.03	-0.01	+0.01	-0.01
Pitch →	2.032 cm		1.684 cm	
Simultaneously make all above changes that individually increase k_{eff}	Δk_{eff} = +0.30%		Δk_{eff} = +0.25%	
Simultaneously make all above changes that individually decrease k_{eff}	Δk_{eff} = -0.29%		Δk_{eff} = -0.20%	

(a) 27-group cross sections with homogenized lattice-cell fuel region (CSASIX); sample input given in Appendix D.
(b) 3σ uncertainty (Reference 13, Vol. 2, p. 3)
(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 ± .001 cm. Therefore, the calculated uncertainty is conservative.

calculations were P_3, S_{16}, with a convergence criterion of 10^{-6}.

2.2 Water Reflector

2.2.1 Top Reflector Thickness - The minimum thickness of the top water reflector is 15 cm above the fuel region. Since the top end plug is 2 inches (5.08 cm) long, the minimum water reflector thickness above the rods is 9.92 cm.

Calculations were performed for a an infinite-slab fuel region with a water reflector on both sides. ONEDANT and 27-group ENDF/B-IV cross sections, with a lattice-cell fuel region homogenized by XSDRNPM, were used. 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 0.002%. 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 less than 0.004%.

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 Thickness - 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 less than 0.002%. Replacing the outermost 8 cm of the 15-cm-thick water with 20% stainless steel in water affects k_{eff} by less than 0.006%. Therefore, lack of specifications about detectors, which were placed in the water reflector, does not affect acceptability of these experiments.

2.3 Gadolinium Impurity

Water impurity sensitivity studies in Appendix C indicate that only gadolinium and boron impurities significantly affect k_{eff}. No gadolinium or boron impurity is reported in references describing all of Cases 1 - 29.

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. ONEDANT calculations with 27-group cross sections, for an infinite slab of fuel pins reflected on both sides by 15 cm of water gave a change in k_{eff} of 0.01% between these two extremes of temperature for a pitch of 2.032 cm and 0.04% for a pitch of 1.684 cm. Therefore, estimates of the uncertainty in k_{eff} due to the effects of

temperature are half of these amounts, namely 0.005% for 2.032-cm pitch and 0.02% for 1.684-cm pitch.

2.5 Cluster Separations

The measurement uncertainties in cluster separation (see Table 3) vary from 0.01 cm to 0.08 cm. To calculate the effect on k_{eff}, cluster separations were reduced by the particular uncertainty for each of the 29 cases. Results are summarized in Table 10.[a] The largest differences in k_{eff} are 0.03% for 2.032-cm pitch and 0.05% for 1.684-cm pitch. These two values may be used as the k_{eff} uncertainty due to uncertainty in cluster separation.

[a] Sensitivity studies described in this section used TWODANT models, with ENDF/B-IV 27-group cross sections. A homogeneous mixture was used to model fuel rod clusters. Reflecting walls were modeled explicitly. The calculations were P_1, S_8, with a convergence criterion of 10^{-5}.

Table 10. 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	2.032	lead	0.01	0.004
2	2.032	lead	0.01	0.002
3	2.032	lead	0.08	0.029
4	2.032	uranium	0.02	0.008
5	2.032	uranium	0.01	0.002
6	2.032	uranium	0.01	0.008
7	2.032	uranium	0.02	0.004
8	2.032	uranium	0.02	0.003
9	2.032	uranium	0.02	0.034
10	2.032	steel	0.03	0.008
11	2.032	steel	0.03	0.006
12	2.032	steel	0.02	0.002
13	2.032	steel	0.02	0.007
14	2.032	steel	0.05	0.018
15	1.684	steel	0.01	0.004
16	1.684	steel	0.07	0.038
17	1.684	steel	0.02	0.010
18	1.684	steel	0.08	0.042
19	1.684	steel	0.03	0.017
20	1.684	steel	0.02	0.013
21	1.684	steel	0.02	0.011

Case No.	Pitch (cm)	Reflecting Wall Material	Uncertainty in Cluster Separation Measurement (cm)	$\%\Delta k_{eff}$ in Uncertainty of Benchmark-Model k_{eff} [(a)]
22	1.684	steel	0.06	0.051
23	1.684	lead	0.03	0.018
24	1.684	lead	0.02	0.011
25	1.684	lead	0.02	0.014
26	1.684	uranium	0.02	0.017
27	1.684	uranium	0.03	0.018
28	1.684	uranium	0.02	0.012
29	1.684	uranium	0.03	0.021

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

2.6 Reflecting Walls

2.6.1 Wall Composition - Three cases were chosen, based on apparent maximum effect of the wall, to determine the influence, if any, of 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, 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 0.022% Δk_{eff}. This can be included in the 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	+0.016
11.03 g/cm^3, 99.71 wt.% Pb	-0.014
11.03 g/cm^3, 99.71 wt.% Pb with 0.29 wt.% Impurities[(a)]	-0.014
Lead Walls Replaced with Water	-2.76

(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	+0.022
18.6 g/cm^3, 99.77 wt.% Uranium	+0.0034
18.6 g/cm^3, 99.87 wt.% Uranium with Impurities[(a)]	+0.016
Uranium Walls Replaced with Water	-2.41

(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).

Description	$\%\Delta k_{eff}$
7.84 g/cm^3, SS with 96.9 wt.% Fe, all other constituents, and 0.66 wt.% Ni	+0.0038
7.84 g/cm^3, SS with 96.64 wt.% Fe, all other constituents, and 0.92 wt.% Ni	+0.0031
Steel Walls Replaced with Water	-2.50

2.6.2 Wall-Cluster Separations - The measurement uncertainties in separation of the walls from the fuel-rod clusters (see Table 3) vary from 0.013 cm to 0.152 cm. To calculate the effect on k_{eff} of this uncertainty, reflecting wall separations were reduced by the particular uncertainty for each of the 29 cases. Results are summarized in Table 14. The largest differences in k_{eff} are 0.04% for 2.032-cm pitch and 0.10% for 1.684-cm pitch. These may represent the uncertainty in k_{eff} due to uncertainty in the wall separation measurement.

Table 14. 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	2.032	lead	0.102	0.028
3	2.032	lead	0.076	0.040
5	2.032	uranium	0.076	0.027
6	2.032	uranium	0.102	0.005
7	2.032	uranium	0.076	0.017
8	2.032	uranium	0.102	0.016
9	2.032	uranium	0.152	0.026
11	2.032	steel	0.102	0.002
12	2.032	steel	0.076	0.002
13	2.032	steel	0.107	0.024
14	2.032	steel	0.132	0.040
16	1.684	steel	0.102	0.014
17	1.684	steel	0.076	0.020
18	1.684	steel	0.013	0.004
19	1.684	steel	0.103	0.032
20	1.684	steel	0.077	0.040
21	1.684	steel	0.132	0.062
22	1.684	steel	0.127	0.036
24	1.684	lead	0.102	0.009
25	1.684	lead	0.148	0.097

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]
27	1.684	uranium	0.076	0.042
28	1.684	uranium	0.107	0.009
29	1.684	uranium	0.132	0.057

(a) Distance between reflecting walls and fuel clusters for Cases 1, 4, 10, 15, 23, and 26 is 0 cm, with no uncertainty. 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 three rectangular clusters, arranged in a row and flanked by two walls of lead, depleted uranium, or steel. Descriptions of the critical configurations, including cluster dimensions, cluster and wall separations, and fuel rod pitch, are given in Table 3 and in Figures 8 and 9.

Several sensitivity studies were performed to justify simplification of the benchmark model.

3.1.1 Clad Composition - In order to test the sensitivity of the critical configurations to the small amounts of alloying substances in the aluminum, a near-critical, cylindrical, water-reflected lattice of rods at pitch 2.032 cm was used. The thickness of the clad was increased so that the clad volume was equal to the volume of the actual clad plus the two end plugs, so that this calculation is a conservative estimate of the effects of varying the clad composition.

Four cases were calculated with ONEDANT. Clad for the four cases were each of the three alloys plus pure aluminum. Results are given in Table 15. The greatest change is 0.17%, for rods at 2.032 cm pitch when pure aluminum clad is used. Therefore, to more accurately represent the fuel rods for this benchmark, nominal amounts of all constituents are included in the specified aluminum alloys.

Table 15. Results of ONEDANT Calculations of k_{eff} for Cylindrical Arrangements of $U(2.35)O_2$ Fuel Rods with Different Aluminum Claddings.[a]

Clad Material (thickness increased from 0.07620 cm to 0.09788 cm)	Δk_{eff} (%) 2.032 cm pitch	Δk_{eff} (%) 1.684 cm pitch
6061 aluminum[b]	-	-
1100 aluminum[b]	0.04	0.01
5052 aluminum[b]	0.12	0.10
aluminum[c]	0.17	0.16

(a) 27-group, ENDF/B-IV homogenized fuel-rod mixture cross sections created by CSASIX.
(b) Alloys contain minimum amounts of aluminum and maximum amounts of other components (See Tables 5 and 15.).
(c) Density is nominal ^{27}Al density of 6061 aluminum alloy (97.325 wt.% of 2.69 g/cm^3)

3.1.2 Water Impurities - The effects on k_{eff} of impurities in the water moderator-reflector for a near-critical cylindrical cluster of $U(2.35)O_2$ fuel pins, as calculated by ONEDANT, are given in Appendix C. All impurities except boron and gadolinium affect the calculated value of k_{eff} by less than 0.005%. No boron or gadolinium impurity was recorded for experiments included in this evaluation, therefore, the uncertainty in k_{eff} can be ignored.

3.1.3 Lattice Plates - The acrylic and polypropylene lattice plates are omitted from the benchmark model. Results of a ONEDANT sensitivity study of a slab of homogenized fuel pins reflected by 15 cm of water are given in Table 16. The lattice plates were placed ~30 cm from the centers of the pins. The calculated estimate (~0.02%) of the effect on k_{eff} of the two lattice plates can be included in the uncertainty of the benchmark-model k_{eff}.

Table 16. Calculated Effect of Two Half-Inch-Thick Lattice Plates on k_{eff}.

Lattice Plate Material	Δk_{eff} (%)	Fuel Pin Pitch (cm)
None	-	2.032 1.684
Acrylic	+0.02	2.032
Polypropylene	+0.015 (top plate) -0.010 (bottom plate)	1.684

3.1.4 Bottom Reflector - The model of the bottom reflector is 2.54 cm of acrylic followed by 15.3 cm of water. The effects on k_{eff} of the one-inch-thick acrylic support plate directly beneath the fuel rods and the carbon steel tank 17.84 cm below the fuel rods were calculated using ONEDANT. Results are shown in Table 17. The conclusions are that replacing the carbon steel tank with water has no effect and replacing the acrylic support plate with water has a small effect (0.06%). Therefore the support plate is retained in the benchmark model.

Because of the negligible effect of materials beyond the water reflector region (see Section 2.2), concrete floors and walls are not included in the benchmark model.

Table 17. Calculated Effect[(a)] of Bottom Reflector Materials on k_{eff}.

Reflector			Δk_{eff} (%) (2.032 cm pitch)	Δk_{eff} (%) (1.684 cm pitch)
Inner 2.54 cm	Middle 15.3 cm	Outer 0.952 cm		
acrylic	water	carbon steel	-	-
acrylic	water	water	+0.00	-0.00
water	water	water	-0.05	-0.06

(a) ONEDANT slab model with CSAS 27-group cross sections and homogeneous fuel region mixture created by XSDRNPM. Reflector materials are on both sides of an infinite slab of the homogenized fuel-pin mixture.

3.2 Dimensions

Fuel rod dimensions, as modeled, are shown in Figure 10. The entire rod has a diameter of 1.27 cm and is 97.79 cm long. The UO_2 fuel region has a diameter of 1.1176 cm and is 91.44 cm long. The clad is 0.0762 cm thick and 93.19 cm long. The clad surrounds the fuel, the lower end plug, and 0.48 cm of the top end plug. There is no gap between the clad and fuel or end plugs. The top end plug is 5.08 cm long. The lower end plug is 1.27 cm long.

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, which includes the reflecting walls on the two sides and extends beyond the ends of the reflecting walls at the ends. The top reflector is 15.2 cm of water.

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.

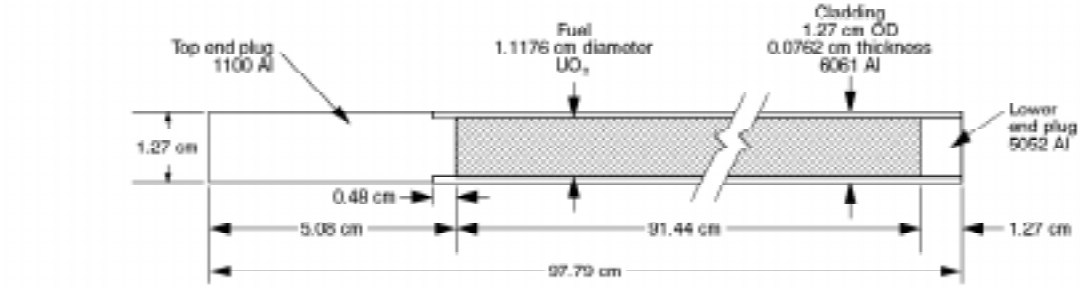


Figure 10. Fuel Rod Model.

3.3 Material Data

3.3.1 Fuel Rods - The fuel region consists of 825 g of UO_2. The mass of ^{235}U in each rod is 17.08 g. The isotopic composition of the uranium is 0.0137 wt.% ^{234}U, 2.35 wt.% ^{235}U, 0.0171 wt.% ^{236}U, and 97.6192 wt.% ^{238}U.[a]

Fuel rods have 6061 aluminum clad, with a 5052 aluminum lower end plug and a 1100 aluminum top end plug, as shown in Figure 12. Aluminum clad and end-plug components are nominal, mid-range, half-maximum, or minimum values, totaling 100 wt.%, as given in Table 5. Fuel rod atom densities are given in Table 18.

[a] This is slightly less than the wt.% for ^{238}U of 97.62 quoted in Section 1, in order that all weight percents add to 100. It is inferred from a footnote to Table I, Reference 13, vol. 2, p. 3, that the wt.% of ^{238}U is the balance. Therefore, the ^{238}U wt.% of the benchmark model is determined by balance.

Table 18. Fuel Rod Atom Densities.

Material	Isotope	Wt.%	Atom Density (barn-cm)$^{-1}$
$U(2.35)O_2$ fuel	^{234}U	-	2.8563×10^{-6}
	^{235}U		4.8785×10^{-4}
	^{236}U		3.5348×10^{-6}
	^{238}U		2.0009×10^{-2}
	O		4.1202×10^{-2}
1100 Aluminum (top end plug; 2.70 g/cm^3)	Al	99.0	5.9660×10^{-2}
	Cu	0.12	3.0705×10^{-5}
	Mn	0.025	7.3991×10^{-6}
	Zn	0.05	1.2433×10^{-5}
	Si	0.4025	2.3302×10^{-4}
	Fe	0.4025	1.1719×10^{-4}
5052 Aluminum (lower end plug; 2.69 g/cm^3)	Al	96.65	5.8028×10^{-2}
	Cr	0.25	7.7888×10^{-5}
	Cu	0.05	1.2746×10^{-5}
	Mg	2.5	1.6663×10^{-3}
	Mn	0.05	1.4743×10^{-5}
	Zn	0.05	1.2387×10^{-5}
	Si	0.225	1.2978×10^{-4}
	Fe	0.225	6.5265×10^{-5}
6061 Aluminum (clad; 2.69 g/cm^3)	Al	97.325	5.8433×10^{-2}
	Cr	0.2	6.2310×10^{-5}
	Cu	0.25	6.3731×10^{-5}
	Mg	1.0	6.6651×10^{-4}
	Mn	0.075	2.2115×10^{-5}
	Ti	0.075	2.5375×10^{-5}
	Zn	0.125	3.0967×10^{-5}
	Si	0.6	3.4607×10^{-4}
	Fe	0.35	1.0152×10^{-4}

3.3.2 Reflecting Walls - Lead, uranium, and steel wall atom densities are given in Table 19.

Table 19. Reflecting Wall Atom Densities.

Material	Isotope	Wt.%	Atom Density (barn-cm)$^{-1}$
Lead (11.07 g/cm^3)	Pb	99.87	3.2132 x 10^{-2}
Depleted Uranium (18.7 g/cm^3)	^{235}U ^{238}U	0.0020 0.9967	9.5220 x 10^{-5} 4.7151 x 10^{-2}
Steel (7.84 g/cm^3)	Fe C Mn P S Si Ni Mo Cr Cu	96.77 0.19 1.28 0.004 0.006 0.22 0.79 0.49 0.12 0.13	8.1810 x 10^{-2} 7.4686 x 10^{-4} 1.1000 x 10^{-3} 6.0971 x 10^{-6} 8.8332 x 10^{-6} 3.6983 x 10^{-4} 6.3552 x 10^{-4} 2.4114 x 10^{-4} 1.0896 x 10^{-4} 9.6587 x 10^{-5}

3.3.3 Moderator-Reflector - Fuel rods rest on an acrylic support plate, with a density of 1.185 g/cm^3 and a composition 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 20.

Table 20. Moderator-Reflector Atom Densities.

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

(a) This is 0.997766 g/cm^3, interpolated from densities at 20 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°C 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 of temperature variation (see Section 2.4) demonstrated that the effects on k_{eff} of temperature were small (less than 0.005% per degree C). The effect is included in the uncertainty of the benchmark-model k_{eff}. Therefore, any reasonable approximation to room temperature may be used in the model.

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 reflector beyond 30.5 cm of water and reflecting walls on the sides, 15.2 cm of water above, and 15.3 cm of water below; no measurement devices in the water, no notch in the top end plug) were judged to have negligible effect on k_{eff}. However, some other experimental uncertainties and model simplifications, described in sensitivity studies in Sections 2 and 3.1, contribute to the estimated uncertainty in the benchmark-model k_{eff}. Those included are listed in Table 21.

Table 21. Uncertainty in Benchmark-Model k_{eff}.

Measurement Uncertainty or Model Simplification	Δk_{eff}	
Pitch→	2.032 cm	1.684 cm
Fuel Rod Characterization	0.0030	0.0025
No Lattice Plates	0.0002	0.0002
Temperature	0.00005	0.0002
Cluster Separation	0.0003	0.0005
Reflecting Wall Composition/Density	0.0002	0.0002
Reflecting Wall Separation	0.0004	0.0010
Total Uncertainty in k_{eff}[(a)]	0.0031	0.0028

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

Therefore, for Cases 1 - 14 at 2.032-cm pitch, the benchmark-model k_{eff} is 1.0000 ± 0.0031. For Cases 15 - 29 at 1.684-cm pitch, the benchmark-model k_{eff} is 1.0000 ± 0.0028.

4.0 RESULTS OF SAMPLE CALCULATIONS

Results of calculations representing the twenty-nine critical configurations are presented in Tables 22 and 23. Code versions and modeling options are discussed briefly in paragraphs preceding the input listings in Appendix A.

For cases at 2.032-cm pitch (Cases 1 - 14), approximately three-quarters of the results are below the range of k_{eff} that includes the estimated uncertainty, and except two cases, k_{eff} is slightly underpredicted for all three codes. For the remaining cases, at 1.684-cm pitch, (Cases 15 - 29), all of the KENO results except two cases are below the range of k_{eff} that includes the estimated uncertainty. KENO with Hansen-Roach cross sections underpredicts k_{eff} by 2.0-3.8%. For the smaller pitch cases (Cases 15 - 29), KENO with Hansen-Roach cross sections predicts k_{eff} about 2% less than the larger pitch cases (Cases 1 - 14). KENO with 27-group ENDF/B-IV cross sections slightly underpredicts k_{eff}. MCNP with ENDF/B-V continuous cross sections also slightly underpredicts k_{eff}.

Table 22. Sample Calculation Results for $U(2.35)O_2$ Fuel Rods, 2.032-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	0.9958 ± .0016	0.9945 ± .0017	1.0036 ± .0016
2	0.9926 ± .0016	0.9947 ± .0017	1.0002 ± .0015
3	0.9951 ± .0017	0.9932 ± .0015	0.9976 ± .0016
4	0.9875 ± .0016	0.9905 ± .0016	0.9960 ± .0017
5	0.9887 ± .0015	0.9923 ± .0016	0.9979 ± .0016
6	0.9909 ± .0013	0.9944 ± .0015	0.9998 ± .0016
7	0.9933 ± .0015	0.9921 ± .0016	0.9975 ± .0015
8	0.9924 ± .0015	0.9919 ± .0015	0.9954 ± .0013
9	0.9937 ± .0016	0.9923 ± .0015	0.9946 ± .0015
10	0.9910 ± .0016	0.9971 ± .0015	0.9993 ± .0018
11	0.9904 ± .0016	0.9953 ± .0018	0.9973 ± .0017
12	0.9928 ± .0017	0.9956 ± .0016	0.9972 ± .0017
13	0.9935 ± .0016	0.9942 ± .0018	0.9986 ± .0015
14	0.9915 ± .0017	0.9953 ± .0017	0.9987 ± .0015

(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, Mg, Mn, Si (XSDRN); Ti, Zn, and Gd (GAM-2).

Table 23. Sample Calculation Results for $U(2.35)O_2$ Fuel Rods, 1.684-cm Pitch in Water, Fractional Rows (United States).

Code (Cross Sections Set)→ Case Number ↓	KENO (Hansen-Roach)[(a)]	KENO (27-Group ENDF/B-IV)	MCNP (Continuous-Energy ENDF/B-V)
15	0.9735 ± .0017	0.9971 ± .0017	0.9917 ± .0016
16	0.9720 ± .0016	0.9930 ± .0017	0.9898 ± .0015
17	0.9770 ± .0017	0.9951 ± .0016	0.9949 ± .0015
18	0.9780 ± .0016	0.9922 ± .0016	0.9962 ± .0018
19	0.9752 ± .0018	0.9969 ± .0016	0.9924 ± .0017
20	0.9748 ± .0016	0.9934 ± .0017	0.9937 ± .0018
21	0.9731 ± .0017	0.9894 ± .0017	0.9967 ± .0017
22	0.9741 ± .0017	0.9889 ± .0016	0.9930 ± .0017
23	0.9759 ± .0018	0.9940 ± .0016	0.9944 ± .0020
24	0.9796 ± .0018	0.9927 ± .0017	0.9940 ± .0015
25	0.9729 ± .0017	0.9914 ± .0016	0.9955 ± .0020
26	0.9623 ± .0014	0.9869 ± .0015	0.9889 ± .0018
27	0.9652 ± .0014	0.9897 ± .0015	0.9941 ± .0015
28	0.9673 ± .0014	0.9946 ± .0016	0.9964 ± .0018
29	0.9716 ± .0016	0.9889 ± .0013	0.9985 ± .0017

(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, Mg, Mn, Si (XSDRN); Ti, Zn, and Gd (GAM-2).

5.0 REFERENCES

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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. Larger 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 0.08602 for 2.032 cm pitch and 0.2011 for 1.684 cm pitch.)

KENO V.a Input Listing for Case 1 of Table 22 (16-Energy-Group Hansen-Roach Cross Sections)

```
phrld21 2.35 wt%, 3 19x16  CLUSTERS, 13.84 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(2.35)02
92400 2.8563-6 92509 3.6755-4 92510 1.2030-4
92600 3.5348-6 92858 2.0009-2 8100 4.1202-2
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
'  1100 Al (top end plug)
13100 5.9660-2  29100 3.0705-5  25100 7.3991-6
30100 1.2433-5  14100 2.3302-4  26100 1.1719-4
MIX=5
' 5052 Al (lower end plug)
13100 5.8028-2  24100 7.7888-5  29100 1.2746-5
12100 1.6663-3  25100 1.4743-5  30100 1.2387-5
14100 1.2978-4  26100 6.5265-5
MIX=6
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=7
' lead
82100  3.2132-2
END MIXT
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
 CUBOID  2 1  4P1.016 96.52 -1.27
UNIT 2
 COM=* 19x16 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* WATER BETWEEN CLUSTERS, 13.1  CM WIDE *
 CUBOID  2 1  13.1  0.0 32.512 0.0 96.52 -1.27
GLOBAL
UNIT 4
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 2 0 0 -1.27
 CUBOID  6 1    142.024 0  32.512 0 96.52 -3.81
 CUBOID  2 1    153.012  -10.988  32.512 0 104.29 -19.11
 REPLICATE 7 1  2R0 2R10.2 2R0 1
 REPLICATE 2 1  2R30.5 2R20.3 7.43 0    1
END GEOM
READ ARRAY  ARA=1 NUX=19 NUY=16  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL 2 3 2 3 2
             END FILL
END ARRAY
```

KENO V.a Input Listing for Case 1 of Table 22 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd)

```
READ PLOT
  XUL=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' END
END PLOT
END DATA
END
```

KENO V.a Input Listing for Case 8 of Table 22 (16-Energy-Group Hansen-Roach Cross Sections)

```
phru25 2.35 wt%, 3 19x16  CLUSTERS, 10.69 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(2.35)02
92400 2.8563-6 92509 3.6755-4 92510 1.2030-4
92600 3.5348-6 92858 2.0009-2 8100 4.1202-2
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
'  1100 Al (top end plug)
13100 5.9660-2  29100 3.0705-5  25100 7.3991-6
30100 1.2433-5  14100 2.3302-4  26100 1.1719-4
MIX=5
' 5052 Al (lower end plug)
13100 5.8028-2  24100 7.7888-5  29100 1.2746-5
12100 1.6663-3  25100 1.4743-5  30100 1.2387-5
14100 1.2978-4  26100 6.5265-5
MIX=6
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=7
' depleted uranium
92512 9.5220-5  92807 4.7151-2
END MIXT
READ GEOM
UNIT 1
 COM=* FUEL PIN *
 CYLINDER  1 1  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
 CUBOID  2 1  4P1.016 96.52 -1.27
UNIT 2
 COM=* 19x16 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* WATER BETWEEN CLUSTERS, 9.95  CM WIDE *
 CUBOID  2 1  9.95  0.0 32.512 0.0 96.52 -1.27
GLOBAL
UNIT 4
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 2 0 0 -1.27
 CUBOID  6 1    135.724       0  32.512 0 96.52 -3.81
 CUBOID  2 1    144.012  -8.288   32.512 0 102.79 -19.11
 REPLICATE 2 1  2R0.0  2R5.405  2R0.0   1
 REPLICATE 7 1  2R0 2R7.65 2R0 1
 REPLICATE 2 1  2R30.5 2R17.445 8.93 0    1
END GEOM
READ ARRAY  ARA=1 NUX=19 NUY=16  FILL F1 END FILL
          ARA=2 NUX=5 NUY=1
          FILL 2 3 2 3 2
             END FILL
```

KENO V.a Input Listing for Case 8 of Table 22 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd)

```
END ARRAY
READ PLOT
  XUL=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' END
END PLOT
END DATA
END
```

KENO V.a Input Listing for Case 17 of Table 23 (16-Energy-Group Hansen-Roach Cross Sections)

```
shr28 2.35 wt%, 1 25x18 2 20x18, 9.51   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(2.35)02
92400 2.8563-6 92509 3.6755-4 92510 1.2030-4
92600 3.5348-6 92858 2.0009-2 8100 4.1202-2
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
'  1100 Al (top end plug)
13100 5.9660-2  29100 3.0705-5  25100 7.3991-6
30100 1.2433-5  14100 2.3302-4  26100 1.1719-4
MIX=5
' 5052 Al (lower end plug)
13100 5.8028-2  24100 7.7888-5  29100 1.2746-5
12100 1.6663-3  25100 1.4743-5  30100 1.2387-5
14100 1.2978-4  26100 6.5265-5
MIX=6
'acrylic
1102 5.6642-2  6100 3.5648-2  8100 1.4273-2
MIX=7
' 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  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
 CUBOID  2 1  4P0.842 96.52 -1.27
UNIT 2
 COM=* 20x18 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* 25x18 ARRAY OF FUEL PINS *
 ARRAY 2 0 0 -1.27
UNIT 4
 COM=* WATER BETWEEN CLUSTERS, 9.096 CM WIDE *
 CUBOID  2 1  9.096 0.0 30.312 0.0 96.52 -1.27
GLOBAL
UNIT 5
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 3 0 0 -1.27
 CUBOID  6 1    127.652     0  30.312 0 96.52 -3.81
 CUBOID  2 1    137.476  -9.824   30.312 0 102.79 -19.11
 REPLICATE 2 1  2R0.0  2R1.321 2R0.0       1
 REPLICATE 7 1  2R0 2R17.85 2R0 1
```

KENO V.a Input Listing for Case 17 of Table 23 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd)

```
 REPLICATE 2 1  2R30.5 2R11.329 8.93 0    1
END GEOM
READ ARRAY  ARA=1 NUX=20 NUY=18  FILL F1 END FILL
          ARA=2 NUX=25 NUY=18  FILL F1 END FILL
          ARA=3 NUX=5 NUY=1
          FILL 2 4 3 4 2
             END FILL
END ARRAY
READ PLOT
  XUL=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' END
END PLOT
END DATA
END
```

KENO V.a Input Listing for Case 1 of Table 22 (27-Energy Group SCALE4 Cross Sections)

```
=CSAS25
pkld21  2.35 wt%, 3 19x16  CLUSTERS, 13.84 CM SEPARATION
27GROUPNDF4 LATTICECELL
' U(2.35)02
U-234  1 0  2.8563-6 295 END
U-235  1 0  4.8785-4 295 END
U-236  1 0  3.5348-6 295 END
U-238  1 0  2.0009-2 295 END
O  1 0  4.1202-2 295 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
'  1100 Al (top end plug)
AL  4 0  5.9660-2 295 END
CU  4 0  3.0705-5 295 END
MN  4 0  7.3991-6 295 END
'       (Zn replaced by Cu)
CU  4 0  1.2433-5 295 END
SI  4 0  2.3302-4 295 END
FE  4 0  1.1719-4 295 END
' 5052 Al (lower end plug)
AL  5 0  5.8028-2 295 END
CR  5 0  7.7888-5 295 END
CU  5 0  1.2746-5 295 END
MG  5 0  1.6663-3 295 END
MN  5 0  1.4743-5 295 END
'       (Zn replaced by Cu)
CU  5 0  1.2387-5 295 END
SI  5 0  1.2978-4 295 END
FE  5 0  6.5265-5 295 END
' acrylic
H   6 0  5.6642-2 295 END
C   6 0  3.5648-2 295 END
O   6 0  1.4273-2 295 END
' lead
PB  7 0  3.2132-2 295 END
END COMP
SQUAREPITCH 2.032 1.1176 1 2 1.27 3 END
pkld21   3 19x16 CLUSTERS, 13.84 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  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
```

KENO V.a Input Listing for Case 1 of Table 22 (27-Energy Group SCALE4 Cross Sections) (cont'd)

```
 CUBOID  2 1  4P1.016 96.52 -1.27
UNIT 2
 COM=* 19x16 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* WATER BETWEEN CLUSTERS, 13.1  CM WIDE *
 CUBOID  2 1  13.1  0.0 32.512 0.0 96.52 -1.27
GLOBAL
UNIT 4
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 2 0 0 -1.27
 CUBOID  6 1    142.024 0  32.512 0 96.52 -3.81
 CUBOID  2 1    153.012  -10.988  32.512 0 104.29 -19.11
 REPLICATE 7 1  2R0 2R10.2 2R0 1
 REPLICATE 2 1  2R30.5 2R20.3 7.43 0    1
END GEOM
READ ARRAY  ARA=1 NUX=19 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=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' END
END PLOT
END DATA
END
```

KENO V.a Input Listing for Case 8 of Table 22 (27-Energy Group SCALE4 Cross Sections)

```
=CSAS25
pku25  2.35 wt%, 3 19x16 CLUSTERS, 10.69 CM SEPARATION
27GROUPNDF4 LATTICECELL
' U(2.35)02
U-234  1 0  2.8563-6 295 END
U-235  1 0  4.8785-4 295 END
U-236  1 0  3.5348-6 295 END
U-238  1 0  2.0009-2 295 END
O  1 0  4.1202-2 295 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
'  1100 Al (top end plug)
AL  4 0  5.9660-2 295 END
CU  4 0  3.0705-5 295 END
MN  4 0  7.3991-6 295 END
'       (Zn replaced by Cu)
CU  4 0  1.2433-5 295 END
SI  4 0  2.3302-4 295 END
FE  4 0  1.1719-4 295 END
' 5052 Al (lower end plug)
AL  5 0  5.8028-2 295 END
CR  5 0  7.7888-5 295 END
CU  5 0  1.2746-5 295 END
MG  5 0  1.6663-3 295 END
MN  5 0  1.4743-5 295 END
'       (Zn replaced by Cu)
CU  5 0  1.2387-5 295 END
SI  5 0  1.2978-4 295 END
FE  5 0  6.5265-5 295 END
' acrylic
H   6 0  5.6642-2 295 END
C   6 0  3.5648-2 295 END
O   6 0  1.4273-2 295 END
' depleted uranium
U-235 7 0  9.5220-5 295 END
U-238 7 0  4.7151-2 295 END
END COMP
SQUAREPITCH 2.032 1.1176 1 2 1.27 3 END
pku25   3 19x16 CLUSTERS, 10.69 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  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
```

KENO V.a Input Listing for Case 8 of Table 22 (27-Energy Group SCALE4 Cross Sections) (cont'd)

```
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
 CUBOID  2 1  4P1.016 96.52 -1.27
UNIT 2
 COM=* 19x16 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* WATER BETWEEN CLUSTERS, 9.95  CM WIDE *
 CUBOID  2 1  9.95  0.0 32.512 0.0 96.52 -1.27
GLOBAL
UNIT 4
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 2 0 0 -1.27
 CUBOID  6 1    135.724       0  32.512 0 96.52 -3.81
 CUBOID  2 1    144.012  -8.288   32.512 0 102.79 -19.11
 REPLICATE 2 1  2R0.0  2R5.405  2R0.0   1
 REPLICATE 7 1  2R0 2R7.65 2R0 1
 REPLICATE 2 1  2R30.5 2R17.445 8.93 0    1
END GEOM
READ ARRAY  ARA=1 NUX=19 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=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' END
END PLOT
END DATA
END
```

KENO V.a Input Listing for Case 17 of Table 23 (27-Energy Group SCALE4 Cross Sections)

```
=CSAS25
sk28    2.35 wt%, 1 25x18 2 20x18  , 9.51 CM SEPARATION,steel walls
27GROUPNDF4 LATTICECELL
' U(2.35)02
U-234  1 0  2.8563-6 295 END
U-235  1 0  4.8785-4 295 END
U-236  1 0  3.5348-6 295 END
U-238  1 0  2.0009-2 295 END
O  1 0  4.1202-2 295 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
'  1100 Al (top end plug)
AL  4 0  5.9660-2 295 END
CU  4 0  3.0705-5 295 END
MN  4 0  7.3991-6 295 END
'       (Zn replaced by Cu)
CU  4 0  1.2433-5 295 END
SI  4 0  2.3302-4 295 END
FE  4 0  1.1719-4 295 END
' 5052 Al (lower end plug)
AL  5 0  5.8028-2 295 END
CR  5 0  7.7888-5 295 END
CU  5 0  1.2746-5 295 END
MG  5 0  1.6663-3 295 END
MN  5 0  1.4743-5 295 END
'       (Zn replaced by Cu)
CU  5 0  1.2387-5 295 END
SI  5 0  1.2978-4 295 END
FE  5 0  6.5265-5 295 END
' acrylic
H   6 0  5.6642-2 295 END
C   6 0  3.5648-2 295 END
O   6 0  1.4273-2 295 END
' STEEL WALLS
FE  7 0  8.1810-2 295 END
C   7 0  7.4686-4 295 END
MN  7 0  1.1000-3 295 END
P   7 0  6.0971-6 295 END
S   7 0  8.8332-6 295 END
SI  7 0  3.6983-4 295 END
NI  7 0  6.3552-4 295 END
MO  7 0  2.4114-4 295 END
CR  7 0  1.0896-4 295 END
CU  7 0  9.6587-5 295 END
END COMP
SQUAREPITCH 1.684 1.1176 1 2 1.27 3 END
sk28   1 25x18 2 20x18 9.51 cm     SEPARATION
```

KENO V.a Input Listing for Case 17 of Table 23 (27-Energy Group SCALE4 Cross Sections) (cont'd)

```
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  0.5588 91.44 0.0
 CYLINDER  4 1  0.5588 91.92 0.0
 CYLINDER  5 1  0.5588 91.92 -1.27
 CYLINDER  3 1  0.635  91.92 -1.27
 CYLINDER  4 1  0.635  96.52 -1.27
 CUBOID  2 1  4P0.842 96.52 -1.27
UNIT 2
 COM=* 20x18 ARRAY OF FUEL PINS *
 ARRAY 1 0 0 -1.27
UNIT 3
 COM=* 25x18 ARRAY OF FUEL PINS *
 ARRAY 2 0 0 -1.27
UNIT 4
 COM=* WATER BETWEEN CLUSTERS, 9.096 CM WIDE *
 CUBOID  2 1  9.096 0.0 30.312 0.0 96.52 -1.27
GLOBAL
UNIT 5
 COM=* ARRAY OF 3 CLUSTERS, 1 IN. ACRYLIC BELOW, WATER REFLECTOR *
 ARRAY 3 0 0 -1.27
 CUBOID  6 1    127.652     0  30.312 0 96.52 -3.81
 CUBOID  2 1    137.476  -9.824   30.312 0 102.79 -19.11
 REPLICATE 2 1  2R0.0  2R1.321 2R0.0       1
 REPLICATE 7 1  2R0 2R17.85 2R0 1
 REPLICATE 2 1  2R30.5 2R11.329 8.93 0    1
END GEOM
READ ARRAY  ARA=1 NUX=20 NUY=18  FILL F1 END FILL
          ARA=2 NUX=25 NUY=18  FILL F1 END FILL
          ARA=3 NUX=5 NUY=1
          FILL 2 4 3 4 2
             END FILL
END ARRAY
READ PLOT
  XUL=-3 YUL=1.016 ZUL=100 XLR=2.032 YLR=1.016
  ZLR=-5  UAX=1  WDN=-1 NAX=30 NDN=110 NCH=' *~ctla~' END
  XUL=-5 YUL=15 ZUL=2 XLR=15 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' *~ctla~' END
  XUL=-5 YUL=1.016 ZUL=100 XLR=150 YLR=1.016
  ZLR=-6   UAX=1  WDN=-1 NAX=120 NCH=' *~ctla~' END
  PIC=UNIT XUL=-5 YUL=40 ZUL=2 XLR=150 YLR=-5
  ZLR=2   UAX=1  VDN=-1 NAX=120 NCH=' 12345' 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 22

```
message:      outp=pmld21.o  runtpe=pmld21.r  srctp=pmld21.s

pmld21       3-19x16   CLUSTERS OF U(2.35)O2 RODS, 13.84 CM SEPR, PITCH 2.032 CM
1     1 .06170524 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2     3 .0597516     1 -2 -9 u=1 imp:n=1 $ clad
3     4 .06006075    -1 8 -9 u=1 imp:n=1 $ top end plug (lower piece)
4     4 .06006075    -2 9 u=1 imp:n=1 $ top end plug (top piece)
5     5 .06000711    -1 -7 u=1 imp:n=1 $ lower end plug
6     2 .100059  2 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 21 -22 23 fill=2 imp:n=1  $ first rod cluster
9     0 -13 12 -20 21 -22 23 fill=2(51.708 0 0) imp:n=1  $ second rod cluster
10    0 -15 14 -20 21 -22 23 fill=2(103.416 0 0) imp:n=1  $ third rod cluster
11    6 .106563  -23 29 -15 11 -20 21 imp:n=1  $ acryl
12    2 .100059 -12 10 -20 21 -22 23 imp:n=1  $ water between clusters
13    2 .100059 -14 13 -20 21 -22 23 imp:n=1  $ water between clusters
14    7 .032132     33 -34 31 -21 35 -36  imp:n=1  $ lead reflector
15    7 .032174     33 -34 20 -32 35 -36  imp:n=1  $ lead reflector
16    2 .100059 (-11:15:20:-21:22:-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 1.016 1.016 .5588  $ fuel cylinder
2     c/z 1.016 1.016 .635  $ clad cylinder
3     px  0.0  $ fuel rod cell boundary
4     px  2.032  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  2.032  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  91.44  $ top of fuel
9     pz  91.92  $ top of clad
10    px  38.6079  $ farthest edge of closest cluster
11    px  .0001  $ closest edge of closest cluster
12    px  51.7081  $ closest edge of center cluster **
13    px  90.3152  $ farthest edge of center cluster
14    px  103.4161 $ closest edge of farthest cluster **
15    px  142.0239  $ farthest end of clusters
20    py  32.5119  $ sides of clusters
21    py  .00001  $ sides of clusters
22    pz  96.52  $ top of fuel rod
23    pz  -1.27  $ bottom of fuel rod
24    px  183.512  $ side of water reflector
25    px  -41.488  $side of water reflector
26    py  63.012  $ side of water reflector
27    py  -30.5  $ side of water reflector
28    pz  111.72  $ top of water
29    pz  -3.81  $ bottom of acrylic support plate
31    py  -10.19999 $lead
32    py   42.7119  $ lead
33    px  -10.988   $ lead
34    px   153.012  $ lead
35    pz  -19.11    $ lead bottom
36    pz   104.29   $ lead

kcode  1500 1 50 160 50000
sdef  x=d1 y=d2 z=d3 cel=d4
si1   0 125
sp1   0 1
si2   0 30
sp2   0 1
```

MCNP Input Listing for Case 1 of Table 22 (cont'd)

```
si3   0 100
sp3   0 1
si4   l 8 9 10
sp4   v
print
c     m1 is UO2 fuel
m1    92234.50c 2.8563e-6 92235.50c 4.8785e-4
      92236.50c 3.5348e-6 92238.50c 2.0009e-2
      8016.50c  4.1202e-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 1100 aluminum (top end plug)
m4    13027.50c  5.9660e-2  29000.50c  3.0705e-5
      25055.50c  7.3991e-6
c       Zn replaced by Cu, below
      29000.50c  1.2433e-5  14000.50c  2.3302e-4
      26000.50c  1.1719e-4
c     m5 is 5052 aluminum (lower end plug)
m5    13027.50c  5.8028e-2  24000.50c  7.7888e-5
      29000.50c  1.2746e-5  12000.50c  1.6663e-3
      25055.50c  1.4743e-5
c       Zn replaced by Cu, below
      29000.50c  1.2387e-5  14000.50c  1.2978e-4
      26000.50c  6.5265e-5
c     m6 is acrylic (support plate)
m6    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt6   poly.01t
c     m7 is lead
m7    82000.50c  3.2132e-2
```

MCNP Input Listing for Case 8 of Table 22

```
message:      outp=pmu25.o  runtpe=pmu25.r  srctp=pmu25.s

pmu25       3 19x16 CLUSTERS OF U(2.35)O2 RODS, 10.69 CM SEPR, PITCH 2.032 CM
1     1 .06170524   -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2     3 .0597516     1 -2 -9 u=1 imp:n=1 $ clad
3     4 .06006075    -1 8 -9 u=1 imp:n=1 $ top end plug (lower piece)
4     4 .06006075    -2 9 u=1 imp:n=1 $ top end plug (top piece)
5     5 .06000711   -1 -7 u=1 imp:n=1 $ lower end plug
6     2 .100059  2 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 21 -22 23 fill=2 imp:n=1  $ first rod cluster
9     0 -13 12 -20 21 -22 23 fill=2(48.558 0 0) imp:n=1  $ second rod cluster
10    0 -15 14 -20 21 -22 23 fill=2(97.116  0 0) imp:n=1  $ third rod cluster
11    6 .106563  -23 29 -15 11 -20 21 imp:n=1  $ acryl
12    2 .100059 -12 10 -20 21 -22 23 imp:n=1  $ water between clusters
13    2 .100059 -14 13 -20 21 -22 23 imp:n=1  $ water between clusters
14    7 .04724622   33 -34 38 -39 35  -36  imp:n=1  $ uranium reflector
15    7 .04724622   33 -34 40 -41 35 -36  imp:n=1  $ uranium reflector
16    2 .100059 (-11:15:20:-21:22:-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 1.016 1.016 .5588  $ fuel cylinder
2     c/z 1.016 1.016 .635  $ clad cylinder
3     px  0.0  $ fuel rod cell boundary
4     px  2.032  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  2.032  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  91.44  $ top of fuel
9     pz  91.92  $ top of clad
10    px  38.6079  $ farthest edge of closest cluster
11    px  .0001  $ closest edge of closest cluster
12    px  48.5581  $ closest edge of center cluster **
13    px  87.1659  $ farthest edge of center cluster
14    px  97.1161  $ closest edge of farthest cluster **
15    px  135.7239  $ farthest end of clusters
20    py  32.5119  $ sides of clusters
21    py  .00001  $ sides of clusters
22    pz  96.52  $ top of fuel rod
23    pz  -1.27  $ bottom of fuel rod
24    px  174.512  $ side of water reflector
25    px  -38.788  $side of water reflector
26    py  63.012  $ side of water reflector
27    py  -30.5  $ side of water reflector
28    pz  111.72  $ top of water
29    pz  -3.81  $ bottom of acrylic support plate
31    py  -7.65     $uranium
32    py   42.712   $uranium
33    px  -8.288    $uranium
34    px   144.012  $uranium
35    pz  -19.11    $uranium
36    pz   102.79   $uranium
38    py  -13.055   $ uranium
39    py  -5.405    $ uranium
40    py   37.917   $ uranium
41    py   45.567   $ uranium

kcode  1500 1 50 160 50000
sdef  x=d1 y=d2 z=d3 cel=d4
```

MCNP Input Listing for Case 8 of Table 22 (cont'd)

```
si1   0 125
sp1   0 1
si2   0 30
sp2   0 1
si3   0 100
sp3   0 1
si4   l 8 9 10
sp4   v
print
c     m1 is UO2 fuel
m1    92234.50c 2.8563e-6 92235.50c 4.8785e-4
      92236.50c 3.5348e-6 92238.50c 2.0009e-2
      8016.50c  4.1202e-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 1100 aluminum (top end plug)
m4    13027.50c  5.9660e-2  29000.50c  3.0705e-5
      25055.50c  7.3991e-6
c       Zn replaced by Cu, below
      29000.50c  1.2433e-5  14000.50c  2.3302e-4
      26000.50c  1.1719e-4
c     m5 is 5052 aluminum (lower end plug)
m5    13027.50c  5.8028e-2  24000.50c  7.7888e-5
      29000.50c  1.2746e-5  12000.50c  1.6663e-3
      25055.50c  1.4743e-5
c       Zn replaced by Cu, below
      29000.50c  1.2387e-5  14000.50c  1.2978e-4
      26000.50c  6.5265e-5
c     m6 is acrylic (support plate)
m6    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt6   poly.01t
c     m7 is uranium
m7    92235.50c  9.5220-5  92238.50c 4.7151-2
```

MCNP Input Listing for Case 17 of Table 23.

```
message:      outp=sm28.o  runtpe=sm28.r  srctp=sm28.s

sm28       U(2.35)O2 RODS, 9.51  CM SEPR, PITCH 1.684 CM
c          1 25x18 2 20x18 CLUSTERS with  steel walls
1     1 .06170524   -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2     3 .0597516     1 -2 -9 u=1 imp:n=1 $ clad
3     4 .06006075    -1 8 -9 u=1 imp:n=1 $ top end plug (lower piece)
4     4 .06006075    -2 9 u=1 imp:n=1 $ top end plug (top piece)
5     5 .06000711   -1 -7 u=1 imp:n=1 $ lower end plug
6     2 .100059  2 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 21 -22 23 fill=2 imp:n=1  $ first rod cluster
9     0 -13 12 -20 21 -22 23 fill=2(42.776 0 0) imp:n=1  $ second rod cluster
10    0 -15 14 -20 21 -22 23 fill=2(93.972 0 0) imp:n=1  $ third rod cluster
11    6 .106563  -23 29 -15 11 -20 21 imp:n=1  $ acryl
12    2 .100059 -12 10 -20 21 -22 23 imp:n=1  $ water between clusters
13    2 .100059 -14 13 -20 21 -22 23 imp:n=1  $ water between clusters
14    7 .08512383   33 -34 38 -39 35  -36  imp:n=1  $ steel reflector
15    7 .08512383   33 -34 40 -41 35 -36  imp:n=1  $ steel reflector
16    2 .100059 (-11:15:20:-21:22:-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 0.842 0.842 .5588  $ fuel cylinder
2     c/z 0.842 0.842 .635  $ clad cylinder
3     px  0.0  $ fuel rod cell boundary
4     px  1.684  $ fuel rod cell boundary
5     py  0.0  $ fuel rod cell boundary
6     py  1.684  $ fuel rod cell boundary
7     pz  0.0  $ bottom of fuel
8     pz  91.44  $ top of fuel
9     pz  91.92  $ top of clad
10    px  33.6799  $ farthest edge of closest cluster
11    px  .0001  $ closest edge of closest cluster
12    px  42.7761  $ closest edge of center cluster **
13    px  84.8759  $ farthest edge of center cluster
14    px  93.9721  $ closest edge of farthest cluster **
15    px  127.6519  $ farthest end of clusters
20    py  30.3119  $ sides of clusters
21    py  .00001  $ sides of clusters
22    pz  96.52  $ top of fuel rod
23    pz  -1.27  $ bottom of fuel rod
24    px  167.976  $ side of water reflector
25    px  -40.324  $side of water reflector
26    py  60.812  $ side of water reflector
27    py  -30.5  $ side of water reflector
28    pz  111.72  $ top of water
29    pz  -3.81  $ bottom of acrylic support plate
31    py  -17.85    $ steel
32    py   50.362   $ steel
33    px  -9.096    $ steel
34    px   137.476  $ steel
35    pz  -19.11    $ steel
36    pz   102.79   $ steel
38    py  -19.171   $ steel
39    py  -1.321    $ steel
40    py   31.633   $ steel
41    py   49.483   $ steel

kcode  1500 1 50 160 50000
```

MCNP Input Listing for Case 17 of Table 23 (cont'd)

```
sdef  x=d1 y=d2 z=d3 cel=d4
si1   0 125
sp1   0 1
si2   0 30
sp2   0 1
si3   0 100
sp3   0 1
si4   l 8 9 10
sp4   v
print
c     m1 is UO2 fuel
m1    92234.50c 2.8563e-6 92235.50c 4.8785e-4
      92236.50c 3.5348e-6 92238.50c 2.0009e-2
      8016.50c  4.1202e-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 1100 aluminum (top end plug)
m4    13027.50c  5.9660e-2  29000.50c  3.0705e-5
      25055.50c  7.3991e-6
c       Zn replaced by Cu, below
      29000.50c  1.2433e-5  14000.50c  2.3302e-4
      26000.50c  1.1719e-4
c     m5 is 5052 aluminum (lower end plug)
m5    13027.50c  5.8028e-2  24000.50c  7.7888e-5
      29000.50c  1.2746e-5  12000.50c  1.6663e-3
      25055.50c  1.4743e-5
c       Zn replaced by Cu, below
      29000.50c  1.2387e-5  14000.50c  1.2978e-4
      26000.50c  6.5265e-5
c     m6 is acrylic (support plate)
m6    1001.50c 5.6642e-2  6000.50c 3.5648e-2
      8016.50c 1.4273e-2
mt6   poly.01t
c     m7 is lead
m7     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/TWODANT Input Listings

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 Box 6 or Box 11. The 2.032-cm-pitch experiments are probably numbered SSC (Simulated Shipping Cask) 2.35-000-143 to -157, dated 7/15/80 to 6/12/81. The 1.684-cm-pitch experiments are likely included in S.C.-2.35-000-001 to -142, dated 1/11/77 to 7/9/80.

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 1.48 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/cm^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	-	-	<.38[f]	2.83[f]
Cr	<0.028	<0.01	<0.01	<0.01	-	.041	<.01	<.005
Zn	0.35±.05	0.26±.07	0.9±1.1	16	10.6	.0613	<.05	.32
Mn	<0.55	<0.01	<0.01	<0.01	-	.041	<.01	<.01
Pb	<0.015	<0.005	.008±.001	<0.005	2.1	1.0220	<.002	<.005
F	0.21±.02	0.15±.04	0.15±.04	0.18	-	-	.12	.12
Fe	<0.06	<0.03	<0.03	24	-	0.21	.12	.20
Cu	<0.06	<0.01	<0.01	<0.01	18.2	.123	<.05	<.05
Cd	0.004±.001	.006±.001	.020±.006	0.001	-	.041	.002	.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	.204	-	-
Nd	-	-	-	-	12.2	2.04	-	-
Si	-	-	-	-	3.1	2.04	-	-
Ni	-	-	-	-	6.8	.204	-	-

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)
Y	-	-	-	-	0.17	.41	-	-
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 the dissolved solids at a concentration of 200 g/m^3, have the same density as water ($\sim$1 g/cm^3), and displace the water. These are conservative assumptions since the 200 g/m^3 concentration is greater than any measured total impurity concentration and since 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 $200/10^6 \times 100 = 0.02\%$. To see the effect of reduced water density, the water volume fraction is reduced by this percentage. The resulting change in k_{eff} is less than 0.04%.[a]

Effect Due to Presence of Individual Impurities. Listed in Table C.2 are the percent changes in k_{eff} for the addition of the maximum measured amounts of each impurity, as calculated by ONEDANT, using the 27-group cross sections processed by CSASIX.[b] No changes are greater than 0.005% except those from boron and gadolinium impurities, with Δk_{eff}'s of 0.9% and 1.7%, 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] 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.

[b] 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.)

All of the experiments from References 3, 5, and 6 evaluated in this report does not include boron or gadolinium impurity in water.

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
Mg	5.70×10^{-06}	1.412×10^{-07}	0
Mn	5.50×10^{-07}	6.029×10^{-09}	0.002
Mo	4.09×10^{-08}	2.564×10^{-10}	0

Impurity	Concentration (g/cm^3)	Atom Density (atoms/barn-cm)	% Δk_{eff}
N	2.83×10^{-06}	1.217×10^{-07}	0.002
Na	1.02×10^{-06}	2.675×10^{-08}	0.002
Nb	3.00×10^{-07}	1.945×10^{-09}	0
Nd	1.22×10^{-05}	5.094×10^{-08}	0.001
Ni	6.80×10^{-06}	6.977×10^{-08}	0.002
Pb	2.10×10^{-06}	6.103×10^{-09}	0
Pt[e]	2.04×10^{-07}	6.305×10^{-10}	0
Rh	1.02×10^{-07}	5.977×10^{-10}	0.001
Ru	1.02×10^{-06}	6.085×10^{-09}	0.001
Si	3.10×10^{-06}	6.647×10^{-08}	0
Sm	2.04×10^{-07}	8.179×10^{-10}	0.001
Sn	1.02×10^{-06}	5.182×10^{-09}	0
SO_3	1.84×10^{-05}	1.384×10^{-07}	0.002
Sr	4.09×10^{-08}	2.808×10^{-10}	0.001
Tb	2.03×10^{-07}	7.709×10^{-10}	0.001
Ti	2.04×10^{-06}	2.568×10^{-08}	0
U	2.04×10^{-07}	5.168×10^{-10}	0
V	4.09×10^{-08}	4.830×10^{-10}	0
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 INPUTS FOR SENSITIVITYSTUDIES USING HOMOGENIZED FUEL ROD REGION

```
=CSASIX
GENERATE 27-GRP LIB FOR 2.35 WT% UO2 PNL FUEL PINS IN WATER
27GROUPNDF4 LATTICECELL
U-234  1 0  2.85626-6 291 END
U-235  1 0  4.87852-4 291 END
U-236  1 0  3.53484-6 291 END
U-238  1 0  2.00094-2 291 END
O  1 0  4.12021-2 291 END
H  2 0  6.67619-2 291 END
O  2 0  3.33809-2 291 END
Al  3 0  6.01507-2 291 END
H  4 0  6.67619-2 291 END
O  4 0  3.33809-2 291 END
END COMP
SQUAREPITCH 2.032 1.1176 1 2 1.27 3 END
END


    1     0     0
SLAB OF U(2.35)O2 FUEL PINS IN WATER, BASE CASE
/  Block 1
igeom=slab ngroup=27 isn=16 niso=5 mt=5 nzone=5 im=4 it=251  T

/  Block 2
xmesh= 0 44.72 45.72 46.72 60.72
xints= 179    8     8     56
zones=   5    5     4      4 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=3 ibl=1 ibr=0 epsi=.000001  T

/  Block 6
pted=0 zned=1  T
```

```
=CSASIX
pkld21  2.35 wt%, 3 19x16  CLUSTERS, 13.84 CM SEPARATION
27GROUPNDF4 LATTICECELL
' U(2.35)02
U-234  1 0  2.8563-6 295 END
U-235  1 0  4.8785-4 295 END
U-236  1 0  3.5348-6 295 END
U-238  1 0  2.0009-2 295 END
O  1 0  4.1202-2 295 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 2.032 1.1176 1 2 1.27 3 END
END

   1     0     0
onel1,slab of u(2.35)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 16.256 17.256 27.456 42.456
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
atwo1, 2.35 wt% 3 19x16 clusters, 13.1 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=220 jm=5
jt=180  maxscm=540000 maxlcm=4500000 t

/  Block 2
xmesh=0 19.304 32.404 71.012 82 92 112.5
xints= 40 30 80 30 20 20
ymesh=0.0 20.3 30.5 63.012 73.212 93.512
yints= 40 20 60 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=110.33  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
```