

**WATER-MODERATED U(4.31)O₂ FUEL RODS
IN 1.892-CM SQUARE-PITCHED ARRAYS
(GADOLINIUM WATER IMPURITY)**

Evaluator

**Virginia F. Dean
Idaho National Engineering Laboratory**

**Internal Reviewer
Carol A. Atkinson**

Independent Reviewer

**Nigel R. Smith
AEA Technology**

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IDENTIFICATION NUMBER: LEU-COMP-THERM-004

SPECTRA

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1.0 DETAILED DESCRIPTION

1.1 Overview of Experiment

A series of critical approach experiments with clusters of aluminum clad U(4.31)O₂ 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. Experiments included rectangular, square-pitched lattice clusters, with pitches of 2.54 cm (LEU-COMP-THERM-002) or 1.892 cm. Some of these experiments were performed with absorber plates of various materials between clusters (LEU-COMP-THERM-009). Others added reflecting walls of depleted uranium, lead, and steel on two opposite sides of the cluster array (LEU-COMP-THERM-010). Some circular, triangular-pitched lattices, with pitches of 2.398, 1.891, 1.801, or 1.598 cm, were used to measure the effect of gadolinium dissolved in the water (LEU-COMP-THERM-005).

Information in this section comes from References 1-10, which are the original PNL reports of these experiments. The primary references for this particular set of experiments are References 4, 5, and 6. References 1-14 provide supplemental information. Details which are from specific references are so noted.

Over the course of performing experiments with this set of fuel rods, analyses were done which resulted in better characterization of the rods over time (Reference 5, p. x; Reference 6, p. xiii^a). For example, the enrichment was originally reported at 4.29 wt.%, but later improved to 4.306 wt.%. Therefore, only the most recent fuel rod data is provide in this evaluation.

This evaluation documents water-reflected clusters with no absorber plates or reflecting walls and with a small, but calculably significant, amount of

^a Confirmed by private communication, Sid Bierman, April 1994.

gadolinium impurity in the water-moderator. A total of 20 experiments were evaluated. All of these were judged to be acceptable as benchmark data.

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 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 are all described in this section), no other apparatus was in the tank.^a (See Figures 1 and 2.)

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

1.2.2 Fuel Rod Support Plate - The bottoms of the fuel rods were supported by a 2.54-cm-thick, acrylic support plate. In the 1- and 3-cluster experiments, 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 15.3 x 5.08 x 0.635 cm 6061-aluminum channel angles resting on the floor of the tank. The angles were oriented so that the bottom surface of the support plate was 15.3 cm above the bottom of the tank. For the 4-cluster experiments, the support plate extended nearly the length and width of the tank and was supported by 6061 aluminum angles attached to the tank walls.^c

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

^b Sid Bierman, private communication, July 1993.

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

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

^a Sid Bierman, private communication, August 1993.



Figure 1. Experiment Tank.



Figure 2. Arranging Fuel Rods.

The top lattice plates were bolted to 5.08 x 5.08 x 0.635 cm aluminum angles, attached at their ends to the walls of the tank. The bottom surfaces of the top lattice plates were approximately 79 cm above the fuel rod support plate. (Reference 4, pp. 11 and 20.) The bottom lattice plates rested on the fuel rod support plate. Lattice plates were 1.27 cm thick.^a

In one experiment with 2.35% enriched UO_2 fuel rods, the aluminum lattice supports were doubled, with no effect on the critical separation between clusters (Reference 1, pp. 26 and 28).

^a Reference 4 (p. 20) gives the uncertainty in the thickness of the polypropylene plates as ± 0.4 cm. The same lattice plates were used in experiments reported in References 5 and 6. (Reference 5, p. x; Reference 6, p. xiii.)

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.^a

1.2.4 Control and Safety Blade Guides - 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 that was either 0.96 cm wide or 0.64 cm wide for the blades.^b During one experiment from a set of similar experiments using 2.35 wt.% enriched UO₂ rods, an extra thickness of aluminum was added to the control and safety blade guides. The results demonstrated "no change in the predicted critical separation between fuel rod clusters." (Reference 1, pp. 13 and 28) These experiments were not repeated with 4.31% enriched rods. However, the experimenters report, "Since the support structures are further from the fuel clusters in the experiments covered by this report, they would have even less of an effect on the data. Consequently, the measurements to determine the effect of the supports were not repeated for these current experiments." (Reference 2, p. 22.)

1.2.5 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, outside the 15-cm-thick water reflector.^c

1.2.6 Water Reflector - The top water surface was always at least 15 centimeters above the top of the fuel region of the rods. (Reference 13, p. 132)^d The bottom water reflector also was at least 15 cm thick, since the aluminum angle supporting

^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.)

^c Private communication, Sid Bierman, July 1993.

^d Confirmed by private communication, Sid Bierman, July 1994.

the fuel-rod support plate above the bottom of the tank was 15.3 cm tall. The minimum side-reflector thickness, assuming that the experiment was centered in the tank and that the longer side of the experiment paralleled the longer side of the tank, was 70 cm.^a

1.2.7 Source - 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.^b 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).

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

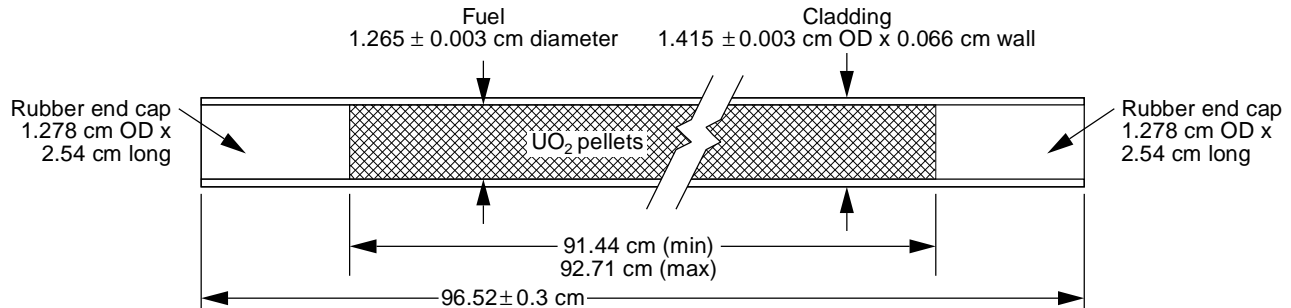


Figure 3. U(4.31) O_2 Fuel Rod.

Diagrams in some of the earlier references showed end plugs protruding from the ends of the rod beyond the aluminum cladding, with total rod length, including protruding plugs, of 96.52 cm. However, later references showed end plugs exactly filling the ends of the clad, which had a length of 96.52 cm. One experimenter recalls that the experimenters carefully inserted rubber plugs in the bottoms of the rods, before filling, so that the rubber plug protruded approximately 1/16

^a Case 11. See Figure 6.

^b Private communication, Sid Bierman, August 1993.

inch uniformly for all rods. Some top end plugs protruded and some were recessed, depending on slight differences between thicknesses of UO_2 pellets. Differences in pellet thicknesses were also the reason for the reported maximum and minimum lengths of 92.71 cm and 91.44 cm for the fuel region. There were no problems with water leakage into the fuel region of the rods.^a

Dimensions of the $\text{U}(4.31)\text{O}_2$ fuel rods are summarized in Table 1. To test the effects of small differences between rods, "experiments were repeated using alternate but identical (within the quality control applied during fabrication) fuel rods and different fuel loading arrangements on the approach to critical. . . the measurement data thus checked were reproduced to within a one sigma limit of 0.3%" in most cases (Reference 2, p. 19). The standard deviations of a few reported critical cluster separations were greater than 0.3%.

Table 1. 4.31 Wt.% Enriched UO_2 Fuel Rod Dimensions.

Component	Length (cm)	Diameter (cm)
UO_2 fuel	91.44 - 92.71	1.265 ± 0.003
Rubber End Caps	2.54	1.278
Gap (not shown)	-	1.283 ± 0.003 OD
Clad (6061 Al)	96.52 ± 0.3	1.415 ± 0.003 OD (.066 cm thick)

1.2.9 Experimental Method for Determining Critical Configuration - Critical configurations were determined by extrapolation to critical, based on count rates of two or three detectors. Rods were added in half or whole-row increments in order that the average fuel-rod worth of the addition was the same as the average fuel-rod worth of an entire row. (See LEU-COMP-THERM-001, Section 1.2 for a more detailed description.)

1.2.10 Critical Cluster Dimensions and Separations - Cluster sizes and separations for the 24 critical configurations are listed in Table 2 and are diagramed in Figures 4-8. Because the critical configuration was determined by extrapolation to critical, the critical number of rods was, in general, not an integral number. Placement of the twenty-five water holes, aluminum clad voids, or water-filled aluminum tubes of Cases 5, 6, and 7 is shown in Figure 8.

^a Sid Bierman, personal communication, April 1994.

Table 2. U(4.31)O₂ Fuel Rod Critical Configurations (See Figures 4-8).

Case Number	Number of Clusters	Cluster Dimensions (number of rods, X x Y) ^(a)	Separation Between Clusters (cm) ^(b)	Reference (pg)
1	1	12 x 18.817 ± 0.008 (225.8 ± 0.1 rods total)	-	4(12)
2	1	14 x 15.443 ± 0.014 (216.2 ± 0.2 rods total)	-	4(12)
3	1	16 x 13.54 ± 0.03 (216.6 ± 0.5 rods total) ^(c)	-	4(12)
4	1	17 x 12.86 ± 0.01 (218.6 ± 0.2 rods total)	-	4(12)
5	1	14 x 13.78 ± 0.01 ^(d) (167.85 ± 0.2 rods total)	-	4(17)
6	1	14 x 16.29 ± 0.01 ^(e) (203.0 ± 0.1 rods total)	-	4(17)
7	1	14 x 14.18 ± 0.01 ^(f) (173.5 ± 0.1 rods total)	-	4(17)
8	2	9 x 12.18 (219.2 ± 0.1 rods total)	2.83 ± 0.02	4(29)
9	3	12 x 16	12.27 ± 0.03	4(31)
10	3	12 x 16	12.493 ± 0.03 ^(g)	5(16), 6(13)
11	4	9 x 12 (two lower) 9 x 2.1 (two upper) (253.8 ± 0.1 rods total)	4.72 ± 0.03 (x- and y-separation)	4(29)
12	4	9 x 12 (two lower) 9 x 12.04 (two upper) (432.7 ± 0.1 rods total)	6.61 ± 0.03 (x- and y-separation)	4(29)
13	4	9 x 12 (two lower) 9 x 0.5 (two upper) (225.0 rods total)	2.83 ± 0.02 (x-separation) 8.38 ± 0.02	4(29)

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Case Number	Number of Clusters	Cluster Dimensions (number of rods, X x Y) ^(a)	Separation Between Clusters (cm) ^(b)	Reference (pg)
14	4	9 x 12 (two lower) 9 x 1 (two upper) (234.0 rods total)	2.83 ± 0.02 (x-separation) 10.86 ± 0.04 (y-separation)	4(29)
15	4	9 x 12 (two lower) 9 x 2 (two upper) (252.0 rods total)	2.83 ± 0.02 (x-separation) 11.29 ± 0.02 (y-separation)	4(29)
16	4	9 x 12 (two lower) 9 x 4 (two upper) (288.0 rods total)	2.83 ± 0.02 (x-separation) 12.02 ± 0.02 (y-separation)	4(29)
17	4	9 x 12 (two lower) 9 x 8 (two upper) (360.0 rods total)	2.83 ± 0.02 (x-separation) 13.64 ± 0.04 (y-separation)	4(29)
18	4	9 x 12 (two lower) 9 x 10 (two upper) (396.0 rods total)	2.83 ± 0.02 (x-separation) 14.98 ± 0.02 (y-separation)	4(29)
19	4	9 x 12 (all four) (432.0 rods total)	2.83 ± 0.02 (x-separation) 19.81 ± 0.05 (y-separation)	4(29)
20	4	9 x 10 (two lower) 9 x 9.3 (two upper) (347.4 ± 0.1 rods total)	2.83 ± 0.02 (x-separation) 8.50 ± 0.04 (y-separation)	4(29)

- (a) For two- or three-cluster configurations, the first dimension is along the direction of cluster placement. Second dimension is the width of facing sides, as shown in Figures 4-8.
- (b) Distance between outermost fuel-rod cell boundaries.
- (c) Average of two experiments, 216.7 ± 0.1 rods total and 216.5 ± 0.5 rods total.
- (d) Includes 25 "water holes" where water replaced fuel rods in the lattice. See Figures 4 and 8.
- (e) Includes 25 "aluminum clad voids" where air-filled aluminum tubes, of the same diameter and length as the fuel rods, replaced fuel rods in the lattice. See Figures 4 and 8.
- (f) Includes 25 "water-filled aluminum tubes" where aluminum tubes, of the same outer diameter and length of the fuel rods, filled with water, replaced fuel rods in the lattice. See Figures 4 and 8.
- (g) This separation is the average of two measurements of rod-surface-to-rod-surface separation reported in Reference 5. The cell boundary separation between clusters is obtained by subtracting (pitch - rod diameter).

Reference 5 reports no gadolinium impurity in the water. As is discussed in Sections 2 and 3, sensitivity studies indicate that the gadolinium impurity affects the calculational results significantly. Therefore, although this configuration contains the same size clusters and arrangement as Case 9 taken from Reference 4, it is considered to be a separate case. This is because a gadolinium impurity is reported in Reference 4, but is not reported for this case, in Reference 5.

1.3 Description of Material Data

1.3.1 UO₂ Fuel Rods - Over the course of performing the experiments, the experimenters improved their analyses of the fuel rods. In Reference 5 (p. x), the experimenters state:

The same UO₂ fuel, lattice grid plates, neutron absorber plates, and reflecting walls have been used throughout these experiments. However, during this period of time some of these parameters have become better defined as a result of repeated analysis. For example, the 4.31 wt% ²³⁵U enriched UO₂ rods were originally identified as having a ²³⁵U enrichment of 4.29 wt%. Multiple analysis of the rods during the course of these five sets of experiments have resulted in the more correct average of 4.31 wt% quoted in this and some of the more recent reports. . . . the values quoted in this report should be considered the latest and, hopefully, the more correct values to use.

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

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

The uranium assay (1059.64 ± 4.80 g/rod) and the ²³⁵U enrichment ($4.306 \pm 0.013\%$) . . . are the average of six assays and six spectrographic analyses made on fuel pellets chosen at random during the reloading. The oxide density (10.40 ± 0.06 g UO₂/cm³) . . . is based on individual volume displacement measurements with 20 pellets selected at random during the reloading operations. The mass of UO₂ per rod (1203.38 ± 4.12 g) is the average mass of the 1865 rods of this type available for use in the experiments. . . . The rubber end cap density (1.321 g/cm³) . . . is the result of a single mass-volume measurement with six end caps selected at random. The composition of the end caps is the result of four analyses on randomly selected end caps.

Uranium isotopic composition is summarized in Table 3.

Table 3. Isotopic Composition of Uranium in 4.31% Enriched UO_2 Fuel Rods
(Reference 10, p. 2.3).

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

Rubber end cap data^a and 6061 aluminum tubing (clad) data are given in Table 4. The 6061 aluminum data includes the measured density and the ASTM Standard chemical composition.^b

^a Reference 10, p. 2.3.

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

Table 4. Rubber End Cap and 6061 Aluminum Clad Data.

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

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

1.3.2 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/cm³.^b

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

^b Interpolated from densities at 20 and 25°C, CRC Handbook of Chemistry and Physics, 68th Edition, p. F-10.

The conclusion of the evaluations of the water impurity analyses in Appendix C and in Sections 2.3 and 3.3 is that the gadolinium impurity reported in Reference 4 is significant. No gadolinium impurity is reported in Reference 5. Therefore, the measurements reported in Reference 6 (p. 13) as two measurements of the same experiment is considered in this evaluation to be two separate configurations, Cases 9 and 10.

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

1.3.4 Support Structures and Tank - Experiment support structures, including lattice plate supports and spacer rods, control/safety blade guides, and tubes housing the proportional counters were 6061 aluminum alloy. (Constituents of 6061 aluminum are given in Table 4.) As mentioned in Section 1.2, doubling the aluminum grid plate supports and the control and safety blade guides did not have a measurable effect on predicted critical separation.

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

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

2.0 EVALUATION OF EXPERIMENTAL DATA

Experiments were well documented and carefully performed. There were no significant omissions of data. However, uncertainties in measurement data contribute to an uncertainty in the benchmark-model k_{eff} . Descriptions of calculations of the effect of the uncertainties on k_{eff} are given below. Results are summarized in Table 5.

2.1 Fuel Rod Characterization

The average length of the fuel region was not given. Rather, a maximum fuel length of 92.71 cm and a minimum fuel length of 91.44 cm were reported. However, using the average of the reported maximum and minimum lengths, the reported fuel diameter, and the reported average mass of UO_2 per rod does give the reported average UO_2 density of 10.40 g/cm^3 . A sensitivity study, with mass of UO_2 per rod held constant over this range in fuel length, gave Δk_{eff} values of 0.05% and 0.08%,^a as shown in Table 5. Therefore, uncertainty in the fuel length contributes a small uncertainty to the benchmark-model k_{eff} value.

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

The uncertainty in fuel diameter was $\pm 0.003 \text{ cm}$. Varying the fuel diameter by this amount, with a corresponding change in UO_2 density, gave a maximum Δk_{eff} of 0.02%.

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

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

The maximum reported uncertainty in pitch was ± 0.003 inch (0.0076 cm).^a The maximum Δk_{eff} calculated was 0.127%.

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

The last two rows of Table 5 are each the result from a model that combines all modifications that contribute to a change in k_{eff} in the same sense, either positive or negative. For example, all changes that produce negative effects on rods are: decreased fuel length, compressed plug, increased fuel diameter, decreased pitch, with minimum UO_2 , maximum U, and minimum enrichment. (Dimensions and atom densities of the model are modified accordingly.) This estimate of the effect on k_{eff} of uncertainties is conservative because it is highly unlikely that all rods differ from the average in all respects that affect k_{eff} in the same sense. Also the estimate of the uncertainty in pitch is itself especially conservative. (See footnote c of Table 7). Nevertheless, an uncertainty of $\pm 0.26\%$ may be included in the benchmark-model k_{eff} to account for fuel rod measurement uncertainties.

^a Reference 8, p. E.4, bottom plate, corrected.

Table 5. 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
Fuel Length (± 0.635 cm)	+0.076	-0.057
Plug Compression (± 0.3175 cm change in length)	+0.0007	-0.0007 ^(b)
Fuel Diameter (± 0.003 cm)	-0.004	+0.023
Pitch (± 0.0076 cm ^(c))	+0.127	-0.122
Combination of Enrichment (± 0.013 wt.%), UO_2 Mass Per Rod (± 4.12 g), U Mass Per Rod (± 4.80 g)	+0.070 ^(d)	-0.054 ^(e)
Combine all changes that individually increase k_{eff}	$\Delta k_{\text{eff}} = 0.26\%$	
Combine all changes that individually decrease k_{eff}	$\Delta k_{\text{eff}} = 0.21\%$	

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

2.2 Reflector Thickness

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

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

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

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

2.3 Gadolinium Impurity

Water impurity sensitivity studies in Appendix C and Section 3.3.2 indicate that the only significant impurity is the gadolinium impurity reported in Reference 4. For all cases from Reference 4 (all cases except Case 10), a gadolinium concentration of $10.4 \pm 3.6 \text{ g/m}^3$ is reported to be present in the water moderator and reflector. However, no gadolinium impurity is reported in References 5 and 6 (Case 10).

One experimenter^a provided the results of the water sample analyses for experiments reported in Reference 4. A letter from Loren J. Maas of the Hanford Environmental Health Foundation to B. M. Durst dated August 31, 1979, stated the results of analyses of three water samples from the set of experiments from Reference 4. The gadolinium results were stated in the letter as 12.0, 6.3 and 13.0 mg/liter of Gd. The average value is 10.4 g/m^3 with a standard deviation of 3.6 g/m^3 , as reported in Reference 4. The three Gd sample values were verified by P. A. Thurman of the water analysis laboratory, who checked the original laboratory worksheet. Recorded values were 12.3, 6.3, and 12.6 mg/l of gadolinium. (Apparently these values were rounded to two significant figures in the letter reporting results.) Ms. Thurman said^b such small amounts could be detected because the sample was concentrated by evaporation before analysis. Another experimenter^c reported information from a recent discussion with Maureen K. Hamilton, Laboratory Director, Environmental Sciences, the Hanford Environmental

^a Private communication, Sid Bierman, September 1993.

^b Private communication, Pam Thurman, April 1994.

^c Private communication, Michael Durst, October 1994.

Health Foundation. Ms. Hamilton said that the 1979 analysis was made just after a new water analysis standard was issued that required analysis for gadolinium. At that time, the standard required analysis of the exact amount of gadolinium present. Later, the standard was revised to require only a determination that the amount of gadolinium was less than 40 ppm. Ms. Hamilton stated that the analysis was made using emission and/or absorption spectroscopy.

A letter from the same laboratory dated August 4, 1980, reporting the analyses of samples from the later experiments in Reference 5^a did not report a value for gadolinium.

Possible sources of the gadolinium are paint on the tank inner wall,^b breach of cladding on gadolinium safety rods used in experiments that were alternated with these experiments,^c and gadolinium solution that was present in the same laboratory at that time. Although all water was replaced as experiments were alternated and precautions were taken to contain gadolinium solutions, the presence of gadolinium impurity is not impossible.^d

(The natural abundance of gadolinium in the earth's crust is 6.1 ppm.^e Several gadolinium compounds are soluble in room-temperature water.^f)

Although calculational results of this set of experiments are significantly low, as discussed in Section 4,^g they cannot be rejected on this basis alone. Evidence indicates that gadolinium impurity at the reported concentration was indeed present. Until and unless other evidence reveals otherwise, these experiments are useful as benchmark experiments, especially for low-enriched fuel rods moderated by water containing low concentrations of gadolinium.

^a Private communication, Sid Bierman, September 1993.

^b Private communication, B. M. Durst, September 1994.

^c B. M. Durst and James Mincey, private communication, September 1994.

^d Private communication, B.M. Durst, February 1995. Although Mr. Durst believes that results of the water sample analyses cannot be discounted, he believes that it is unlikely that such a large amount of Gd could have been present in the tank. (The 10.4 g/m³ represents about 60 grams of gadolinium in the tank.)

^e N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, Pergamon Press, New York, p. 1426, 1984.

^f In particular, gadolinium bromide, chloride, fluoride, iodide, dimethylphosphate, nitrate, selenate, and sulfate. (*CRC Handbook of Chemistry and Physics*, R.C. Weast, ed., CRC Press, Inc., Boca Raton, Florida, 68th edition, p. B-91, 1987.)

^g However, see calculational results in Appendix E.

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 gave a change in k_{eff} of 0.023% between these two extremes of temperature. (The gadolinium impurity was not included.) Therefore, estimates of the uncertainty in k_{eff} due to the effects of temperature are half of these amounts, namely 0.01%.

2.5 Cluster Separations

The measurement uncertainties in cluster separation (See Table 2.) vary from 0.02 cm to 0.05 cm. To calculate the effect on k_{eff} of this uncertainty, cluster separations were reduced for several cases. Average results of KENO V.a 27-group calculations for four groups are summarized in Table 6.

Table 6. Effect on k_{eff} of Uncertainty in Measured Cluster Separation.

Case Number	$\Delta k_{\text{eff}}(\%)$ per 0.01 cm reduction in separation ^(a)
8, 9	0.041
10-13, 15, 16, 18	0.041 ^(b)
14, 17, 19, 20	0.061 ^(c)

- (a) KENO V.a with 27-group ENDF/B-IV cross sections; difference between averages of at least six calculations with at least 165,000 active neutrons/calculation.
- (b) Both x and y-separations were reduced by 0.03 cm; the resulting Δk_{eff} was then divided by 3 to find the effect per 0.01 cm.
- (c) Y-separation was reduced by 0.04 cm (the average y-separation uncertainty) and x-separation was reduced by 0.02 cm; the resulting Δk_{eff} was then divided by 2 to find the effect per 0.01 cm.

The uncertainties to be included in the benchmark-model k_{eff} due to uncertainty in the cluster separation measurement are listed in Table 7. Cases that are not listed were single-cluster configurations.

Table 7. Uncertainties in Benchmark-Model k_{eff} Due to Cluster Separation Measurement Uncertainty.

Case Number	Uncertainty in Separation Measurement (cm)	$\Delta k_{\text{eff}}(\%)$ to Include in Uncertainty of Benchmark-Model k_{eff}
8	0.02	0.08
9-12	0.03	0.12
13, 15, 16, 18	0.02	0.08
14, 17, 19, 20	0.02 ^(a)	0.12

- (a) This is x-separation uncertainty. Y-separation uncertainty is 0.04, except for Case 19, where it is 0.05. (See footnote c of preceding table.)

3.0 BENCHMARK SPECIFICATIONS

3.1 Description of Model

The calculational models consist of square-pitched, aluminum-clad cylindrical fuel pins in water arranged in rectangular clusters. Descriptions of the benchmark critical configurations, including cluster dimensions, separations, and fuel rod pitch, are given in Table 8 and are shown in Figures 4-8.

A fraction of a rod is rounded to the nearest whole rod. Fractional rows for the single-cluster cases are modeled by a partial row along one side of the array that begins at the corner of the array. For Cases 8, 11, 12, 13, and 20, with two or four clusters, the rods of the two partial rows for each case are added from the upper left corners. (See Figure 9.)

Table 8. U(4.31)O₂ Fuel Rod Critical Configurations (See Figures 4-9).

Case Number	Number of Clusters	Dimensions of Complete Rectangular Cluster ^(a) (number of rods, X x Y)	Number of Rods in Partial Row(s) (X ~)	Separation Between Clusters (cm)
1	1	12 x 18	10	-
2	1	14 x 15	6	-
3	1	16 x 13	9	-
4	1	17 x 12	15	-
5	1	14 x 13 ^(b)	11	-
6	1	14 x 16 ^(c)	4	-
7	1	14 x 14 ^(d)	3	-
8	2	9 x 12	1 on one cluster, 2 on the other cluster	2.83
9	3	12 x 16	-	12.27
10 ^(e)	3	12 x 16	-	12.493
11	4	9 x 12 (two lower) 9 x 2 (two upper)	1 on each of two upper clusters	4.72
12	4	9 x 12 (all four)	1 on one upper cluster only	6.61
13	4	9 x 12 (two lower) upper clusters are partial rows only	5 on one upper cluster, 4 on other upper cluster	2.83 (x-separation), 8.38 (y-separation)
14	4	9 x 12 (two lower) 9 x 1 (two upper)	-	2.83 (x-separation) 10.86 (y-separation)
15	4	9 x 12 (two lower) 9 x 2 (two upper)	-	2.83 (x-separation) 11.29 (y-separation)
16	4	9 x 12 (two lower) 9 x 4 (two upper)	-	2.83 (x-separation) 12.02 (y-separation)
17	4	9 x 12 (two lower) 9 x 8 (two upper)	-	2.83 (x-separation) 13.64 (y-separation)
18	4	9 x 12 (two lower) 9 x 10 (two upper)	-	2.83 (x-separation) 14.98 (y-separation)
19	4	9 x 12 (all four)	-	2.83 (x-separation) 19.81 (y-separation)
20	4	9 x 10 (two lower) 9 x 9 (two upper)	2 on one upper cluster, 3 on other upper cluster	2.83 (x-separation) 8.50 (y-separation)

(a) This is the portion of the cluster or clusters that does not contain partial rows.

(b) Includes 25 "water holes" where water replaces fuel rods in the lattice. See Figures 4 and 8.

(c) Includes 25 "aluminum clad voids" where plugged, air-filled aluminum tubes, of the same material and dimensions as the fuel rod clad and end plugs, replace fuel rods in the lattice. See Figures 4 and 8.

(d) Includes 25 "water-filled aluminum tubes" where open aluminum tubes, of the same material and dimensions as the fuel rod clad and filled with water, replace fuel rods in the lattice. See Figures 4 and 8.

(e) No gadolinium impurity is present in the water moderator-reflector for this case.

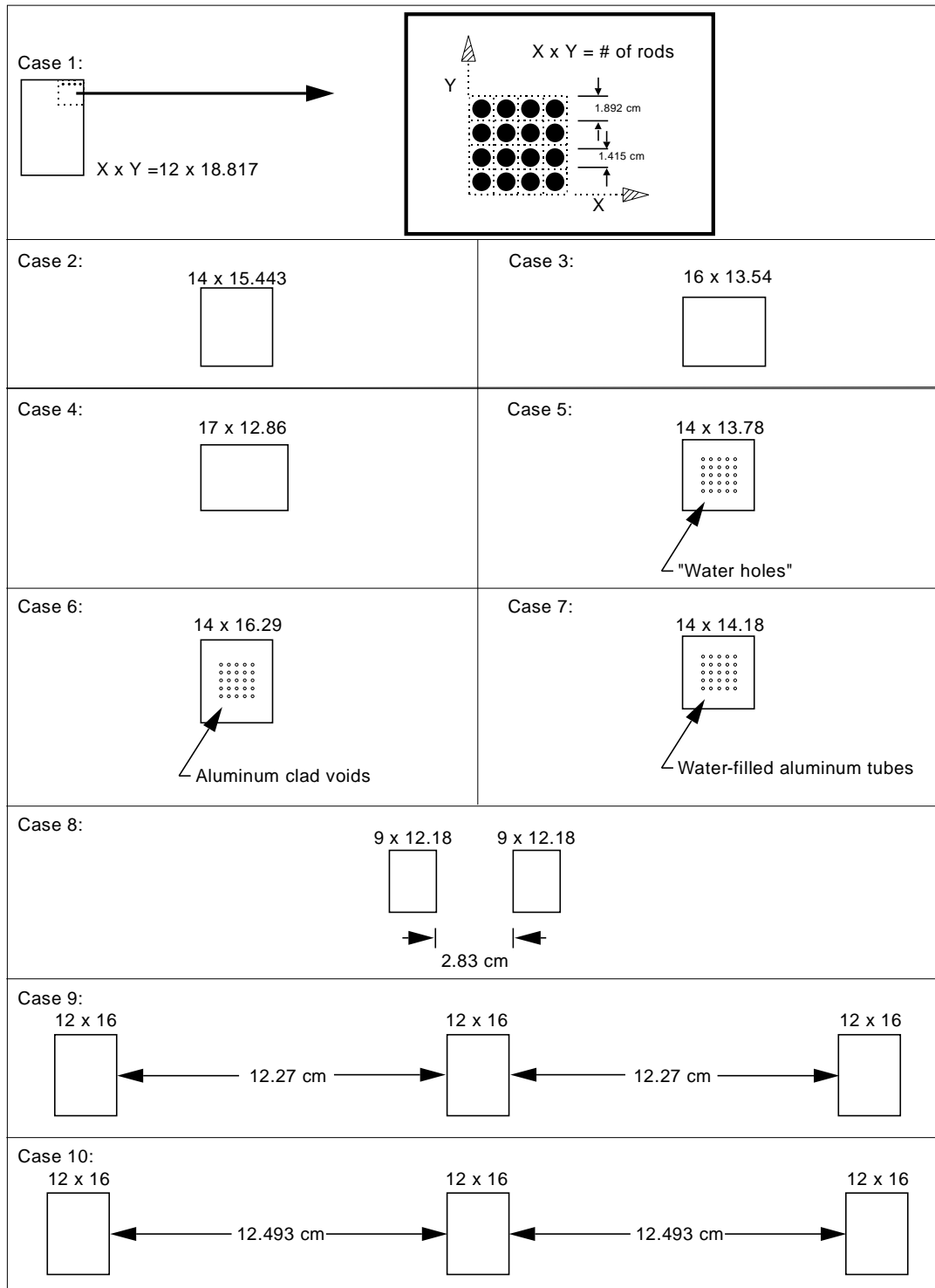


Figure 4. Critical Configurations of Clusters of $U(4.31)O_2$ Fuel Rods at 1.892 Centimeter Pitch (Cases 1-10).

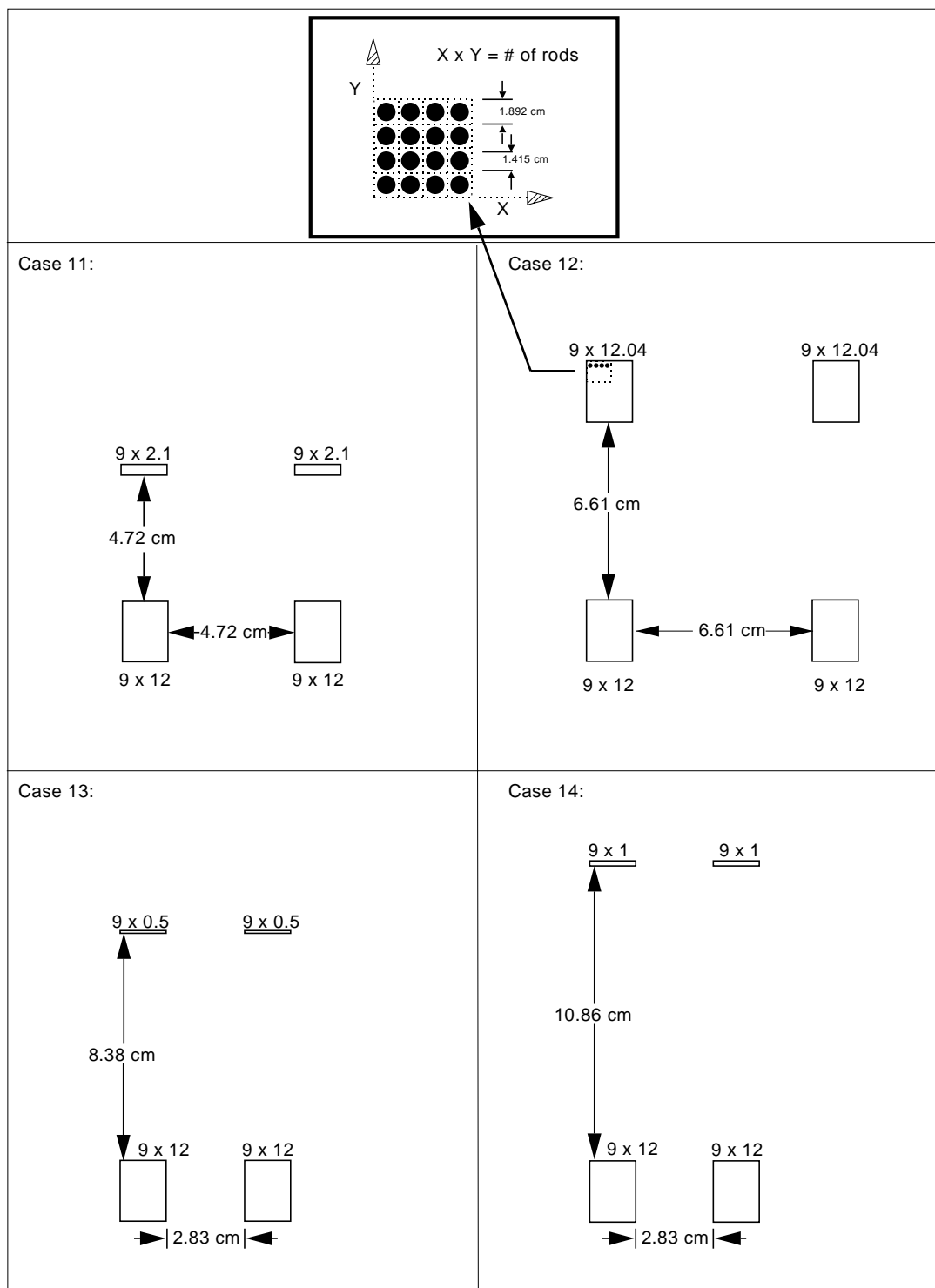


Figure 5. Critical Configurations of Clusters of $U(4.31)O_2$ Fuel Rods at 1.892 Centimeter Pitch (Cases 11-14).

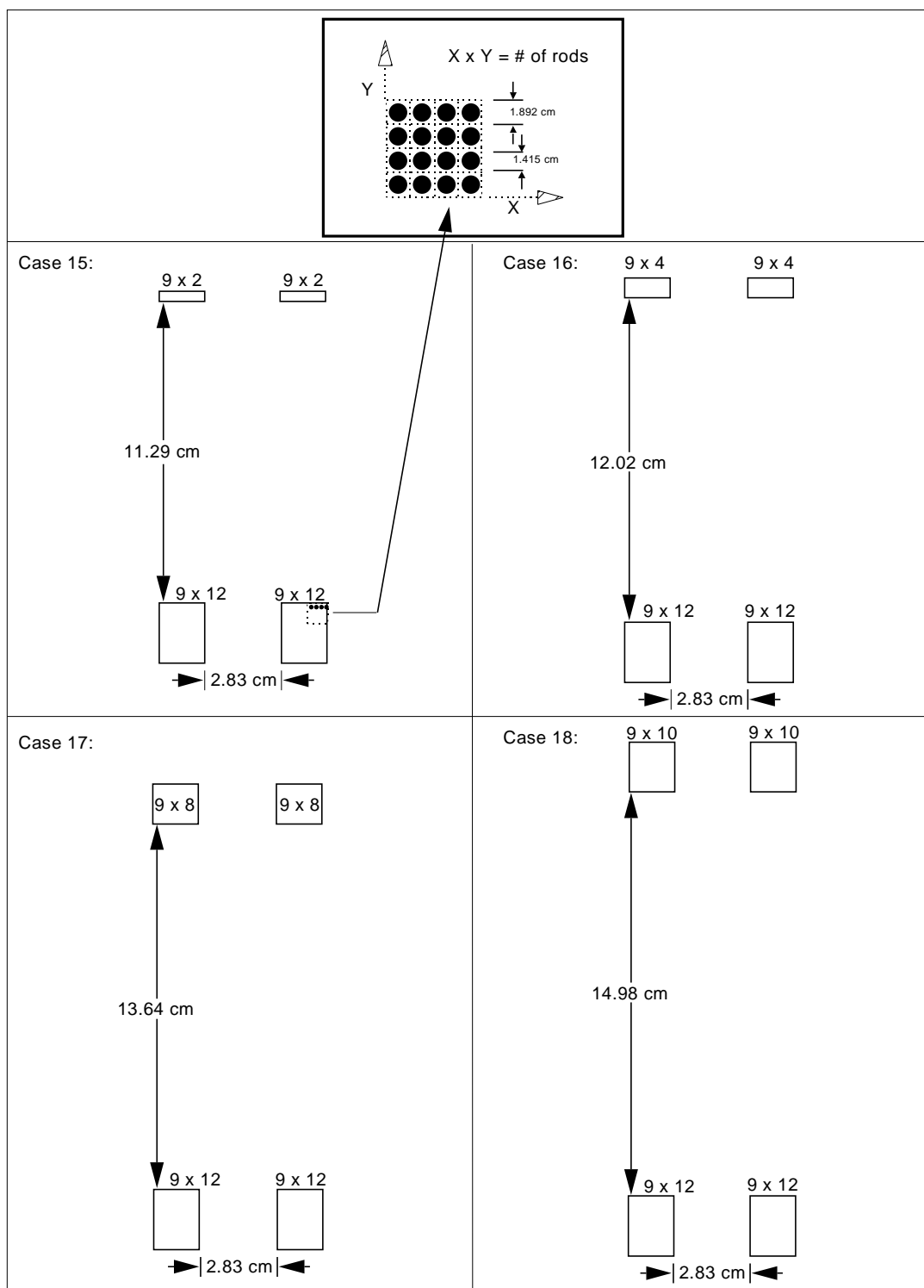


Figure 6. Critical Configurations of Clusters of $U(4.31)O_2$ Fuel Rods at 1.892 Centimeter Pitch (Cases 15-18).

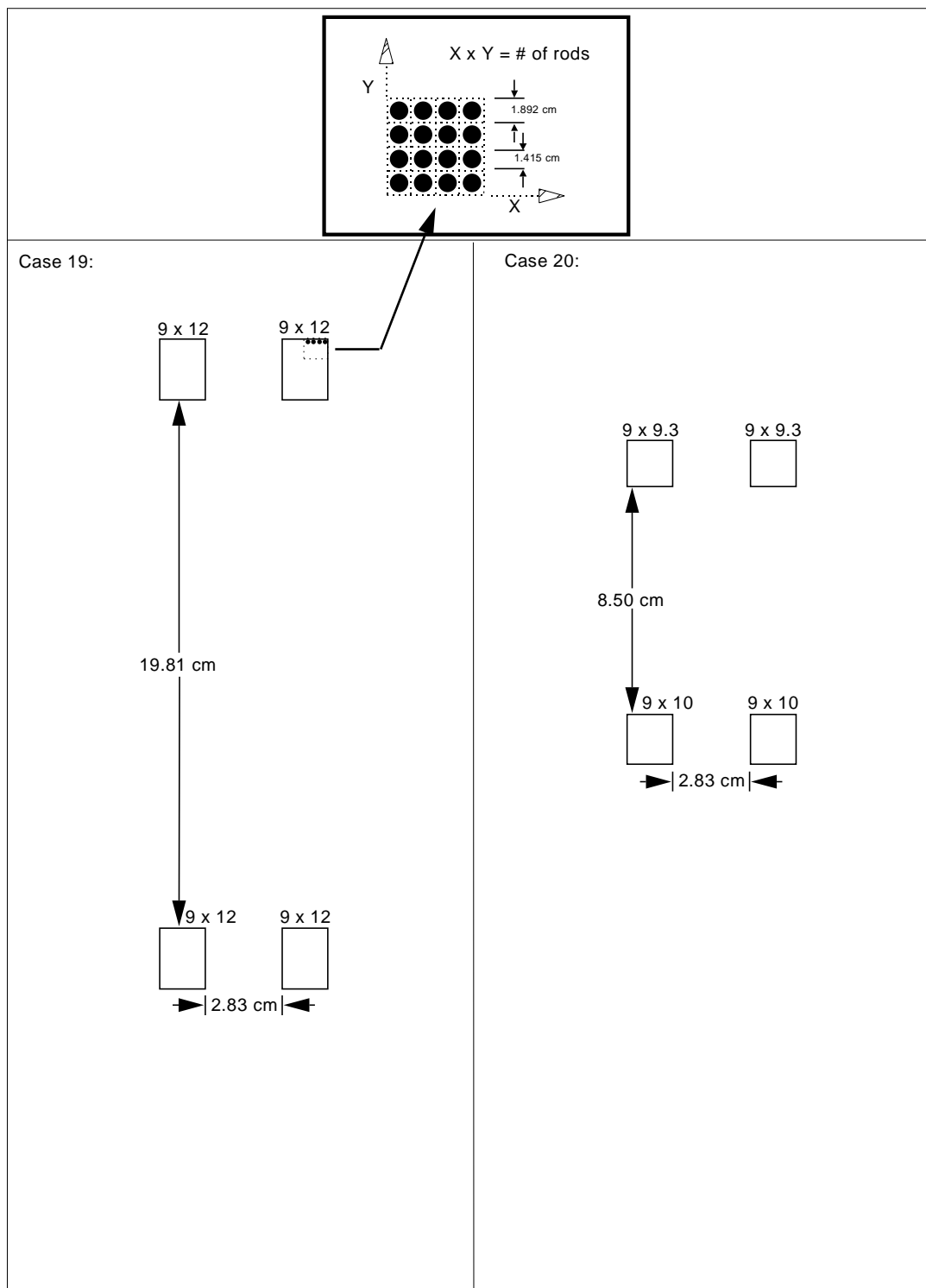


Figure 7. Critical Configurations of Clusters of $\text{U}(4.31)\text{O}_2$ Fuel Rods at 1.892 Centimeter Pitch (Cases 19 and 20).

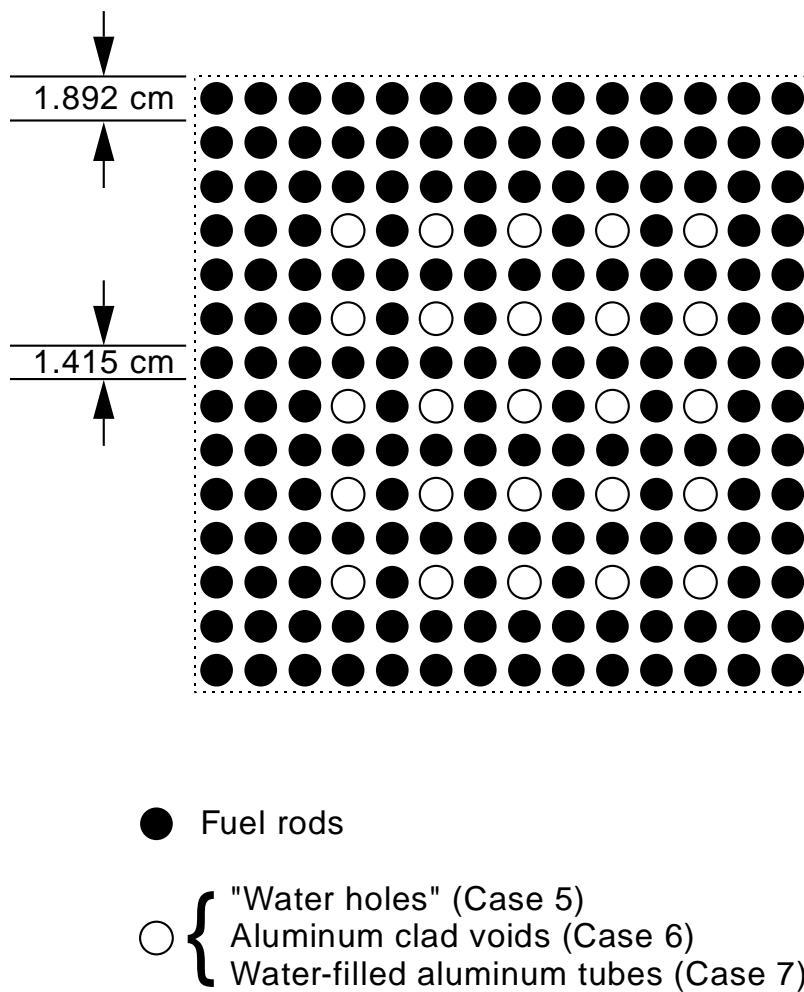


Figure 8. 14 x 14 Array of $\text{U}(4.31)\text{O}_2$ Fuel Rods at 1.892 Centimeter Pitch Showing Placement of Water Holes, Aluminum Clad Voids, and Water-Filled Aluminum Tubes (Cases 5-7).

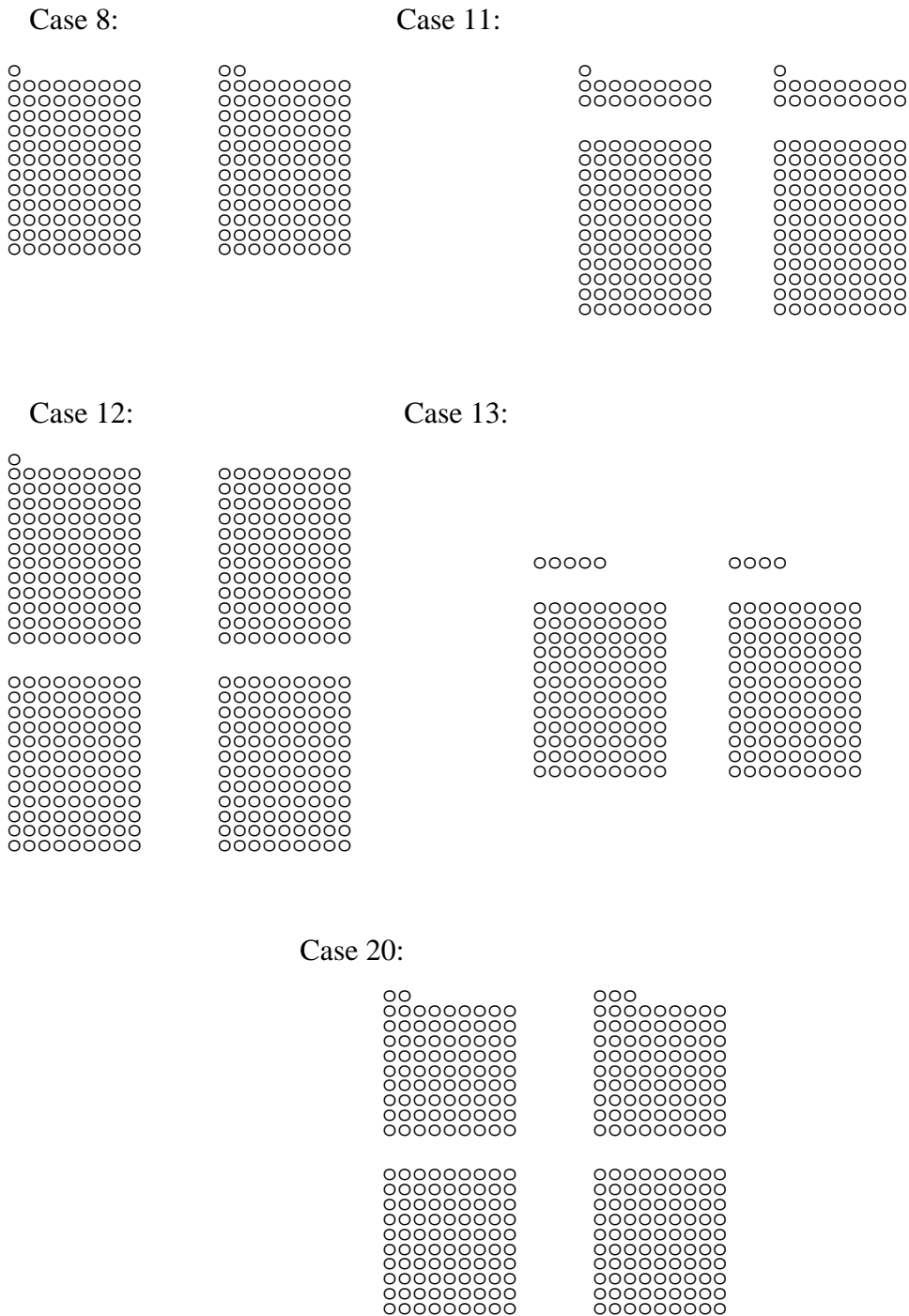


Figure 9. Partial Row Placement for Cases 8, 11-13, and 20.

Sensitivity Studies. Two studies were performed to determine the sensitivity of the model to the method of representing the partial rows. One study calculated the effect of adding an extra rod to provide an estimate of twice the maximum effect of dropping the fractional rod. A ONEDANT cylindrical homogeneous model of an array of pins was used, with the extra rod adding to the diameter of the cylinder and, therefore, effectively spread out around the outer radius of the cylinder. The effect was $0.06\% \Delta k_{\text{eff}}$. This indicates that rounding the fraction of a rod to the nearest whole rod in the benchmark model will have a small effect on k_{eff} . Half the calculated effect, 0.03% , may be added to the uncertainty in the benchmark model k_{eff} .

Another study compared rods of the partial row placed at the end of the row, as in the benchmark model, to the rods of the partial row placed at the center of the side. This comparison was made for five typical cases. Results for several calculations by KENO V.a with the 27-group ENDF/B-IV cross sections were statistically combined. The difference was 0.09% . Half of this amount should be added to the uncertainty in the benchmark model k_{eff} .

3.2 Dimensions

Fuel rod dimensions are shown in Figure 10. The rod has an outer diameter of 1.415 cm and is 96.52 cm long. The UO_2 fuel region has a diameter of 1.265 cm and is 92.075 cm long. The clad is 0.066 cm thick. Therefore, the gap between UO_2 and clad is 0.009 cm thick with an outer radius of 0.6415 cm. The compressed rubber end plugs are 2.2225 cm long with a radius of 0.6415, to fit exactly within the ends of the fuel rod.

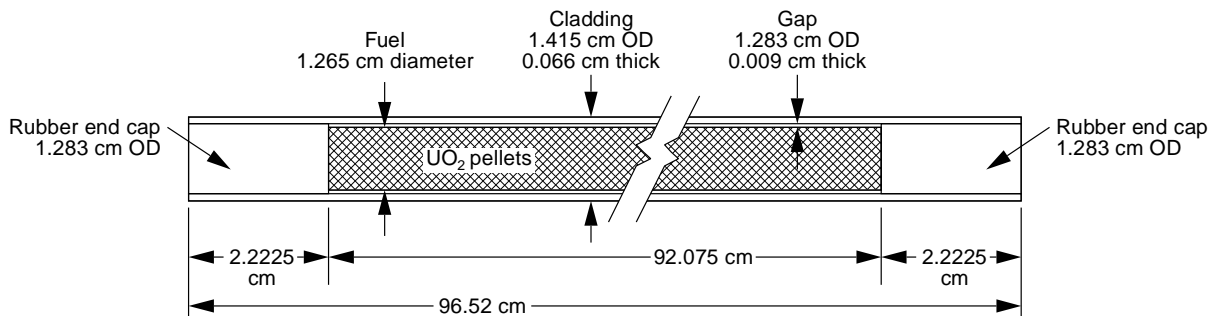


Figure 10. Fuel Rod Model.

The twenty-five aluminum clad voids and water-filled aluminum tubes were modeled with aluminum tubes with the same length and diameters as the fuel tubes. The water-filled aluminum tubes were open, while the aluminum clad voids were closed on both ends by compressed rubber plugs.

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-cm-thick water. The top reflector is 12.7775 cm of water.

3.3 Material Data

3.3.1 Fuel Rods - The fuel region consists of 1203.38 g of UO_2 . The mass of uranium in each rod is 1059.64 g. The isotopic composition of the uranium is 0.022 wt.% ^{234}U , 4.306 wt.% ^{235}U , 0.022 wt.% ^{236}U , and 95.650 wt.% ^{238}U . Fuel rods have 6061 aluminum clad and compressed rubber end plugs of density 1.498 g/cm³.^a Atom densities are given in Table 9.

^a This density is more than the reported density of the plugs in Table 4 because of the compression of the plugs.

Table 9. Fuel Rod Atom Densities.

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

3.3.2 Moderator-Reflector - Fuel rods rest on an acrylic support plate. The support plate has a density of 1.185 g/cm³ 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. The water contains 10.4 g/m³ of gadolinium impurity for all cases except Case 10, which contains no gadolinium. Atom densities are given in Table 10.

Table 10. Moderator-Reflector Atom Densities.

Material	Isotope	Atom Density (barn-cm) ⁻¹
Water ^(a)	H	6.6706×10^{-2}
	O	3.3353×10^{-2}
	Gd ^(b)	3.9828×10^{-8}
Acrylic	H	5.6642×10^{-2}
	C	3.5648×10^{-2}
	O	1.4273×10^{-2}

- (a) This is 0.997766 g/cm³, interpolated from densities at 20°C and 25°C (CRC Handbook of Chemistry and Physics, 68th edition, p F-10.)
- (b) This is 10.4 g/m³ of gadolinium, which is the analyzed average concentration for critical configurations from Reference 4. Case 10 from Reference 5 is the only case with no gadolinium in the water.

Sensitivity Studies. Water Impurities. The effects on k_{eff} of impurities in the water moderator-reflector for a near-critical cylindrical cluster of UO₂ 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 impurity was recorded for experiments included in this evaluation. However, the reported gadolinium concentration of 10.4 g/m³ caused a significant reduction (~1%) in k_{eff} . Results of a sensitivity study with ONEDANT slab and cylindrical geometries are given in Table 11 and shown in Figure 11.

Table 11. Effects on k_{eff} for $\text{U}(4.31)\text{O}_2$ Fuel Pins of Gadolinium Impurity in the Water Moderator-Reflector.

Quantity	Gadolinium Concentration (g/m ³)	Gadolinium Atom Density (atoms/barn-cm)	$\Delta k_{\text{eff}}(\%)$, ONEDANT slab geometry	$\Delta k_{\text{eff}}(\%)$, ONEDANT cylindrical geometry
no impurity	0	0	-	-
standard deviation of three sample measurements of impurity	3.6	1.3787×10^{-8}	-0.11	-0.19
average measured concentration minus the standard deviation	6.8	2.6042×10^{-8}	-0.21	-0.38
average measured concentration	10.4	3.9828×10^{-8}	-0.33	-0.56
average measured concentration plus the standard deviation	14.0	5.3615×10^{-8}	-0.46	-0.77

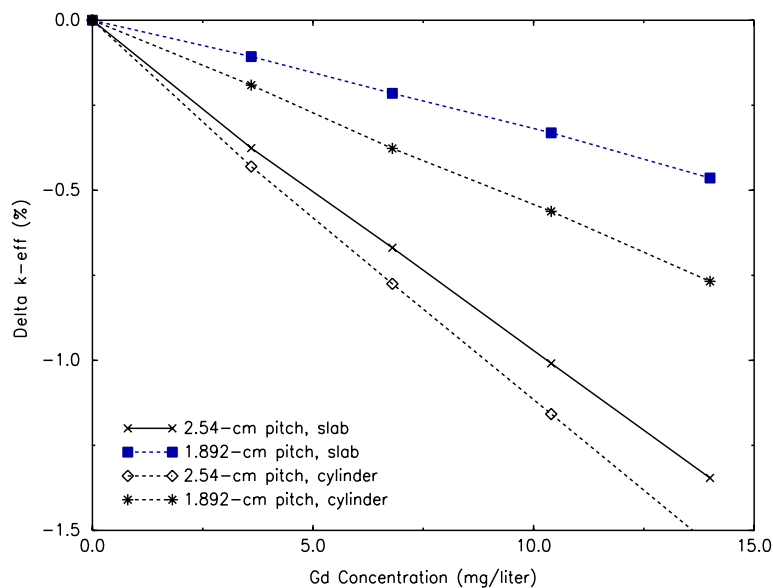


Figure 11. Change in k_{eff} with Gd Concentration (ONEDANT).

Note that the magnitude of the effect of gadolinium is greater for the near-critical cylinders than for infinite slabs. Because a reflected cylindrical cluster includes more water reflector and, therefore, better represents the critical configurations evaluated here, the cylindrical results are used to determine an uncertainty in k_{eff} due to the gadolinium impurity.

The effect of the 3.6 g/m^3 uncertainty in gadolinium concentration on k_{eff} for a cylindrical cluster is -0.19% for 1.892-cm pitch rods. This may be added to the uncertainty in k_{eff} for the benchmark model. For Reference 5, which does not report a gadolinium impurity, it is not known whether gadolinium was not measured or was measured and found to be too small to report. Therefore, this uncertainty in k_{eff} may apply to all cases.^a

Note that if the gadolinium cross sections are in error, then the magnitudes of the calculated uncertainties in the benchmark-model k_{eff} due to gadolinium will also be in error.

Table 12 gives calculated results for nineteen critical configurations with and without gadolinium in the water of the reflector and moderator. As expected, gadolinium reduces k_{eff} by approximately 1%. Therefore, the benchmark models of configurations from Reference 4 (all cases except Case 10) include gadolinium.

^a A more conservative estimate of the uncertainty in k_{eff} is the effect of the entire average measured Gd impurity. This can be used if the validity of Gd impurity measurements of all reports is questioned. The effect on k_{eff} of the average 10.4 g/m^3 is 0.79% for 1.684-cm pitch rods. This uncertainty may then be included in the uncertainty in the benchmark-model k_{eff} for all cases.

Table 12. Calculated Results U(4.31)O₂ Fuel Rods, 1.892-cm Pitch in Water, with and without Gd Impurity in Water.^(a)

Code (Cross Section Set)→ Case Number ↓	KENO (27-Group ENDF/B-IV)	KENO (27-Group ENDF/B-IV) w/o Gd in water	MCNP (ENDF/B-V)	MCNP (ENDF/B-V) w/o Gd in water
1	.9876	.9934	.9899	.9971
2	.9882	.9960	.9925	1.0009
3	.9899	.9933	.9899	.9989
4	.9857	.9945	.9898	.9991
5	.9850	.9971	.9899	.9970
6	.9868	.9932	.9894	.9957
7	.9877	.9962	.9901	.9923
8	.9805	.9931	.9855	.9978
9,10	.9817	.9895	.9874	.9970
11	.9806	.9935	.9820	.9956
12	.9767	.9879	.9814	.9927
13	.9817	.9954	.9893	.9974
14	.9829	.9927	.9856	.9945
15	.9822	.9933	.9880	.9919
16	.9844	.9901	.9868	.9916
17	.9806	.9897	.9855	.9956
18	.9856	.9922	.9893	.9979
19	.9816	.9965	.9856	.9982
20	.9817	.9920	.9811	.9930
Average of above cases	.9837	.9931	.9873	.9960
Average change in k _{eff} when Gd is removed	-	0.96%	-	0.88%

(a) The gadolinium concentration was 10.4 g/m³. Standard deviations of the calculations were between 0.0012 and 0.0021. Some cases in this table vary slightly from the final benchmark models described in Section 3.

Lattice Plates. ONEDANT calculations of an infinite slab of fuel pins, with and without polypropylene lattice plates present and reflected by 15 centimeters of water, were performed. The effect on k_{eff} of the lattice plates located at 0 cm and 79 cm above the fuel rod support plate is 0.02%. Because the lattice plates are omitted from the benchmark models, this small positive reactivity should be subtracted from the benchmark-model k_{eff} .

Bottom Reflector. The effects on k_{eff} of the one-inch-thick acrylic support plate directly beneath an infinite slab of fuel rods and of the carbon steel tank 17.84 cm below the fuel rods was calculated using ONEDANT. Results are shown in Table 13. As expected, the carbon steel tank had practically no effect on k_{eff} , while the acrylic support plate had a small measurable effect. Therefore, the acrylic support plate is retained in the benchmark model. As discussed in Section 2.2, concrete or stainless steel beyond 15 centimeters of water reflector have a negligible effect on k_{eff} . Therefore, the model of the bottom reflector is 2.54 cm of acrylic followed by 15.3 cm of water.

Table 13. Effect of Bottom Reflector Materials on k_{eff} ^(a)

Reflector			Δk_{eff} (%)
Inner 2.54 cm	Middle 15.3 cm	Outer 0.952 cm	
acrylic	water	carbon steel	-
acrylic	water	water	0.000
water	water	water	-0.06

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

3.4 Temperature Data

Temperature data for the individual experiments were not published.

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

A sensitivity study in Section 2.4 demonstrated that the effects on k_{eff} of temperature are small (approximately 0.01%). Therefore, any reasonable

approximation to room temperature may be used in the model. (Temperature uncertainty is included in the uncertainty in benchmark-model k_{eff} .)

3.5 Experimental and Benchmark-Model k_{eff}

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

Because of small calculated positive effects of lattice plates, which are omitted from the benchmark model, the benchmark-model k_{eff} is slightly below 1.0. The benchmark-model k_{eff} is 0.9998.

Other model simplifications (no aluminum support structures; no reflection beyond 30 cm of water on the sides, 15 cm of water above, and 15.3 cm of water below; no measurement devices in the reflector beyond 15 cm; uniform end plugs filling the ends of the clad) were judged to have negligible effect on k_{eff} . However, some experimental uncertainties or model simplifications, whose effects were described in sensitivity studies above, contribute to an estimated uncertainty in the benchmark model k_{eff} . Uncertainties included are listed in Table 14.

Table 14. Uncertainty in Benchmark-Model k_{eff} .

Measurement Uncertainty or Model Simplification	Δk_{eff}	
Fuel rod characterization	0.0026	
Temperature	0.0001	
Cluster Separations	Cases 8, 13, 15, 16, 18	0.0008
	Cases 9-12, 14, 17, 19, 20	0.0012
Omit fractional rod	0.0003	
Placement of partial row	0.0005	
Gadolinium impurity uncertainty	0.0019	
Total Uncertainty in k_{eff} ^(a)	Cases 1-7	0.0033 ^(b)
	Cases 8-20	0.0035 ^(c)

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

(b) If the entire Gd impurity is considered uncertain, this value is 0.0062.

(c) If the entire Gd impurity is considered uncertain, this value is 0.0063.

Therefore, the benchmark model k_{eff} is 0.9998 ± 0.0033 for Cases 1-7 and is 0.9998 ± 0.0035 for Cases 8-20.



4.0 RESULTS OF SAMPLE CALCULATIONS

Results of calculations representing the 20 critical configurations are presented in the following three tables. Code versions and modelling options are discussed briefly in paragraphs preceding the input listings in Appendix A. Appendix E provides an additional set of calculational results of the benchmark model configurations.

Calculated results are 1-2% low for MCNP, 1-2% low for KENO V.a with 27-group cross sections, and 3-3.5% low for KENO V.a with Hansen Roach cross sections. This bias in k_{eff} could be due to a bias in the experimental data (e.g., pitch, extrapolation to critical, cluster separation measurements, gadolinium impurity) and/or a bias in cross sections that are significant in this problem (e.g., Gd, ^{238}U capture resonances).^a Note, however, that all calculated results are below the benchmark-model k_{eff} by more than the estimated uncertainty in k_{eff} ,^b even if the entire reported gadolinium impurity is considered as uncertain. (This uncertainty is approximately ± 0.0063 , as mentioned in a footnote to Table 14.)

Note also that the 16-group gadolinium cross section set is not a Hansen-Roach cross-section set. See footnote to Table 15.

A possible cause of the low results for the KENO 27-group calculations is provided by the SCALE4 reference manual. Section M4.B.4, Known Cross-Section Irregularities states the following:

Systems containing gadolinium have not calculated well with the 27-group library. The problem stems from the characteristic of the gadolinium data in the thermal range. Gadolinium has low energy resonance data down to 10^{-5} eV. The resonances are so broad that the implementation of the Nordheim treatment in NITAWL-II fails to have a mesh point in group 27 of the 27-group structure. This has been addressed by setting the bottom energy of the resonance data to that

^a A possible contribution to low MCNP results is a slight Doppler broadening at 300 K of the sharp, tall Gd resonances. This temperature, which is the temperature of the ENDF/B-V cross sections used in the calculations, is just above the temperature range of the experiments.

A possible contribution to low 27-group results is the ENDF/B-IV evaluation of ^{238}U . According to W. Rothenstein, "Thermal-Reactor Lattice Analysis Using ENDF/B-IV Data with Monte Carlo Resonance Reaction Rates," Nuclear Science and Engineering, 1976, vol. 59, pp. 337-349, the ENDF/B-IV representation of the low-lying ^{238}U resonances leads to low eigenvalues (by approximately 1%) for water-reflected low-enriched UO_2 lattices.

^b Except for four cases, the additional calculational results in Appendix E are within the uncertainty range of the benchmark-model k_{eff} .

of group 26 and carrying infinite dilution cross sections in group 27 of the master library. Use of the gadolinium in the SCALE system, especially for very dilute systems, should be done with caution.

Note that the highest calculated value for all three codes is for Case 10, a case with no gadolinium impurity. However even for this case, codes underpredict by 1% (MCNP and KENO 27-group) and 2% (KENO Hansen-Roach). This indicates that, besides a possible overestimation by the codes of the negative effect of gadolinium, there is some other negative influence biasing the result.

Table 15. Sample Calculation Results (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	0.9679 ± .0019	0.9882 ± .0018	0.9899 ± .0022
2	0.9697 ± .0017	0.9841 ± .0017	0.9925 ± .0017
3	0.9686 ± .0020	0.9873 ± .0022	0.9918 ± .0020
4	0.9653 ± .0019	0.9862 ± .0019	0.9913 ± .0018
5	0.9707 ± .0018	0.9843 ± .0020	0.9899 ± .0021
6	0.9728 ± .0017	0.9879 ± .0021	0.9894 ± .0018
7	0.9698 ± .0017	0.9839 ± .0019	0.9870 ± .0019
8	0.9747 ± .0017	0.9860 ± .0020	0.9855 ± .0020
9	0.9684 ± .0020	0.9845 ± .0017	0.9856 ± .0019
10	0.9707 ± .0016	0.9925 ± .0018	0.9973 ± .0018

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

Table 16. Sample Calculation Results (United States).

Code (Cross Sections Set)→ Case Number ↓	KENO (Hansen-Roach) ^(a)	KENO (27-Group ENDF/B-IV)	MCNP (Continuous Energy ENDF/B-V)
11	0.9709 ± .0018	0.9798 ± .0019	0.9820 ± .0018
12	0.9695 ± .0020	0.9783 ± .0018	0.9814 ± .0019
13	0.9659 ± .0017	0.9823 ± .0019	0.9893 ± .0017
14	0.9693 ± .0021	0.9814 ± .0019	0.9856 ± .0020
15	0.9687 ± .0018	0.9789 ± .0022	0.9880 ± .0021
16	0.9717 ± .0020	0.9834 ± .0018	0.9868 ± .0018
17	0.9690 ± .0017	0.9851 ± .0019	0.9855 ± .0019
18	0.9675 ± .0018	0.9819 ± .0022	0.9893 ± .0021
19	0.9754 ± .0020	0.9821 ± .0017	0.9856 ± .0021
20	0.9718 ± .0018	0.9756 ± .0019	0.9811 ± .0020

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

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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. Cuboids of water were used to complete partial rows. 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

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

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 0.17271 for 1.892 cm pitch.)

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KENO-V.a Input Listing for Case 1 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections).

```
K406 12X18.817 CLUSTER (12X18 + 10 RODS), 1.892 CM PITCH
READ PARA TME=300 GEN=160 NPG=1500 NSK=50 NUB=YES
LIB=41 XS1=YES RUN=YES LNG=60000 END PARA
READ MIXT SCT=3
MIX=1
' U(4.31)02 for 1.892 cm pitch
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end plugs)
6100 4.3562-2 1102 5.8178-2 20100 2.5660-3
16100 4.7820-4 14100 9.6360-5 8100 1.2461-2
MIX=5
' acrylic
1102 5.6642-2 6100 3.5648-2 8100 1.4273-2
MIX=6
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* FUEL PINS AT END OF SIDE *
ARRAY 2 3R0
GLOBAL
UNIT 5
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 3 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=12 NUY=18 FILL F1 END FILL
ARA=2 NUX=12 NUY=1 FILL 10R1 2R2 END FILL
ARA=3 NUX=1 NUY=2 FILL 3 4 END FILL
END ARRAY
END DATA
END
```

KENO-V.a Input Listing for Case 5 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections).

```
K410 14X13.78 CLUSTER (14X13 + 11 RODS, WITH 25
WATER-HOLES), 1.892 CM PITCH
READ PARA TME=300 GEN=160 NPG=1500 NSK=50 NUB=YES
LIB=41 XS1=YES RUN=YES LNG=60000 END PARA
READ MIXT SCT=3
MIX=1
' U(4.31)02 for 1.892 cm pitch
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end plugs)
6100 4.3562-2 1102 5.8178-2 20100 2.5660-3
16100 4.7820-4 14100 9.6360-5 8100 1.2461-2
MIX=5
' acrylic
1102 5.6642-2 6100 3.5648-2 8100 1.4273-2
MIX=6
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ONE ROW OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* ONE ROW OF FUEL PINS AND 5 WATER-HOLES *
ARRAY 2 3R0
UNIT 5
COM=* PARTIAL ROW OF FUEL PINS *
ARRAY 3 3R0
GLOBAL
UNIT 6
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 4 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=14 NUY=1 FILL F1 END FILL
ARA=2 NUX=14 NUY=1 FILL 3R1 2 1 2 1 2 1 2 2R1
END FILL
ARA=3 NUX=14 NUY=1 FILL 11R1 3R2 END FILL
```


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KENO-V.a Input Listing for Case 5 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd).

```

      ARA=4 NUX=1 NUY=14 FILL 2R3 4 3 4 3 4 3 4 3 4 3 3 5 END
FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=44 ZUL=20 XLR=37 YLR=-4
  ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 8 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections).

```

K413 TWO 9X12.18 CLUSTERS(TWO 9X12 + 1 AND 2 RODS),1.892
CM PITCH,2.83 CM SEP
READ PARA TME=300 GEN=160 NPG=1500 NSK=50 NUB=YES
LIB=41 XS1=YES RUN=YES LNG=70000 END PARA
READ MIXT SCT=3
MIX=1
' U(4.31)02 for 1.892 cm pitch
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end plugs)
6100 4.3562-2 1102 5.8178-2 20100 2.5660-3
16100 4.7820-4 14100 9.6360-5 8100 1.2461-2
MIX=5
' acrylic
1102 5.6642-2 6100 3.5648-2 8100 1.4273-2
MIX=6
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* FUEL PINS OF PARTIAL ROW *
ARRAY 2 3R0
UNIT 5
COM=* FUEL PINS OF OTHER PARTIAL ROW *
ARRAY 3 3R0
UNIT 6
COM=* WATER BETWEEN CLUSTERS *
CUBOID 2 1 2.83 0 24.596 0 94.2975 -2.2225
UNIT 7
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 4 3R0
UNIT 8
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 5 3R0
GLOBAL
UNIT 9
COM=* TWO CLUSTERS WITH WATER BETWEEN *

```

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KENO-V.a Input Listing for Case 8 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd).

```

ARRAY 6 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=1 FILL 1R1 8R2 END FILL
      ARA=3 NUX=9 NUY=1 FILL 2R1 7R2 END FILL
      ARA=4 NUX=1 NUY=2 FILL 3 4 END FILL
      ARA=5 NUX=1 NUY=2 FILL 3 5 END FILL
      ARA=6 NUX=3 NUY=1 FILL 7 6 8 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=25 ZUL=20 XLR=37 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 11 of Table 16 (16-Energy-Group Hansen-Roach Cross Sections).

```

K415 FOUR CLUSTERS, TWO 9X12 AND TWO 9X2.1, 1.892 CM
PITCH, 4.72 CM SEPARATION
READ PARA TME=300 GEN=160 NPG=1500 NSK=50 NUB=YES
LIB=41 XS1=YES RUN=YES LNG=71000 END PARA
READ MIXT SCT=3
MIX=1
' U(4.31)02 for 1.892 cm pitch
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end plugs)
6100 4.3562-2 1102 5.8178-2 20100 2.5660-3
16100 4.7820-4 14100 9.6360-5 8100 1.2461-2
MIX=5
' acrylic
1102 5.6642-2 6100 3.5648-2 8100 1.4273-2
MIX=6
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* ARRAY OF FUEL PINS *
ARRAY 2 3R0
UNIT 5
COM=* PARTIAL ROW OF FUEL PINS *
ARRAY 3 3R0
UNIT 6
COM=* Y-WATER BETWEEN CLUSTERS *
CUBOID 2 1 17.028 0 4.72 0 94.2975 -2.2225
UNIT 7
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 4 3R0
UNIT 8
COM=* X-WATER BETWEEN CLUSTERS *
CUBOID 2 1 4.72 0 33.1 0 94.2975 -2.2225
GLOBAL
UNIT 9
COM=* CLUSTERS WITH WATER BETWEEN *

```

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KENO-V.a Input Listing for Case 11 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd).

```

ARRAY 5 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=2 FILL F1 END FILL
      ARA=3 NUX=9 NUY=1 FILL 1 8R2 END FILL
      ARA=4 NUX=1 NUY=4 FILL 3 6 4 5 END FILL
      ARA=5 NUX=3 NUY=1 FILL 7 8 7 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=68 ZUL=20 XLR=44 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

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

```

K420 FOUR CLUSTERS, TWO 9X12 & TWO 9X4, 1.892 CM P, 2.83 &
12.02 CM SEP
READ PARA TME=300 GEN=160 NPG=1500 NSK=50 NUB=YES
LIB=41 XS1=YES RUN=YES LNG=71000 END PARA
READ MIXT SCT=3
MIX=1
' U(4.31)02 for 1.892 cm pitch
92400 5.1835-6 92508 9.1530-4 92509 9.4904-5
92600 5.1395-6 92857 1.1216-2 92858 1.0941-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end plugs)
6100 4.3562-2 1102 5.8178-2 20100 2.5660-3
16100 4.7820-4 14100 9.6360-5 8100 1.2461-2
MIX=5
' acrylic
1102 5.6642-2 6100 3.5648-2 8100 1.4273-2
MIX=6
' water
1102 6.6706-2 8100 3.3353-2 64100 3.9828-8
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* FOUR ROWS OF FUEL PINS *
ARRAY 2 3R0
UNIT 5
COM=* Y-WATER BETWEEN CLUSTERS *
CUBOID 2 1 17.028 0 12.02 0 94.2975 -2.2225
UNIT 6
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 3 3R0
UNIT 7
COM=* X-WATER BETWEEN CLUSTERS *
CUBOID 2 1 2.83 0 42.292 0 94.2975 -2.2225
GLOBAL
UNIT 8
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 4 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1

```

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KENO-V.a Input Listing for Case 16 of Table 15 (16-Energy-Group Hansen-Roach Cross Sections) (cont'd).

```

END GEOM
READ ARRAY  ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=4 FILL F1 END FILL
      ARA=3 NUX=1 NUY=3 FILL 3 5 4 END FILL
      ARA=4 NUX=3 NUY=1 FILL 6 7 6 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=68 ZUL=20 XLR=44 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 1 of Table 15 (27-Energy-Group SCALE4 Cross Sections).

```

=CSAS25
C406 12X18.817 CLUSTER (12X18 + 10 RODS), 1.892 CM PITCH
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234 1 0 5.1835-6 295 END
U-235 1 0 1.0102-3 295 END
U-236 1 0 5.1395-6 295 END
U-238 1 0 2.2157-2 295 END
O 1 0 4.6753-2 295 END
' water
H 2 0 6.6706-2 295 END
O 2 0 3.3353-2 295 END
GD 2 0 3.9828-8 295 END
' 6061 Al (clad)
AL 3 0 5.8433-2 295 END
CR 3 0 6.2310-5 295 END
CU 3 0 6.3731-5 295 END
MG 3 0 6.6651-4 295 END
MN 3 0 2.2115-5 295 END
TI 3 0 2.5375-5 295 END
' (Zn replaced by Cu)
CU 3 0 3.0967-5 295 END
SI 3 0 3.4607-4 295 END
FE 3 0 1.0152-4 295 END
' rubber end plug
C 4 0 4.3562-2 295 END
H 4 0 5.8178-2 295 END
CA 4 0 2.5660-3 295 END
S 4 0 4.7820-4 295 END
SI 4 0 9.6360-5 295 END
O 4 0 1.2461-2 295 END
' acrylic
H 5 0 5.6642-2 295 END
C 5 0 3.5648-2 295 END
O 5 0 1.4273-2 295 END
' water
H 6 0 6.6706-2 295 END
O 6 0 3.3353-2 295 END
GD 6 0 3.9828-8 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
C406 12X18.817 CLUSTER (12X18 + 10 RODS), 1.892 CM PITCH
READ PARA TME=200 GEN=160 NPG=1500 NSK=50 NUB=YES
XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* FUEL PINS AT END OF SIDE *

```

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KENO-V.a Input Listing for Case 1 of Table 15 (27-Energy-Group SCALE4 Cross Sections) (cont'd).

```

ARRAY 2 3R0
GLOBAL
UNIT 5
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 3 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=12 NUY=18 FILL F1 END FILL
      ARA=2 NUX=12 NUY=1 FILL 10R1 2R2 END FILL
      ARA=3 NUX=1 NUY=2 FILL 3 4 END FILL
END ARRAY
READ PLOT
  XUL=-4 YUL=44 ZUL=20 XLR=37 YLR=-4
  ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~cpa~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 5 of Table 15 (27-Energy-Group SCALE4 Cross Sections).

```

=CSAS25
C410 14X13.78 CLUSTER (14X13 + 11 RODS, WITH 25
WATER-HOLES), 1.892 CM PITCH
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234 1 0 5.1835-6 295 END
U-235 1 0 1.0102-3 295 END
U-236 1 0 5.1395-6 295 END
U-238 1 0 2.2157-2 295 END
O 1 0 4.6753-2 295 END
' water
H 2 0 6.6706-2 295 END
O 2 0 3.3353-2 295 END
GD 2 0 3.9828-8 295 END
' 6061 Al (clad)
AL 3 0 5.8433-2 295 END
CR 3 0 6.2310-5 295 END
CU 3 0 6.3731-5 295 END
MG 3 0 6.6651-4 295 END
MN 3 0 2.2115-5 295 END
TI 3 0 2.5375-5 295 END
' (Zn replaced by Cu)
CU 3 0 3.0967-5 295 END
SI 3 0 3.4607-4 295 END
FE 3 0 1.0152-4 295 END
' rubber end plug
C 4 0 4.3562-2 295 END
H 4 0 5.8178-2 295 END
CA 4 0 2.5660-3 295 END
S 4 0 4.7820-4 295 END
SI 4 0 9.6360-5 295 END
O 4 0 1.2461-2 295 END
' acrylic
H 5 0 5.6642-2 295 END
C 5 0 3.5648-2 295 END
O 5 0 1.4273-2 295 END
' water
H 6 0 6.6706-2 295 END
O 6 0 3.3353-2 295 END
GD 6 0 3.9828-8 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
C410 14X13.78 CLUSTER (14X13 + 11 RODS, WITH 25
WATER-HOLES), 1.892 CM PITCH
READ PARA TME=200 GEN=160 NPG=1500 NSK=50 NUB=YES
XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ONE ROW OF FUEL PINS *
ARRAY 1 3R0

```

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KENO-V.a Input Listing for Case 5 of Table 15 (27-Energy-Group SCALE4 Cross Sections) (cont'd).

```
UNIT 4
COM=* ONE ROW OF FUEL PINS AND 5 WATER-HOLES *
ARRAY 2 3R0
UNIT 5
COM=* PARTIAL ROW OF FUEL PINS *
ARRAY 3 3R0
GLOBAL
UNIT 6
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 4 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=14 NUY=1 FILL F1 END FILL
      ARA=2 NUX=14 NUY=1 FILL 3R1 2 1 2 1 2 1 2 2R1 END
FILL
      ARA=3 NUX=14 NUY=1 FILL 11R1 3R2 END FILL
      ARA=4 NUX=1 NUY=14 FILL 2R3 4 3 4 3 4 3 4 3 3 5 END
FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=44 ZUL=20 XLR=37 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END
```

KENO-V.a Input Listing for Case 8 of Table 15 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
C413 TWO 9X12.18 CLUSTERS(TWO 9X12 + 1 AND 2 RODS),1.892
CM PITCH,2.83 CM SEP
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234 1 0 5.1835-6 295 END
U-235 1 0 1.0102-3 295 END
U-236 1 0 5.1395-6 295 END
U-238 1 0 2.2157-2 295 END
O 1 0 4.6753-2 295 END
' water
H 2 0 6.6706-2 295 END
O 2 0 3.3353-2 295 END
GD 2 0 3.9828-8 295 END
' 6061 Al (clad)
AL 3 0 5.8433-2 295 END
CR 3 0 6.2310-5 295 END
CU 3 0 6.3731-5 295 END
MG 3 0 6.6651-4 295 END
MN 3 0 2.2115-5 295 END
TI 3 0 2.5375-5 295 END
' (Zn replaced by Cu)
CU 3 0 3.0967-5 295 END
SI 3 0 3.4607-4 295 END
FE 3 0 1.0152-4 295 END
' rubber end plug
C 4 0 4.3562-2 295 END
H 4 0 5.8178-2 295 END
CA 4 0 2.5660-3 295 END
S 4 0 4.7820-4 295 END
SI 4 0 9.6360-5 295 END
O 4 0 1.2461-2 295 END
' acrylic
H 5 0 5.6642-2 295 END
C 5 0 3.5648-2 295 END
O 5 0 1.4273-2 295 END
' water
H 6 0 6.6706-2 295 END
O 6 0 3.3353-2 295 END
GD 6 0 3.9828-8 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
C413 TWO 9X12.18 CLUSTERS(TWO 9X12 + 1 AND 2 RODS),1.892
CM PITCH,2.83 CM SEP
READ PARA TME=200 GEN=160 NPG=1500 NSK=50 NUB=YES
XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
```

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KENO-V.a Input Listing for Case 8 of Table 15 (27-Energy-Group SCALE4 Cross Sections) (cont'd).

```

UNIT 4
COM=* FUEL PINS OF PARTIAL ROW *
ARRAY 2 3R0
UNIT 5
COM=* FUEL PINS OF OTHER PARTIAL ROW *
ARRAY 3 3R0
UNIT 6
COM=* WATER BETWEEN CLUSTERS *
CUBOID 2 1 2.83 0 24.596 0 94.2975 -2.2225
UNIT 7
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 4 3R0
UNIT 8
COM=* ARRAY WITH PARTIAL ROW OF FUEL PINS ADDED *
ARRAY 5 3R0
GLOBAL
UNIT 9
COM=* TWO CLUSTERS WITH WATER BETWEEN *
ARRAY 6 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=1 FILL 1R1 8R2 END FILL
      ARA=3 NUX=9 NUY=1 FILL 2R1 7R2 END FILL
      ARA=4 NUX=1 NUY=2 FILL 3 4 END FILL
      ARA=5 NUX=1 NUY=2 FILL 3 5 END FILL
      ARA=6 NUX=3 NUY=1 FILL 7 6 8 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=25 ZUL=20 XLR=37 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 11 of Table 16 (27-Energy-Group SCALE4 Cross Sections).

```

=CSAS25
C415 FOUR CLUSTERS, TWO 9X12 AND TWO 9X2.1, 1.892 CM
PITCH, 4.72 CM SEPARATION
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234 1 0 5.1835-6 295 END
U-235 1 0 1.0102-3 295 END
U-236 1 0 5.1395-6 295 END
U-238 1 0 2.2157-2 295 END
O 1 0 4.6753-2 295 END
' water
H 2 0 6.6706-2 295 END
O 2 0 3.3353-2 295 END
GD 2 0 3.9828-8 295 END
' 6061 Al (clad)
AL 3 0 5.8433-2 295 END
CR 3 0 6.2310-5 295 END
CU 3 0 6.3731-5 295 END
MG 3 0 6.6651-4 295 END
MN 3 0 2.2115-5 295 END
TI 3 0 2.5375-5 295 END
' (Zn replaced by Cu)
CU 3 0 3.0967-5 295 END
SI 3 0 3.4607-4 295 END
FE 3 0 1.0152-4 295 END
' rubber end plug
C 4 0 4.3562-2 295 END
H 4 0 5.8178-2 295 END
CA 4 0 2.5660-3 295 END
S 4 0 4.7820-4 295 END
SI 4 0 9.6360-5 295 END
O 4 0 1.2461-2 295 END
' acrylic
H 5 0 5.6642-2 295 END
C 5 0 3.5648-2 295 END
O 5 0 1.4273-2 295 END
' water
H 6 0 6.6706-2 295 END
O 6 0 3.3353-2 295 END
GD 6 0 3.9828-8 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
C415 FOUR CLUSTERS, TWO 9X12 AND TWO 9X2.1, 1.892 CM
PITCH, 4.72 CM SEPARATION
READ PARA TME=200 GEN=160 NPG=1500 NSK=50 NUB=YES
XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0

```

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KENO-V.a Input Listing for Case 11 of Table 16 (27-Energy-Group SCALE4 Cross Sections) (cont'd).

```

UNIT 4
COM=* ARRAY OF FUEL PINS *
ARRAY 2 3R0
UNIT 5
COM=* PARTIAL ROW OF FUEL PINS *
ARRAY 3 3R0
UNIT 6
COM=* Y-WATER BETWEEN CLUSTERS *
CUBOID 2 1 17.028 0 4.72 0 94.2975 -2.2225
UNIT 7
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 4 3R0
UNIT 8
COM=* X-WATER BETWEEN CLUSTERS *
CUBOID 2 1 4.72 0 33.1 0 94.2975 -2.2225
GLOBAL
UNIT 9
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 5 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=2 FILL F1 END FILL
      ARA=3 NUX=9 NUY=1 FILL 1 8R2 END FILL
      ARA=4 NUX=1 NUY=4 FILL 3 6 4 5 END FILL
      ARA=5 NUX=3 NUY=1 FILL 7 8 7 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=68 ZUL=20 XLR=44 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END

```

KENO-V.a Input Listing for Case 16 of Table 16 (27-Energy-Group SCALE4 Cross Sections).

```

=CSAS25
C420 FOUR CLUSTERS, TWO 9X12 & TWO 9X4, 1.892 CM P, 2.83 &
12.02 CM SEP
27GROUPNDF4 LATTICECELL
' U(4.306)02
U-234 1 0 5.1835-6 295 END
U-235 1 0 1.0102-3 295 END
U-236 1 0 5.1395-6 295 END
U-238 1 0 2.2157-2 295 END
O 1 0 4.6753-2 295 END
' water
H 2 0 6.6706-2 295 END
O 2 0 3.3353-2 295 END
GD 2 0 3.9828-8 295 END
' 6061 Al (clad)
AL 3 0 5.8433-2 295 END
CR 3 0 6.2310-5 295 END
CU 3 0 6.3731-5 295 END
MG 3 0 6.6651-4 295 END
MN 3 0 2.2115-5 295 END
TI 3 0 2.5375-5 295 END
' (Zn replaced by Cu)
CU 3 0 3.0967-5 295 END
SI 3 0 3.4607-4 295 END
FE 3 0 1.0152-4 295 END
' rubber end plug
C 4 0 4.3562-2 295 END
H 4 0 5.8178-2 295 END
CA 4 0 2.5660-3 295 END
S 4 0 4.7820-4 295 END
SI 4 0 9.6360-5 295 END
O 4 0 1.2461-2 295 END
' acrylic
H 5 0 5.6642-2 295 END
C 5 0 3.5648-2 295 END
O 5 0 1.4273-2 295 END
' water
H 6 0 6.6706-2 295 END
O 6 0 3.3353-2 295 END
GD 6 0 3.9828-8 295 END
END COMP
SQUAREPITCH 1.892 1.265 1 2 1.415 3 1.283 0 END
C420 FOUR CLUSTERS, TWO 9X12 & TWO 9X4, 1.892 CM P, 2.83 &
12.02 CM SEP
READ PARA TME=200 GEN=160 NPG=1500 NSK=50 NUB=YES
XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P.946 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P.946 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0

```


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KENO-V.a Input Listing for Case 16 of Table 16 (27-Energy-
Group SCALE4 Cross Sections) (cont'd).

```
UNIT 4
COM=* FOUR ROWS OF FUEL PINS *
ARRAY 2 3R0
UNIT 5
COM=* Y-WATER BETWEEN CLUSTERS *
CUBOID 2 1 17.028 0 12.02 0 94.2975 -2.2225
UNIT 6
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 3 3R0
UNIT 7
COM=* X-WATER BETWEEN CLUSTERS *
CUBOID 2 1 2.83 0 42.292 0 94.2975 -2.2225
GLOBAL
UNIT 8
COM=* CLUSTERS WITH WATER BETWEEN *
ARRAY 4 3R0
REPLICATE 5 1 5R0.0 2.54 1
REPLICATE 6 1 4R30.0 12.7775 15.3 1
END GEOM
READ ARRAY ARA=1 NUX=9 NUY=12 FILL F1 END FILL
      ARA=2 NUX=9 NUY=4 FILL F1 END FILL
      ARA=3 NUX=1 NUY=3 FILL 3 5 4 END FILL
      ARA=4 NUX=3 NUY=1 FILL 6 7 6 END FILL
END ARRAY
READ PLOT
      XUL=-4 YUL=68 ZUL=20 XLR=44 YLR=-4
      ZLR=20 UAX=1 VDN=-1 NAX=120 NCH='*~ctla~' END
END PLOT
END DATA
END
```

A.2 MCNP Input Listings

MCNP4 was used.

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

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

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MCNP Input Listing for Case 1 of Table 15.

M406 12X18 +10 CLUSTER OF U(4.31)O2 RODS, 1.892 CM PITCH

```

1  1 .069930523 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2  0 -2 1 7 -8 u=1 imp:n=1 $ gap
3  3 .059751598 -12 2 u=1 imp:n=1 $ clad
4  4 .11734156 -2 8 u=1 imp:n=1 $ rubber end plug (top)
5  4 .11734156 -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6  2 .1000590398 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 21 -9 23 fill=2 imp:n=1 $ rod cluster
9  0 -13 11 -21 19 -9 23 imp:n=1 fill=2 $ partial row of fuel rods
10 2 .1000590398 13 -10 -21 19 -9 23 imp:n=1 $ water of partial row
11 5 .106563 19 -20 11 -10 -23 29 imp:n=1 $ acrylic support plate
12 2 .1000590398 (-11:10:20:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
13 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z .946 .946 .6325 $ fuel cylinder
2  c/z .946 .946 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 1.892 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 1.892 $ fuel rod cell boundary
7  pz 0.0 $ bottom of fuel
8  pz 92.075 $ top of fuel
9  pz 94.2975 $ top of clad
10 px 22.7039 $ farthest edge of closest cluster ***
11 px .0001 $ closest edge of closest cluster
12 c/z .946 .946 .7075 $ clad outer surface
13 px 18.919 $ edge of partial row ***
19 py 0.0001 $ close edge of cluster + partial row
20 py 35.9479 $ sides of clusters ***
21 py 1.8921 $ side of partial row and full cluster
23 pz -2.2225 $ bottom of fuel rod
24 px 52.704 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 65.948 $ side of water reflector ***
27 py -30 $ side of water reflector
28 pz 107.075 $ top of water
29 pz -4.7625 $ bottom of acrylic support plate
30 pz -20.0625 $ bottom of water

```

kcode 1500 1 50 160 50000

sdef x=d1 y=d2 z=d3 cel=d4

si1 0 23

sp1 0 1

si2 0 36

sp2 0 1

si3 0 93

sp3 0 1

si4 1 8

sp4 v

print

c

c MATERIALS FOR U(4.31)O2 RODS

c

c m1 is UO2 fuel

m1 92234.50c 5.1835e-6 92235.50c 1.0102e-3

92236.50c 5.1395e-6 92238.50c 2.2157e-2

8016.50c 4.6753e-2

c m2 is water with 10.4 mg/liter Gd

m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2

64152.50c 7.9656e-11 64154.50c 8.6825e-10

64155.50c 5.8946e-9 64156.50c 8.1528e-9

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MCNP Input Listing for Case 1 of Table 15 (cont'd).

```
64157.50c 6.2331e-9 64158.50c 9.8933e-9
64160.50c 8.7064e-9
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-2 1001.50c 5.8178e-2
20000.50c 2.5660e-3 16032.50c 4.7820e-4
14000.50c 9.6360e-5 8016.50c 1.2461e-2
mt4 poly.01t
c m5 is acrylic (support plate)
m5 1001.50c 5.6642e-2 6000.50c 3.5648e-2
8016.50c 1.4273e-2
mt5 poly.01t
```

MCNP Input Listing for Case 5 of Table 15.

M410 14X13 +11 CLUSTER OF U(4.31)O2 RODS, 1.892 CM PITCH, 25 WATER HOLES

```

1 1.069930523 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2 0 -2 1 7 -8 u=1 imp:n=1 $ gap
3 3.059751598 -12 2 u=1 imp:n=1 $ clad
4 .11734156 -2 8 u=1 imp:n=1 $ rubber end plug (top)
5 4.11734156 -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6 2.1000590398 12 u=1 imp:n=1 $ water
7 2.1000590398 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=0:13 0:13 0:0
      1 30r 2 1 2 1 2 1 2 1 2 1 18r
          2 1 2 1 2 1 2 1 2 1 18r
              2 1 2 1 2 1 2 1 2 1 18r
                  2 1 2 1 2 1 2 1 2 1 18r
                      2 1 2 1 2 1 2 1 2 1 40r 2 2 2
8 0 -10 11 -20 19 -9 23 fill=2 imp:n=1 $ rod cluster
9 5.106563 19 -20 11 -10 -23 29 imp:n=1 $ acrylic support plate
10 2.1000590398 (-11:10:20:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
11 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z .946 .946 .6325 $ fuel cylinder
2  c/z .946 .946 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 1.892 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 1.892 $ fuel rod cell boundary
7  pz 0.0 $ bottom of fuel
8  pz 92.075 $ top of fuel
9  pz 94.2975 $ top of clad
10 px 26.4879 $ farthest edge of cluster ***
11 px .0001 $ closest edge of cluster
12 c/z .946 .946 .7075 $ clad outer surface
19 py .0001 $ side of cluster
20 py 26.4879 $ side of cluster ***
23 pz -2.2225 $ bottom of fuel rod
24 px 56.488 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 56.488 $ side of water reflector ***
27 py -30 $ side of water reflector
28 pz 107.075 $ top of water
29 pz -4.7625 $ bottom of acrylic support plate
30 pz -20.0625 $ bottom of water

```

```
kcode 1500 1 50 160 50000
sdef x=d1 y=d2 z=d3 cel=d4
si1 0 33
sp1 0 1
si2 0 27
sp2 0 1
si3 0 93
sp3 0 1
si4 18
sp4 v
print
c
c MATERIALS FOR U(4.31)O2 RODS
c
c m1 is UO2 fuel
m1 92234.50c 5.1835e-6 92235.50c 1.0102e-3
92236.50c 5.1395e-6 92238.50c 2.2157e-2
8016.50c 4.6753e-2
c m2 is water with 10.4 mg/liter Gd
m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2
64152.50c 7.9656e-11 64154.50c 8.6825e-10
```

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MCNP Input Listing for Case 5 of Table 15 (cont'd).

```
64155.50c 5.8946e-9 64156.50c 8.1528e-9
64157.50c 6.2331e-9 64158.50c 9.8933e-9
64160.50c 8.7064e-9
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-2 1001.50c 5.8178e-2
20000.50c 2.5660e-3 16032.50c 4.7820e-4
14000.50c 9.6360e-5 8016.50c 1.2461e-2
mt4 poly.01t
c m5 is acrylic (support plate)
m5 1001.50c 5.6642e-2 6000.50c 3.5648e-2
8016.50c 1.4273e-2
mt5 poly.01t
```

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MCNP Input Listing for Case 8 of Table 15.

M413 TWO 9X12 CLUSTERS + 3 OF U(4.31)O2 RODS, 1.892 CM PITCH, 2.83 CM SEP

```

1  1 .069930523 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2  0 -2 1 7 -8 u=1 imp:n=1 $ gap
3  3 .059751598 -12 2 u=1 imp:n=1 $ clad
4  4 .11734156 -2 8 u=1 imp:n=1 $ rubber end plug (top)
5  4 .11734156 -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6  2 .1000590398 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 21 -9 23 fill=2 imp:n=1 $ first rod cluster
9  0 -14 15 -20 21 -9 23 fill=2(19.858 0 0) imp:n=1 $ second rod cluster
10 0 -13 15 -21 19 -9 23 imp:n=1 fill=2(19.858 0 0) $ one partial row
11 0 -10 11 -21 19 -9 23 imp:n=1 fill=1 $ other partial row of fuel rods
12 2 .1000590398 13 -14 -21 19 -9 23 imp:n=1 $ water of partial row
13 2 .1000590398 10 -15 -20 19 -9 23 imp:n=1 $ water between clusters
14 5 .106563 19 -20 11 -14 -23 29 imp:n=1 $ acrylic support plate
15 2 .1000590398 (-11:14:20:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
16 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z .946 .946 .6325 $ fuel cylinder
2  c/z .946 .946 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 1.892 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 1.892 $ fuel rod cell boundary
7  pz 0.0 $ bottom of fuel
8  pz 92.075 $ top of fuel
9  pz 94.2975 $ top of clad
10 px 17.0279 $ farthest edge of first cluster ***
11 px .0001 $ closest edge of first cluster
12 c/z .946 .946 .7075 $ clad outer surface
13 px 23.6419 $ edge of partial row ***
14 px 36.8859 $ farthest edge of second cluster ***
15 px 19.8581 $ closest edge of second cluster
19 py 0.0001 $ close edge of cluster + partial row
20 py 24.5959 $ sides of clusters ***
21 py 1.8921 $ side of partial rows
23 pz -2.2225 $ bottom of fuel rod
24 px 66.886 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 54.596 $ side of water reflector ***
27 py -30 $ side of water reflector
28 pz 107.075 $ top of water
29 pz -4.7625 $ bottom of acrylic support plate
30 pz -20.0625 $ bottom of water

```

kcode 1500 1 50 160 50000

sdef x=d1 y=d2 z=d3 cel=d4

si1 0 37

sp1 0 1

si2 0 25

sp2 0 1

si3 0 93

sp3 0 1

si4 1 8 9

sp4 v

print

c

c MATERIALS FOR U(4.31)O2 RODS

c

c m1 is UO2 fuel

m1 92234.50c 5.1835e-6 92235.50c 1.0102e-3

92236.50c 5.1395e-6 92238.50c 2.2157e-2

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MCNP Input Listing for Case 8 of Table 15 (cont'd).

8016.50c 4.6753e-2
c m2 is water with 10.4 mg/liter Gd
m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2
64152.50c 7.9656e-11 64154.50c 8.6825e-10
64155.50c 5.8946e-9 64156.50c 8.1528e-9
64157.50c 6.2331e-9 64158.50c 9.8933e-9
64160.50c 8.7064e-9
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-2 1001.50c 5.8178e-2
20000.50c 2.5660e-3 16032.50c 4.7820e-4
14000.50c 9.6360e-5 8016.50c 1.2461e-2
mt4 poly.01t
c m5 is acrylic (support plate)
m5 1001.50c 5.6642e-2 6000.50c 3.5648e-2
8016.50c 1.4273e-2
mt5 poly.01t

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MCNP Input Listing for Case 11 of Table 16.

M415 FOUR CLUSTERS OF U(4.31)O₂ RODS, 9X12 + 9X2+1, 1.892 CM PITCH, 4.72 CM SEP

```

1  1 .069930523 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2  0 -2 1 7 -8 u=1 imp:n=1 $ gap
3  3 .059751598 -12 2 u=1 imp:n=1 $ clad
4  4 .11734156 -2 8 u=1 imp:n=1 $ rubber end plug (top)
5  4 .11734156 -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6  2 .1000590398 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 19 -9 23 fill=2 imp:n=1 $ first 9x12 rod cluster
9  0 -14 15 -20 19 -9 23 fill=2(21.748 0 0) imp:n=1 $ second 9x12 rod clstr
10 0 -10 11 -22 21 -9 23 fill=2(0 27.424 0) imp:n=1 $ third rod cluster
11 0 -10 11 -18 22 -9 23 fill=1(0 31.208 0) imp:n=1 $ partial row of 3rd cls
12 0 -14 15 -22 21 -9 23 fill=2(21.748 27.424 0) imp:n=1 $ fourth rod cluster
13 0 -16 15 -18 22 -9 23 fill=2(21.748 27.424 0) imp:n=1 $ partial row
14 2 .1000590398 16 -14 -18 22 -9 23 imp:n=1 $ water of partial row of 4th clstr
15 2 .1000590398 11 -10 -21 20 -9 23 imp:n=1 $ y-water between clusters
16 2 .1000590398 15 -14 -21 20 -9 23 imp:n=1 $ other y-water betwn clusters
17 2 .1000590398 10 -15 -18 19 -9 23 imp:n=1 $ x-water between clusters
18 5 .106563 19 -18 11 -14 -23 29 imp:n=1 $ acrylic support plate
19 2 .1000590398 (-11:14:18:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
20 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z .946 .946 .6325 $ fuel cylinder
2  c/z .946 .946 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 1.892 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 1.892 $ fuel rod cell boundary
7  pz 0.0 $ bottom of fuel
8  pz 92.075 $ top of fuel
9  pz 94.2975 $ top of clad
10 px 17.0279 $ farthest edge of first cluster ***
11 px .0001 $ closest edge of first cluster
12 c/z .946 .946 .7075 $ clad outer surface
14 px 38.7759 $ farthest edge of second cluster ***
15 px 21.7481 $ closest edge of second cluster
16 px 23.639 $ edge of partial row of fourth cluster
18 py 33.099 $ farthest sides of farthest clusters - partial rows
19 py 0.0001 $ closest sides of closest clusters
20 py 22.7039 $ farthest sides of closest clusters ***
21 py 27.4241 $ closest sides of farthest clusters
22 py 31.2079 $ farthest sides of farthest clusters ***
23 pz -2.2225 $ bottom of fuel rod
24 px 68.776 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 63.1 $ side of water reflector ***
27 py -30 $ side of water reflector
28 pz 107.075 $ top of water
29 pz -4.7625 $ bottom of acrylic support plate
30 pz -20.0625 $ bottom of water

```

```

kcode 1500 1 50 160 50000
sdef x=d1 y=d2 z=d3 cel=d4
si1 0 39
sp1 0 1
si2 0 34
sp2 0 1
si3 0 93
sp3 0 1
si4 1 8 9 10 12
sp4 v
print

```

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MCNP Input Listing for Case 11 of Table 16 (cont'd).

c
c MATERIALS FOR U(4.31)O2 RODS
c
c m1 is UO2 fuel
m1 92234.50c 5.1835e-6 92235.50c 1.0102e-3
92236.50c 5.1395e-6 92238.50c 2.2157e-2
8016.50c 4.6753e-2
c m2 is water with 10.4 mg/liter Gd
m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2
64152.50c 7.9656e-11 64154.50c 8.6825e-10
64155.50c 5.8946e-9 64156.50c 8.1528e-9
64157.50c 6.2331e-9 64158.50c 9.8933e-9
64160.50c 8.7064e-9
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-2 1001.50c 5.8178e-2
20000.50c 2.5660e-3 16032.50c 4.7820e-4
14000.50c 9.6360e-5 8016.50c 1.2461e-2
mt4 poly.01t
c m5 is acrylic (support plate)
m5 1001.50c 5.6642e-2 6000.50c 3.5648e-2
8016.50c 1.4273e-2
mt5 poly.01t

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MCNP Input Listing for Case 16 of Table 16.

M420 FOUR CLUSTERS OF U(4.31)O₂ RODS, TWO 9X12, TWO 9X4, 2.83 X-SEP, 12.02 Y-SEP

```

1  1 .069930523 -1 7 -8 u=1 imp:n=1 $ uo2 fuel
2  0 -2 1 7 -8 u=1 imp:n=1 $ gap
3  3 .059751598 -12 2 u=1 imp:n=1 $ clad
4  4 .11734156 -2 8 u=1 imp:n=1 $ rubber end plug (top)
5  4 .11734156 -2 -7 u=1 imp:n=1 $ rubber end plug (bottom)
6  2 .1000590398 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 19 -9 23 fill=2 imp:n=1 $ first 9x12 rod cluster
9  0 -14 15 -20 19 -9 23 fill=2(19.858 0 0) imp:n=1 $ second 9x12 rod clstr
10 0 -10 11 -22 21 -9 23 fill=2(0 34.724 0) imp:n=1 $ third cluster
11 0 -14 15 -22 21 -9 23 fill=2(19.858 34.724 0) imp:n=1 $ fourth cluster
12 2 .1000590398 11 -10 -21 20 -9 23 imp:n=1 $ y-water between clusters
13 2 .1000590398 15 -14 -21 20 -9 23 imp:n=1 $ other y-water betwn clusters
14 2 .1000590398 10 -15 -22 19 -9 23 imp:n=1 $ x-water between clusters
15 5 .106563 19 -22 11 -14 -23 29 imp:n=1 $ acrylic support plate
16 2 .1000590398 (-11:14:22:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
17 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z .946 .946 .6325 $ fuel cylinder
2  c/z .946 .946 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 1.892 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 1.892 $ fuel rod cell boundary
7  pz 0.0 $ bottom of fuel
8  pz 92.075 $ top of fuel
9  pz 94.2975 $ top of clad
10 px 17.0279 $ farthest edge of first cluster ***
11 px .0001 $ closest edge of first cluster
12 c/z .946 .946 .7075 $ clad outer surface
14 px 36.8859 $ farthest edge of second cluster ***
15 px 19.8581 $ closest edge of second cluster ***
19 py 0.0001 $ closest sides of closest clusters
20 py 22.7039 $ farthest sides of closest clusters ***
21 py 34.7241 $ closest sides of farthest clusters ***
22 py 42.2919 $ farthest sides of farthest clusters ***
23 pz -2.2225 $ bottom of fuel rod
24 px 66.886 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 72.292 $ side of water reflector ***
27 py -30 $ side of water reflector
28 pz 107.075 $ top of water
29 pz -4.7625 $ bottom of acrylic support plate
30 pz -20.0625 $ bottom of water

```

kcode 1500 1 50 160 50000

sdef x=d1 y=d2 z=d3 cel=d4

si1 0 41

sp1 0 1

si2 0 53

sp2 0 1

si3 0 93

sp3 0 1

si4 1 8 9 10 11

sp4 v

print

c

c MATERIALS FOR U(4.31)O₂ RODS

c

c m1 is UO₂ fuel

m1 92234.50c 5.1835e-6 92235.50c 1.0102e-3

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MCNP Input Listing for Case 16 of Table 16 (cont'd).

92236.50c 5.1395e-6 92238.50c 2.2157e-2
8016.50c 4.6753e-2
c m2 is water with 10.4 mg/liter Gd
m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2
64152.50c 7.9656e-11 64154.50c 8.6825e-10
64155.50c 5.8946e-9 64156.50c 8.1528e-9
64157.50c 6.2331e-9 64158.50c 9.8933e-9
64160.50c 8.7064e-9
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-2 1001.50c 5.8178e-2
20000.50c 2.5660e-3 16032.50c 4.7820e-4
14000.50c 9.6360e-5 8016.50c 1.2461e-2
mt4 poly.01t
c m5 is acrylic (support plate)
m5 1001.50c 5.6642e-2 6000.50c 3.5648e-2
8016.50c 1.4273e-2
mt5 poly.01t

A.3 ONEDANT/TWODANT Input Listings

Because of the heterogeneity of the fuel rod lattice, neither ONEDANT nor TWODANT calculations were performed.

APPENDIX B: CORRELATION BETWEEN CASE NUMBER AND ORIGINAL EXPERIMENT NUMBER

Table B.1 correlates the experiment "Case" number, as used in this evaluation, with the original experiment number. Logbooks are stored at the Los Alamos National Laboratory (LANL) Archives under the original experiment number. Logbooks for most experiments below were listed on the "Abbreviated Inventory List for Critical Experiment Data Log Books from Hanford Plutonium Critical Mass Laboratory (Boxes No. 1 through 15)," available at the LANL Archives, for the shipment from Hanford to Los Alamos as being in Box 6. Box numbers from that list are given below.

Table B.1. Correlation of Case Number with Original Experiment Number.

Case Number	Shipment Box	Original Experiment Number
1	6	SSC-4.31-000-046
2	6	SSC-4.31-000-045
3	6, 11	SSC-4.31-000-044, -130
4	6	SSC-4.31-000-043
5	6,11	SSC-4.31-000-047, -122
6	6	SSC-4.31-000-048
7	11	SSC-4.31-000-121
8	6	SSC-4.31-000-062
9	10, 11	SSC-4.31-000-131,161-172
10	6	SSC-4.31-000-051
11	6	SSC-4.31-000-053
12	6	SSC-4.31-000-061
13	6	SSC-4.31-000-060
14	6	SSC-4.31-000-059
15	6	SSC-4.31-000-058
16	6	SSC-4.31-000-057
17	6	SSC-4.31-000-055
18	6	SSC-4.31-000-056
19	11	SSC-4.31-000-119

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/cm³). 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 $\text{Gd}(\text{NO}_3)_3 \times 4.91 \text{ H}_2\text{O}$, giving a molecular weight of 431.72. Therefore, assuming a solution concentration of 1.481 g Gd/liter, the concentration of the impurity in solution from the given weight percent of the impurity in the gadolinium nitrate powder (Reference 8, p. C.3) is

$$\begin{aligned}
 .001481 \frac{\text{g}}{\text{cm}^3} \frac{(\text{wt.}\% \text{ impurity})}{(\text{wt.}\% \text{ Gd})} &= \frac{.001481 \frac{\text{g}}{\text{cm}^3} (\text{wt.}\% \text{ impurity})}{[100 - \sum (\text{wt.}\% \text{ impurities})] \frac{A_{\text{W,Gd}}}{M_{\text{W,Gd powder}}}} \\
 &= \frac{0.001481 \frac{\text{g}}{\text{cm}^3} (\text{wt.}\% \text{ impurity})}{[100 - 0.4735] \frac{157.25}{431.72}} = 4.08534 \times 10^{-5} (\text{wt.}\% \text{ impurity}) \frac{\text{g}}{\text{cm}^3}
 \end{aligned}$$

Table C.1. Impurity Components of Water (g/m³).^(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	-	0.041	<0.01	<0.005
Zn	0.35±. 05	0.26±. 07	0.9±1. 1	16	10.6	0.0613	<0.05	0.32
Mn	<0.55	<0.01	<0.01	<0.01	-	0.041	<0.01	<0.01
Pb	<0.015	<0.005	0.008± .001	<0.005	2.1	1.0220	<0.002	<0.005
F	0.21±. 02	0.15±. 04	0.15±. 04	0.18	-	-	0.12	0.12
Fe	<0.06	<0.03	<0.03	24	-	0.21	0.12	0.20
Cu	<0.06	<0.01	<0.01	<0.01	18.2	0.123	<0.05	<0.05
Cd	0.004± .001	0.006± .001	0.020± .006	0.001	-	0.041	0.002	0.0006
Gd	-	-	10.4±3 .6	-	-	-	-	<10
SO ₃	6.7±.4	6.6±.0 4	13.4±5 .0	14.5	-	-	21	16
CaCO ₃	-	-	-	-	19.2 ^g	1.02 ^g	51.2	35
B	-	-	-	-	0.09	1.02	-	<25
Al	-	-	-	-	7.3	2.04	-	-
Eu	-	-	-	-	0.08	1.23	-	-
Mg	-	-	-	-	5.7	0.204	-	-
Nd	-	-	-	-	12.2	2.04	-	-
Si	-	-	-	-	3.1	2.04	-	-
Ni	-	-	-	-	6.8	0.204	-	-
Y	-	-	-	-	0.17	.41	-	-

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

(a) If one cubic centimeter has a mass of 1 gram, then this is the same as PPM (parts per million) by weight.

(b) Average of samples taken at the beginning and near the end of the experiments.

(c) Error limits are standard deviations observed in three samples.

(d) In Reference 7, analysis is prior to boron additions (Reference 7, p. 2).

(e) Largest values of three samples.

(f) "Nitrate (as N) mg/liter."

(g) As Ca.

Effect Due to Water Density Reduction - The maximum amount of dissolved solids reported was 137 grams per cubic meter of solution. Assume that dissolved solids is 200 g/m³, has the same density as water (~1 g/cm³), and displaces the water. (These are all conservative assumptions: This concentration is greater than any measured total impurity concentration; also, many materials are denser than water and, when dissolved in water, do not displace as much water as their dry volume.) The percentage of water volume displaced by the solute is then $200/10^6 \times 100 = 0.02$ percent. To see the effect of reduced water density, the water volume

fraction is reduced by this percentage. The resulting change in k_{eff} is less than 0.04 percent.^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, for U(2.35)O₂ fuel rods at 2.032 cm pitch, using the 27-group cross sections processed by CSASIX.^b No changes are greater than 0.005 percent except those from boron and gadolinium impurities, with Δk_{eff} values of 0.9 percent and 1.7 percent, respectively.

Additional calculations for Gd and B impurities in the water of arrays of 4.31 wt.% enriched fuel rods at two pitches, 2.54 cm and 1.892 cm, were performed. For U(4.31)O₂ rods at 2.54 cm pitch, B at 25 g/m³ and Gd at 14 g/m³ gave Δk_{eff} values of -0.81 percent and -1.48 percent, respectively. These same concentrations of B and Gd for U(4.31)O₂ rods at 1.892 cm pitch gave Δk_{eff} values of -0.41 percent and -0.69 percent, respectively. Therefore, critical configurations from the two references with these maximal possible impurity concentrations, References 4 and 10, should include these two impurities in the water.

^a This is based on ONEDANT calculations of U(2.35)O₂ 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.)

Table C.2. Calculated Effect of Impurities on Δk_{eff} (U(2.35)O₂ Rods at 2.032 cm pitch).

Impurity	Concentration (g/cm ³)	Atom Density (atoms/barn-cm)	% Δk_{eff}
Ag	4.09x10 ⁻⁰⁸	2.281x10 ⁻¹⁰	0
Al	7.30x10 ⁻⁰⁶	1.629x10 ⁻⁰⁷	0
Au	4.09x10 ⁻⁰⁸	1.249x10 ⁻¹⁰	0
B	2.50x10 ⁻⁰⁵	1.393x10 ⁻⁰⁶	-0.885 -0.784 ^(a)
	1.02x10 ^{-06(b)}	5.682x10 ⁻⁰⁸	-0.009
Ba	4.09x10 ⁻⁰⁸	1.791x10 ⁻¹⁰	0
Be	2.04x10 ⁻⁰⁶	1.365x10 ⁻⁰⁷	0.002
CaCO ₃	5.12x10 ⁻⁰⁵	3.081x10 ⁻⁰⁷	0.005
Cd	4.09x10 ⁻⁰⁸	2.189x10 ⁻¹⁰	0
Ce	1.02x10 ⁻⁰⁷	4.390x10 ⁻¹⁰	0.001
Cl	3.60x10 ⁻⁰⁵	6.115x10 ⁻⁰⁷	0.004
Co	4.09x10 ⁻⁰⁸	4.175x10 ⁻¹⁰	0
Cr	4.09x10 ⁻⁰⁸	4.732x10 ⁻¹⁰	0
Cu	1.82x10 ⁻⁰⁵	1.725x10 ⁻⁰⁷	0.002
Eu	1.22x10 ⁻⁰⁶	4.838x10 ⁻⁰⁹	-0.005
F	2.30x10 ⁻⁰⁷	7.291x10 ⁻⁰⁹	0
Fe	2.40x10 ⁻⁰⁵	2.588x10 ⁻⁰⁷	0.003
Gd	1.40x10 ⁻⁰⁵	5.361x10 ⁻⁰⁸	-1.653 -1.830 ^(a)
	1.00x10 ^{-05(c)}	3.830x10 ⁻⁰⁸	-1.200
	5.00x10 ^{-06(d)}	1.915x10 ⁻⁰⁸	-0.592
Hf	4.09x10 ⁻⁰⁸	1.378x10 ⁻¹⁰	0
K	2.04x10 ⁻⁰⁷	3.146x10 ⁻⁰⁹	0
Li	4.09x10 ⁻⁰⁸	3.544x10 ⁻⁰⁹	0
La	2.04x10 ⁻⁰⁷	8.856x10 ⁻¹⁰	0
Mg	5.70x10 ⁻⁰⁶	1.412x10 ⁻⁰⁷	0
Mn	5.50x10 ⁻⁰⁷	6.029x10 ⁻⁰⁹	0.002

LEU-COMP-THERM-004

Impurity	Concentration (g/cm ³)	Atom Density (atoms/barn-cm)	% Δk_{eff}
Mo	4.09×10^{-08}	2.564×10^{-10}	0
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 AND ONEDANT INPUTS FOR SENSITIVITY STUDIES USING HOMOGENIZED FUEL ROD REGION

=CSASIX

GENERATE 27-GRP LIB FOR PNL FUEL PINS IN WATER

27GROUPNDF4 LATTICECELL

U-234 1 0 5.21951-6 295 END

U-235 1 0 1.01724-3 295 END

U-236 1 0 5.17519-6 295 END

U-238 1 0 2.23108-2 295 END

O 1 0 4.70776-2 295 END

H 2 0 6.67619-2 295 END

O 2 0 3.33809-2 295 END

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

AL 4 0 2.53336-3 295 END

CR 4 0 2.70145-6 295 END

CU 4 0 2.76306-6 295 END

MG 4 0 2.88965-5 295 END

MN 4 0 9.58796-7 295 END

TI 4 0 1.10013-6 295 END

C 4 0 7.63823-3 295 END

H 4 0 6.06879-2 295 END

CA 4 0 4.49928-4 295 END

S 4 0 8.38481-5 295 END

O 4 0 2.74185-2 295 END

SI 4 0 1.68960-5 295 END

H 5 0 6.67619-2 295 END

O 5 0 3.33809-2 295 END

END COMP

SQUAREPITCH 2.54 1.265 1 2 1.415 3 1.283 0 END

END

1 0 0

SLAB OF U(4.31)O2 FUEL PINS IN WATER, 15 CM WATER REFL, 91.44
CM LENGTH

/ Block 1

igeom=slab ngroup=27 isn=16 niso=6 mt=6 nzone=6 im=5 it=129
T

/ Block 2

xmesh= 0 44 45.72 48.26 50 63.26

xints= 68 8 13 10 30

zones= 6 6 4 5 5 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=1 zned=0 edoutf=3 T

APPENDIX E: ADDITIONAL CALCULATIONAL RESULTS OF BENCHMARK MODEL CONFIGURATIONS

The following results, using inputs from Appendix A, were provided by Charles F. Sanders of the Commercial Nuclear Fuel Division of Westinghouse Electric Corporation. Calculations were performed using SCALE with processing through BONAMI-S and NITAWL-II. The ENDF/B-V 227-group cross section set, which was collapsed to the SCALE 27-group structure using XSDRNPM-S, is a proprietary cross-section set which has been modified by Westinghouse. The 227-group library is P_3 with a 10^{-5} eV to 20 MeV energy range, with 79 thermal groups below 3 eV. The reference for this P_3 cross-section library is W.E. Ford, III, et al., "CSRL-V: 227-Neutron-Group and Pointwise Cross-Section Libraries for Criticality Safety, Reactor and Shielding Studies," NUREG/CR-2306 (ORNL/CSD/TM-160), May 1982.

Table E.1. Calculational Results for U(4.31)O₂ Fuel Rods at 1.892-cm Pitch.

Case Number	BONAMI/NITAWL/XSDRN with 227-Group Westinghouse ENDF/B-V cross sections, collapsed to 27 groups
1	1.00161 ± 0.00103
2	1.00074 ± 0.00067
3	0.99984 ± 0.00100
4	1.00226 ± 0.00112
5	0.99878 ± 0.00106
6	1.00068 ± 0.00106
7	0.99740 ± 0.00104
8	0.99828 ± 0.00104
11	0.99598 ± 0.00101
12	0.99332 ± 0.00107
13	0.99727 ± 0.00108
14	0.99712 ± 0.00105
15	0.99774 ± 0.00100
16	0.99716 ± 0.00111
17	0.99772 ± 0.00106
18	0.99617 ± 0.00109
19	0.99817 ± 0.00102
20	0.99382 ± 0.00105