

**WATER-MODERATED U(4.31)O₂ FUEL RODS
IN 2.54-CM SQUARE-PITCHED ARRAYS**

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WATER-MODERATED U(4.31)O₂ FUEL RODS IN 2.54-CM SQUARE-PITCHED ARRAYS

IDENTIFICATION NUMBER: LEU-COMP-THERM-002

SPECTRA

KEY WORDS: low enriched fuel rods, low enriched uranium, PNL, ²³⁵U, uranium dioxide

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 or 1.892 cm (LEU-COMP-THERM-004). 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 set of experiments at 2.54-cm pitch are References 2, 3, and 5. 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.

References 11 - 14 provide supplemental information. Details which are from specific references are so noted.

This evaluation documents water-reflected clusters with no absorber plates or reflecting walls. A total of five experiments were evaluated. All of these were judged to be acceptable as benchmark data.

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

1.2 Description of Experimental Configuration

1.2.1 Experiment Tank and Surroundings - Experiments were performed in a 0.952-cm-thick, open-top, carbon-steel tank. Tank inside dimensions were 1.8 x 3.0 x 2.1 meters deep. The experiment was centered in the tank to within one-quarter inch. The 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 is located approximately four feet from the two closest corner walls.^b

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

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

The top lattice plates were bolted to 5.08 x 5.08 x 0.635 cm aluminum angles, attached at their ends to the walls of the tank. In one experiment with 2.35% enriched UO₂ fuel rods, these aluminum lattice supports were doubled, with no effect on the critical separation between clusters (Reference 1, pp. 26 and 28).

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

^b Sid Bierman, private communication, July 1993.

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

^d Sid Bierman, private communication, August 1993.



Figure 1. Experiment Tank.



Figure 2. Arranging Fuel Rods.

For the 3-cluster experiment from Reference 2, the lattice plates were positioned by twelve 1.27-cm-diameter, vertical aluminum spacer rods at the corners of the lattice plates. The spacer rods were 83.9 cm long. The bottom set of lattice plates was raised approximately 5 or 6 inches above the fuel rod support plate by pieces of Tygon tubing placed on four or five fuel rods in each cluster.^a In all other experiments, the bottom lattice plates rested on the fuel rod support plate.

A summary of the vertical positions of the lattice plates is given in Table 1. Lattice plates were 1.27-cm thick.^b

^a Sid Bierman, private communication, August 1993.

^b 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.)

Table 1. Dimensions and Positions of Lattice Plates.

Experiments	Height of bottom surface above fuel rod support plate
single cluster and 3- cluster experiments in Reference 2 (Cases 1-4)	Bottom plate: ~14 cm ^(a) Top plate: 66 cm ^(b)
3-cluster experiment in References 3 and 5 (Case 5)	Bottom plate: 0 cm Top plate: 66 cm ^(b)

(a) Sid Bierman, personal communication, August 4, 1993.

(b) Estimated from Figure 1, Reference 3, p. 3.

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 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.^b

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

^a Private communication, Sid Bierman, August 1993.

^b Private communication, Sid Bierman, July 1993.

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

the tank and that the longer side of the experiment paralleled the longer side of the tank, was 77 cm.^a

1.2.6 Others - A ^{252}Cf source of approximately 0.6 micrograms was placed near the center of each experimental assembly. The source was mounted in an open acrylic tube, 0.6 cm in diameter (Reference 8, p. 2.3) and two or three inches long.^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).

The aluminum control and safety blade guides were located between clusters in multi-cluster experiments. The blade guides, two for the control blade and two for the safety blade, extended from the bottom of the fuel pin array to well above the water surface. Two slightly different sizes of guides were used throughout the series of experiments. Guides were 3.8 cm wide and were 2.54 cm thick (Reference 3, p. 5), with a slot that was 0.96 cm wide for the blades.^c During one experiment from a set of similar experiments using 2.35 wt.% enriched UO_2 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)

1.2.7 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)

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.

^a Case 1. See Figure 4.

^b Private communication, Sid Bierman, August 1993.

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

One experimenter recalls that the experimenters carefully inserted rubber plugs in the bottoms of the rods, before filling, so that the rubber plug protruded approximately 1/16 inch uniformly for all rods. Some top end plugs protruded and some were recessed, depending on slight differences between thicknesses of UO_2 pellets. Differences in pellet thicknesses were also the reason for the reported 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 2. To test the effects of small differences between rods, "experiments were repeated using alternate but identical (within the quality control applied during fabrication) fuel rods and different fuel loading arrangements on the approach to critical. ... the measurement data thus checked were reproduced to within a one sigma limit of 0.3%" in most cases (Reference 2, p. 19). The standard deviations of a few reported critical cluster separations were greater than 0.3%.

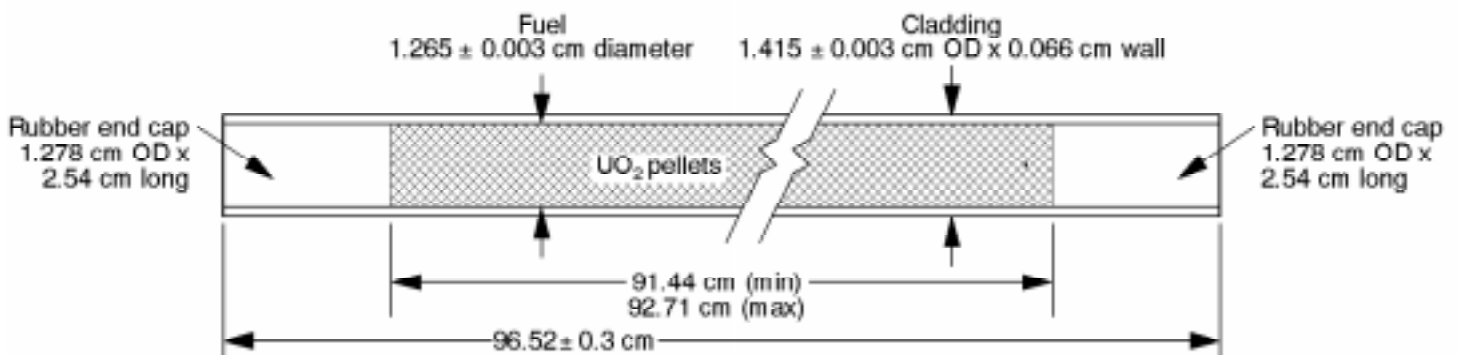


Figure 3. $\text{U}(4.31)\text{O}_2$ Fuel Rod.

^a Sid Bierman, personal communication, April 1994.

Table 2. 4.31 Wt.% Enriched UO₂ 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)

1.2.8 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.)

1.2.9 Critical Cluster Dimensions and Separations - Cluster sizes and separations for the five critical configurations are listed in Table 3 and are diagramed in Figure 4. Because the critical configuration was determined by extrapolation to critical, the critical number of rods for single cluster experiments was not an integral number.

Table 3. U(4.31)O₂ Fuel Rod Critical Configurations. (See Figure 4.)

Case Number	Number of Clusters	Cluster Dimensions (number of rods, X x Y) ^(a)	Separation Between Clusters (cm) ^(b)	Reference (pg)
1	1	10 x 11.51 ± 0.04	-	2(9)
2	1	9 x 13.35 ± 0.01	-	2(9)
3	1	8 x 16.37 ± 0.03	-	2(9)
4	3	15 x 8	10.62 ± .01 ^(c)	2(9)
5	3	13 x 8	7.11 ± .04 ^(d)	3(14), 5(16)

- (a) For three-cluster configurations, the first dimension is along the direction of cluster placement. Second dimension is the width of facing sides, as shown in Figure 4.
- (b) Distance between outermost fuel-rod cell boundaries.
- (c) Average of two values, 10.64 cm and 10.60 cm. (Sid Bierman, personal communication, March 1993. Reported separations in Reference 2 were rod-surface to rod-surface separations.)
- (d) Average of two reported separations of 8.24 and 8.23 ± 0.3 cm. These separations were rod-surface to rod-surface (Sid Bierman, private communication, July 1993) or lattice plate hole-edge to hole-edge (Sid Bierman, private communication, February 1994). Cell boundary separation is equal to (rod-surface separation) - (pitch) + (rod diameter) = 8.235 - 2.54 + 1.415 = 7.11 cm.

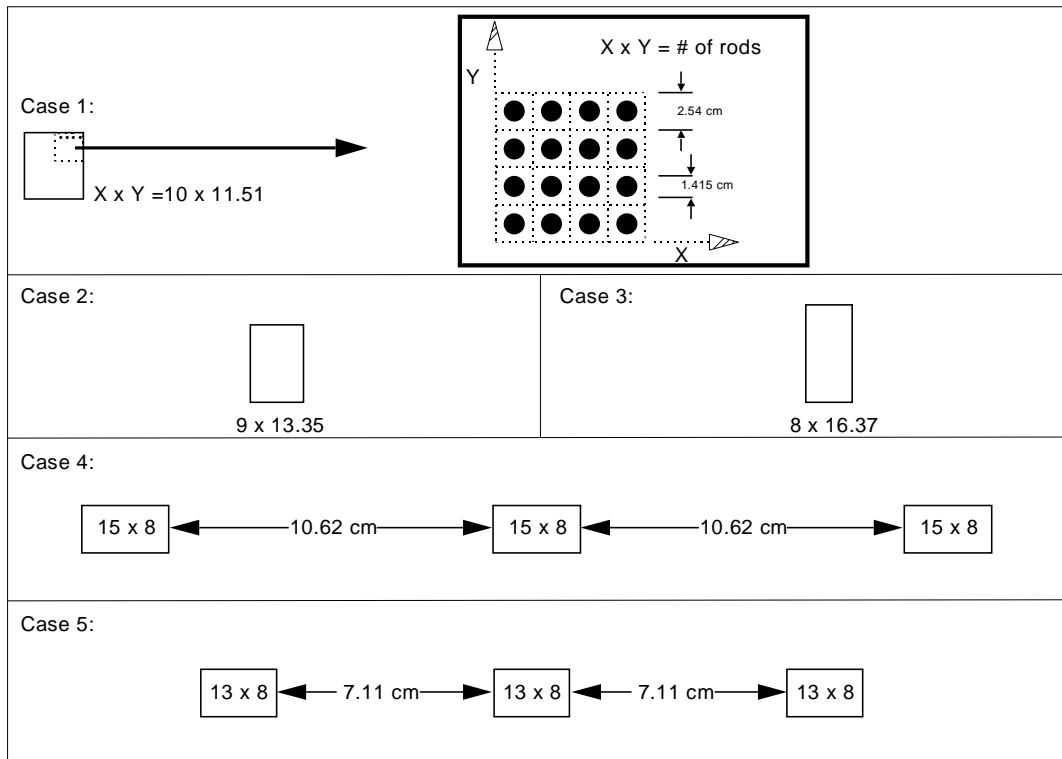


Figure 4. Arrangement of Fuel Rod Clusters for Critical Configurations of $U(4.31)O_2$ Fuel Rods at 2.54 Centimeter Pitch.

1.3 Description of Material Data

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

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

more recent reports. . . . the values quoted in this report should be considered the latest and, hopefully, the more correct values to use.

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

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

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

Uranium isotopic composition is summarized in Table 4.

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

Uranium Isotope	Wt. %
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 5. The 6061 aluminum data includes the measured density and the ASTM Standard chemical composition.^b

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

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

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

^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.

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

1.3.3 Lattice Plates and Fuel Rod Support Plates - The acrylic fuel rod support plates and lattice plates had a density of 1.185 g/cm³ and were 8 wt.% hydrogen, 60 wt.% carbon, and 32 wt.% oxygen. (Reference 4, pp. 11 and 20; Reference 10, p. 2.5; Reference 13, p. 133) Uncertainties and methods of determination were not given.

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 5.) As mentioned in Section 1.2, doubling the aluminum grid plate supports and the control and safety blade guides did not have a measurable effect on predicted critical separation.

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

^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.

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

2.0 EVALUATION OF EXPERIMENTAL DATA

Experiments were well documented and carefully performed. There were no significant omissions of data. However, uncertainties in measurement data contribute to an uncertainty in the benchmark-model k_{eff} . Descriptions of calculations of the effect of the uncertainties on k_{eff} are given below. Results are summarized in Table 6.

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 0.020 and 0.026%,^a as shown in Table 6. 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%. Replacing the plugs with water changed k_{eff} by -0.011%. 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 0.103% for 2.54-cm-pitch rods.

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} was for the minimum UO_2 mass, the maximum U mass, and the maximum enrichment. The calculated Δk_{eff} , as compared to models having the average amounts of these variables, was +0.083%. The lowest calculated k_{eff} was for maximum UO_2 , minimum U, and minimum enrichment, with a Δk_{eff} of -0.147%. These two worst-case results should also contribute to the uncertainty in the benchmark model k_{eff} .

The last two rows of Table 6 are each the results from a model that combines all modifications that contribute to a change in k_{eff} in the same sense, either positive or negative. This estimate of the effect on k_{eff} is conservative because it is assumed that all rods differ from the average in all respects that affect k_{eff} in the same sense, which is unlikely. The estimate for the uncertainty in pitch is itself especially conservative. (See footnote c of Table 6). Nevertheless, an uncertainty of $\pm 0.18\%$ 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 6. 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)	-0.020	-0.026
Plug Compression (± 0.3175 cm change in length)	+0.0007	-0.0007 ^(b)
Fuel Diameter (± 0.003 cm)	+0.021	+0.005
Pitch (± 0.0076 cm ^(c))	-0.103	+0.074
Combination of Enrichment (± 0.013 wt.%), UO ₂ Mass Per Rod (± 4.12 g), U Mass Per Rod (± 4.80 g)	+0.083 ^(d)	-0.147 ^(e)
Combine all changes that individually increase k_{eff}	$\Delta k_{\text{eff}} = +0.13\%$	
Combine all changes that individually decrease k_{eff}	$\Delta k_{\text{eff}} = -0.18\%$	

- (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 UO₂, maximum U, and maximum enrichment.
- (e) Lowest k_{eff} value; for a model with maximum UO₂, minimum U, and minimum enrichment.

2.2 Reflector

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

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 Water Impurities

Water impurity sensitivity studies in Appendix C and Section 3.3 indicate that only boron and gadolinium impurities significantly affect k_{eff} . No boron or gadolinium impurities were reported in References 2, 3, and 5, which describe this set of experiments.

2.4 Temperature Data

Water temperatures were recorded in logbooks for approximately ten percent of the experiments. Measured temperatures ranged from 18°C to 26°C. Calculations gave a change in k_{eff} of 0.072% between these two extremes of temperature. Therefore, an estimate of the uncertainty in k_{eff} due to the effects of temperature is half of this, namely 0.04%.

2.5 Cluster Separations

The measurement uncertainties in cluster separation for Cases 4 and 5 (See Table 3.) are 0.01 cm and 0.04 cm. The effect as calculated by KENO V.a with 27-group cross sections was 0.011% Δk_{eff} per centimeter of reduction in separation of clusters. The uncertainties to be included in the benchmark-model k_{eff} due to uncertainty in the cluster separation measurement are, therefore, 0.01% for Case 4 and 0.04% for Case 5.

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 7 and are shown in Figure 4.

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.

Table 7. U(4.31)O₂ Fuel Rod Critical Configurations (See Figure 4).

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	10 x 11	5	-
2	1	9 x 13	3	-
3	1	8 x 16	3	-
4	3	15 x 8	-	10.62
5	3	13 x 8	-	7.11

(a) This is the portion of the cluster that does not contain a partial row.

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 0.10% Δk_{eff} . Half of this, 0.05%, should 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. Results for several calculations by KENO V.a with the 27-group ENDFB/IV

cross sections were statistically combined. The differences were $0.13\% \Delta k_{\text{eff}}$. Half of this, 0.07% , should be added to the uncertainty in the benchmark model k_{eff} .

3.2 Dimensions

Fuel rod dimensions are shown in Figure 5. 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.

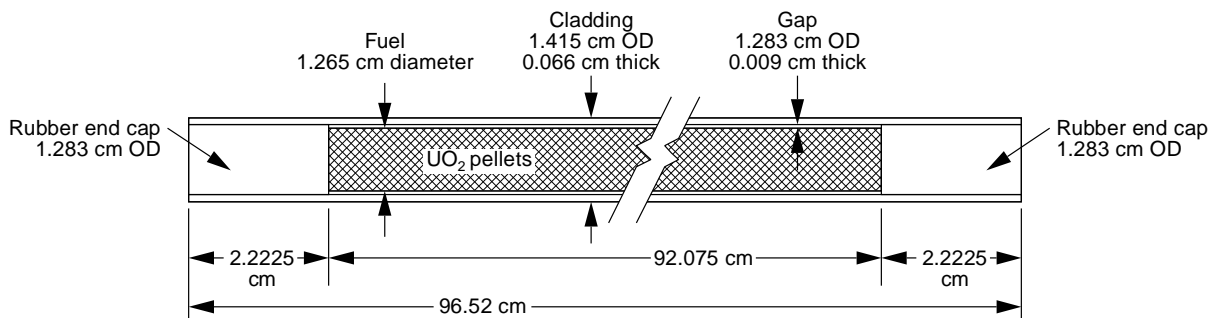


Figure 5. Fuel Rod Model.

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 8.

Table 8. Fuel Rod Atom Densities.

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

3.3.2 Moderator-Reflector - Fuel rods rest on an acrylic support plate. The support plate density is 1.185 g/cm³ and is composed of 8 wt.% hydrogen, 60 wt.% carbon, and 32 wt.% oxygen. The moderator-reflector is water at a temperature of 22°C. Atom densities are given in Table 9.

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

Table 9. Moderator-Reflector Atom Densities.

Material	Isotope	Atom Density (barn-cm) ⁻¹
Water ^(a)	H	6.6706×10^{-2}
	O	3.3353×10^{-2}
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.)

Lattice Plates. ONEDANT calculations of an infinite slab of fuel pins, with and without acrylic lattice plates present (using two fuel mixtures, one with acrylic moderator and one with water moderator) and reflected by 15 centimeters of water, were performed. The effect of the lattice plates of the specified thickness and at the specified locations on k_{eff} was 0.03%. Because the acrylic 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 10. As expected, the carbon-steel tank had practically no effect on k_{eff} , while the acrylic support plate had a small measurable effect (0.02% for one support plate). Therefore, the acrylic support plate is retained in the benchmark model. As discussed in Section 2.2, concrete or stainless steel beyond 15 centimeters of water reflector have a negligible effect on k_{eff} . Therefore, the model of the bottom reflector is 2.54 cm of acrylic followed by 15.3 cm of water.

Table 10. Effect of Reflector Materials on k_{eff} .^(a)

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

(a) ONEDANT infinite slab of fuel pins with reflector materials on both sides. CSAS 27-group 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 effect on k_{eff} of half the temperature range is small (approximately 0.04%). 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 calculated positive effects of lattice plates which are omitted from the benchmark model, the benchmark-model k_{eff} is slightly below 1.0. Therefore, the benchmark-model k_{eff} is 0.9997.

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 effects on k_{eff} . However, some experimental uncertainties or model simplifications, whose effects were

described in sensitivity studies, contribute to an estimated uncertainty in the benchmark model k_{eff} . Uncertainties included are summarized listed in Table 11.

Table 11. Uncertainty in Benchmark-Model k_{eff} .

Measurement Uncertainty or Model Simplification	Δk_{eff}	
Fuel rod characterization	0.0018	
Temperature	0.0004	
Cluster Separations	Case 4	0.0001
	Case 5	0.0004
Omit fractional rod	Case 1-3	0.0005
Placement of partial row	Cases 1-3	0.0007
Total Uncertainty in $k_{\text{eff}}^{(a)}$	Cases 1-3	0.0020
	Case 4	0.0018
	Case 5	0.0019

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

Therefore, the benchmark model k_{eff} is 0.9997 ± 0.0020 .

4.0 RESULTS OF SAMPLE CALCULATIONS



Results of calculations representing the five critical configurations are presented in Table 12. Code versions and modelling options are discussed briefly in paragraphs preceding the input listings in Appendix A. In general, calculated k_{eff} values are slightly low, by approximately 0.5%.^a Only one result (Case 2, MCNP) is within the estimated uncertainty of the benchmark-model k_{eff} .

Table 12. 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	0.9923 ± .0018	0.9948 ± .0021	0.9970 ± .0017
2	0.9951 ± .0018	0.9972 ± .0018	1.0016 ± .0018
3	0.9921 ± .0017	0.9937 ± .0018	0.9951 ± .0019
4	0.9975 ± .0016	0.9922 ± .0018	0.9974 ± .0018
5	0.9975 ± .0017	0.9949 ± .0019	0.9950 ± .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, and Ca (GAM-2).

^a 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 ²³⁸U resonances leads to low eigenvalues (by approximately 1%) for water-reflected low-enriched UO₂ lattices.

5.0 REFERENCES

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13. S. R. Bierman and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 and 4.31 wt.% ^{235}U -Enriched UO_2 Rods in Water with Steel Reflecting Walls," Nuc. Technol., **54**, August 1981.
14. S. R. Bierman, B. M. Durst, and E. D. Clayton, "Criticality Experiments with Subcritical Clusters of Low Enriched UO_2 Rods in Water with Uranium or Lead Reflecting Walls," Nuc. Technol., **47**, January 1980.

APPENDIX A: TYPICAL INPUT LISTINGS

A.1 KENO Input Listings

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

KENO V.a input files were created with arrays of fuel rod units. Cuboids of water 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 0.03894.)

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KENO-V.a Input Listing for Case 2 of Table 12 (16-Energy-Group Hansen-Roach Cross Sections).

```
K402 9X13.35 CLUSTER (9X13 + 3 RODS), 2.54 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 2.54 cm pitch
92400 5.1835-6 92508 8.0955-4 92509 2.0065-4
92600 5.1395-6 92857 5.9286-3 92858 1.6228-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end 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
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P1.27 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P1.27 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=9 NUY=13 FILL F1 END FILL
      ARA=2 NUX=9 NUY=1 FILL 3R1 6R2 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 4 of Table 12 (16-Energy-Group Hansen-Roach Cross Sections).

```
K404 THREE 15X8 CLUSTERS, 10.62 CM SEPARATION, 2.54 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 2.54 cm pitch
92400 5.1835-6 92508 8.0955-4 92509 2.0065-4
92600 5.1395-6 92857 5.9286-3 92858 1.6228-2
8100 4.6753-2
MIX=2
' water
1102 6.6706-2 8100 3.3353-2
MIX=3
' 6061 Al (clad)
13100 5.8433-2 24100 6.2310-5 29100 6.3731-5
12100 6.6651-4 25100 2.2115-5 22100 2.5375-5
30100 3.0967-5 14100 3.4607-4 26100 1.0152-4
MIX=4
' rubber (end 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
END MIXT
READ GEOM
UNIT 1
COM=* FUEL PIN *
CYLINDER 1 1 0.6325 92.075 0.0
CYLINDER 0 1 0.6415 92.075 0.0
CYLINDER 4 1 0.6415 94.2975 -2.2225
CYLINDER 3 1 0.7075 94.2975 -2.2225
CUBOID 2 1 4P1.27 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P1.27 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* WATER BETWEEN FUEL PINS *
CUBOID 6 1 10.62 0 20.32 0 94.2975 -2.2225
GLOBAL
UNIT 5
COM=* THREE FUEL-ROD CLUSTERS *
ARRAY 2 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=15 NUY=8 FILL F1 END FILL
      ARA=2 NUX=5 NUY=1 FILL 3 4 3 4 3 END FILL
END ARRAY
END DATA
END
```

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KENO-V.a Input Listing for Case 2 of Table 12 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
C402 9X13.35 CLUSTER (9X13 + 3 RODS), 2.54 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
' 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
END COMP
SQUAREPITCH 2.54 1.265 1 2 1.415 3 1.283 0 END
C402 9X13.35 CLUSTER (9X13 + 3 RODS), 2.54 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 4P1.27 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P1.27 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=9 NUY=13 FILL F1 END FILL
ARA=2 NUX=9 NUY=1 FILL 3R1 6R2 END FILL
ARA=3 NUX=1 NUY=2 FILL 3 4 END FILL
END ARRAY
END DATA
END
```

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KENO-V.a Input Listing for Case 4 of Table 12 (27-Energy-Group SCALE4 Cross Sections).

```
=CSAS25
C404 THREE 15X8 CLUSTERS, 10.62 CM SEPARATION, 2.54 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
' 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
END COMP
SQUAREPITCH 2.54 1.265 1 2 1.415 3 1.283 0 END
C404 THREE 15X8 CLUSTERS, 10.62 CM SEPARATION, 2.54 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 4P1.27 94.2975 -2.2225
UNIT 2
COM=* WATER FUEL PIN *
CUBOID 6 1 4P1.27 94.2975 -2.2225
UNIT 3
COM=* ARRAY OF FUEL PINS *
ARRAY 1 3R0
UNIT 4
COM=* WATER BETWEEN FUEL PINS *
CUBOID 6 1 10.62 0 20.32 0 94.2975 -2.2225
GLOBAL
```

```
UNIT 5
COM=* THREE FUEL-ROD CLUSTERS *
ARRAY 2 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=15 NUY=8 FILL F1 END FILL
          ARA=2 NUX=5 NUY=1 FILL 3 4 3 4 3 END FILL
END ARRAY
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 2 of Table 12.

M402 9X13 +3 CLUSTER OF U(4.31)O2 RODS, 2.54 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 .100059 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 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 .100059 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 .100059 (-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 1.27 1.27 .6325 $ fuel cylinder
2  c/z 1.27 1.27 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 2.54 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 2.54 $ 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 22.859 $ farthest edge of closest cluster ***
11 px .0001 $ closest edge of closest cluster
12 c/z 1.27 1.27 .7075 $ clad outer surface
13 px 7.619 $ edge of partial row ***
19 py 0.0001 $ close edge of cluster + partial row
20 py 35.559 $ sides of clusters ***
21 py 2.541 $ side of partial row and full cluster
23 pz -2.2225 $ bottom of fuel rod
24 px 52.86 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 65.56 $ 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 37

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

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

mt2 lwtr.01t

c m3 is 6061 Al (clad)

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MCNP Input Listing for Case 2 of Table 12 (cont'd).

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 4 of Table 12.

M404 THREE 15X8 CLUSTERS OF U(4.31)O2 RODS, 2.54 CM PITCH, 10.62 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 .100059 12 u=1 imp:n=1 $ water
7  0 -4 3 -6 5 imp:n=1 lat=1 u=2 fill=1 $ lattice of fuel rods
8  0 -10 11 -20 19 -9 23 fill=2 imp:n=1 $ first rod cluster
9  0 -13 14 -20 19 -9 23 fill=2(48.72 0 0) imp:n=1 $ second rod cluster
10 0 -15 16 -20 19 -9 23 fill=2(97.44 0 0) imp:n=1 $ third rod cluster
11 2 .100059 10 -14 -20 19 -9 23 imp:n=1 $ water between clusters
12 2 .100059 13 -16 -20 19 -9 23 imp:n=1 $ water between clusters
13 5 .106563 19 -20 11 -15 -23 29 imp:n=1 $ acrylic support plate
14 2 .100059 (-11:15:20:-19:9:-29) -24 25 -26 27 -28 30 imp:n=1 $ water
15 0 24:-25:26:-27:28:-30 imp:n=0

```

```

1  c/z 1.27 1.27 .6325 $ fuel cylinder
2  c/z 1.27 1.27 .6415 $ clad inner surface
3  px 0.0 $ fuel rod cell boundary
4  px 2.54 $ fuel rod cell boundary
5  py 0.0 $ fuel rod cell boundary
6  py 2.54 $ 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 38.099 $ farthest edge of closest cluster ***
11 px .0001 $ closest edge of closest cluster
12 c/z 1.27 1.27 .7075 $ clad outer surface
13 px 86.819 $ farthest edge of middle cluster ***
14 px 48.721 $ closest edge of middle cluster ***
15 px 135.539 $ farthest edge of farthest cluster ***
16 px 97.441 $ closest edge of farthest cluster ***
19 py 0.0001 $ close edge of clusters
20 py 20.319 $ sides of clusters ***
23 pz -2.2225 $ bottom of fuel rod
24 px 165.54 $ side of water reflector ***
25 px -30 $ side of water reflector
26 py 50.32 $ 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 0 136

sp1 0 1

si2 0 21

sp2 0 1

si3 0 93

sp3 0 1

si4 1 8 9 10

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

MCNP Input Listing for Case 4 of Table 12 (cont'd).

c m2 is water
m2 8016.50c 3.3353e-2 1001.50c 6.6706e-2
mt2 lwtr.01t
c m3 is 6061 Al (clad)
m3 13027.50c 5.8433e-2 24000.50c 6.2310e-5
29000.50c 6.3731e-5 12000.50c 6.6651e-4
25055.50c 2.2115e-5 22000.50c 2.5375e-5
c Zn replaced by Cu, below
29000.50c 3.0967e-5 14000.50c 3.4607e-4
26000.50c 1.0152e-4
c m4 is rubber (end plugs)
m4 6000.50c 4.3562e-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 the 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.

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

Case Number	Original Experiment Number
1	SSC-4.31-000-001
2	SSC-4.31-000-003
3	SSC-4.31-000-002
4	SSC-4.31-000-004, -032
5	SSC-4.31-000-0xx ^(a)

(a) Exact experiment number is not known.

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 (0.001481 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

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

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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	-	-	<0.38 ^(f)	2.83 ^(f)
Cr	<0.028	<0.01	<0.01	<0.01	-	0.041	<0.01	<0.005
Zn	0.35±.05	0.26±.07	0.9±1.1	16	10.6	0.0613	<0.05	0.32
Mn	<0.55	<0.01	<0.01	<0.01	-	0.041	<0.01	<0.01
Pb	<0.015	<0.005	0.008±.0 01	<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±.0 01	0.006±.0 01	0.020±.0 06	0.001	-	0.041	0.002	0.0006
Gd	-	-	10.4±3.6	-	-	-	-	<10
SO ₄	6.7±.4	6.6±.04	13.4±5.0	14.5	-	-	21	16
CaCO ₃	-	-	-	-	19.2 ^g	1.02 ^g	51.2	35
B	-	-	-	-	0.09	1.02	-	<25
Al	-	-	-	-	7.3	2.04	-	-
Eu	-	-	-	-	0.08	1.23	-	-
Mg	-	-	-	-	5.7	0.204	-	-
Nd	-	-	-	-	12.2	2.04	-	-
Si	-	-	-	-	3.1	2.04	-	-
Ni	-	-	-	-	6.8	0.204	-	-
Y	-	-	-	-	0.17	0.41	-	-

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

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

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

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

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

(e) Largest values of three samples.

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

(g) As Ca.

Effect Due to Water Density Reduction - The maximum amount of dissolved solids reported was 137 grams per cubic meter of solution. Assume that dissolved solids is 200 g/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} for this conservative model is less than 0.04 percent.^a

^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.

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 $\text{U}(2.35)\text{O}_2$ fuel rods at 2.032 cm pitch, using the 27-group cross sections processed by CSASIX.^a No changes are greater than 0.005 percent except those from boron and gadolinium impurities, with Δk_{eff} values of 0.9 percent and 1.7 percent, respectively.

Additional calculations for Gd and B impurities in the water of arrays of 4.31 wt.% enriched fuel rod at two pitches, 2.54 cm and 1.892 cm, were performed. For $\text{U}(4.31)\text{O}_2$ 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 $\text{U}(4.31)\text{O}_2$ rods at 1.892 cm pitch gave Δk_{eff} values of -0.41 percent and -0.69 percent, respectively. Therefore, critical configurations from the two references with these maximal possible impurity concentrations, References 4 and 10, should include these two impurities in the water.

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

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

Impurity	Concentration (g/cm ³)	Atom Density (atoms/barn-cm)	% Δk_{eff}
Ag	4.09×10^{-08}	2.281×10^{-10}	0
Al	7.30×10^{-06}	1.629×10^{-07}	0
Au	4.09×10^{-08}	1.249×10^{-10}	0
B	2.50×10^{-05}	1.393×10^{-06}	-0.885 -0.784 ^(a)
	$1.02 \times 10^{-06(b)}$	5.682×10^{-08}	-0.009
Ba	4.09×10^{-08}	1.791×10^{-10}	0
Be	2.04×10^{-06}	1.365×10^{-07}	0.002
CaCO ₃	5.12×10^{-05}	3.081×10^{-07}	0.005
Cd	4.09×10^{-08}	2.189×10^{-10}	0
Ce	1.02×10^{-07}	4.390×10^{-10}	0.001
Cl	3.60×10^{-05}	6.115×10^{-07}	0.004
Co	4.09×10^{-08}	4.175×10^{-10}	0
Cr	4.09×10^{-08}	4.732×10^{-10}	0
Cu	1.82×10^{-05}	1.725×10^{-07}	0.002
Eu	1.22×10^{-06}	4.838×10^{-09}	-0.005
F	2.30×10^{-07}	7.291×10^{-09}	0
Fe	2.40×10^{-05}	2.588×10^{-07}	0.003
Gd	1.40×10^{-05}	5.361×10^{-08}	-1.653 -1.830 ^(a)
	$1.00 \times 10^{-05(c)}$	3.830×10^{-08}	-1.200
	$5.00 \times 10^{-06(d)}$	1.915×10^{-08}	-0.592
Hf	4.09×10^{-08}	1.378×10^{-10}	0
K	2.04×10^{-07}	3.146×10^{-09}	0
Li	4.09×10^{-08}	3.544×10^{-09}	0
La	2.04×10^{-07}	8.856×10^{-10}	0
Mg	5.70×10^{-06}	1.412×10^{-07}	0
Mn	5.50×10^{-07}	6.029×10^{-09}	0.002
Mo	4.09×10^{-08}	2.564×10^{-10}	0

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Impurity	Concentration (g/cm ³)	Atom Density (atoms/barn-cm)	% Δk_{eff}
N	2.83×10^{-06}	1.217×10^{-07}	0.002
Na	1.02×10^{-06}	2.675×10^{-08}	0.002
Nb	3.00×10^{-07}	1.945×10^{-09}	0
Nd	1.22×10^{-05}	5.094×10^{-08}	0.001
Ni	6.80×10^{-06}	6.977×10^{-08}	0.002
Pb	2.10×10^{-06}	6.103×10^{-09}	0
Pt ^(e)	2.04×10^{-07}	6.305×10^{-10}	0
Rh	1.02×10^{-07}	5.977×10^{-10}	0.001
Ru	1.02×10^{-06}	6.085×10^{-09}	0.001
Si	3.10×10^{-06}	6.647×10^{-08}	0
Sm	2.04×10^{-07}	8.179×10^{-10}	0.001
Sn	1.02×10^{-06}	5.182×10^{-09}	0
SO ₃	1.84×10^{-05}	1.384×10^{-07}	0.002
Sr	4.09×10^{-08}	2.808×10^{-10}	0.001
Tb	2.03×10^{-07}	7.709×10^{-10}	0.001
Ti	2.04×10^{-06}	2.568×10^{-08}	0
U	2.04×10^{-07}	5.168×10^{-10}	0
V	4.09×10^{-08}	4.830×10^{-10}	0
W	1.02×10^{-07}	3.345×10^{-10}	0
Y	4.09×10^{-07}	2.767×10^{-09}	0
Zn ^(f)	1.60×10^{-05}	1.474×10^{-07}	0.003
Zr	4.09×10^{-08}	2.697×10^{-10}	0

(a) MCNP calculation.

(b) This is an actual measured value, from Reference 8.

(c) Measured maximum value from Reference 10.

(d) Half of measured maximum value from Reference 10.

(e) Because platinum was not in the cross section library, gold was substituted.

(f) Because zinc was not in the cross section library, copper was substituted.

APPENDIX D: SAMPLE CSASIX 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