NEA/NSC/DOC/(95)03/IV
Volume IV

LEU-COMP-THERM-014

WATER-REFLECTED ARRAYS OF U(4.31)O_2 FUEL RODS (1.890-CM AND 1.715-CM SQUARE PITCH) IN BORATED WATER

Evaluator

Virginia F. Dean
Subcontractor to INEEL

Internal Reviewer
Soon S. Kim
INEEL

Independent Reviewer

David Hanlon
Serco Assurance

WATER-REFLECTED ARRAYS OF U(4.31)O_2 FUEL RODS (1.890-CM AND 1.715-CM SQUARE PITCH) IN BORATED WATER

IDENTIFICATION NUMBER: LEU-COMP-THERM-014 SPECTRA

KEY WORDS: absorber, acceptable, boric acid, boron, fuel rods, low-enriched, Plexiglas, PNL, poison, thermal, ^{235}U, unacceptable, uranium, uranium dioxide, water-reflected

1.0 DETAILED DESCRIPTION

1.1 Overview of Experiment

A series of critical-approach experiments with arrays of 36-inch-long aluminum-clad U(4.31)O_2 fuel rods in a large water-filled tank was performed over the course of several years at the Critical Mass Laboratory at the Pacific Northwest Laboratories (PNL). Most of the experiments were square-pitched lattice clusters, or arrays. Some were simply rod arrays in water (LEU-COMP-THERM-002 and LEU-COMP-THERM-004). Others had lead, depleted-uranium, or steel reflecting walls on two opposite sides of a row of clusters (LEU-COMP-THERM-010). Others had absorber plates between the arrays (LEU-COMP-THERM-009). One set of experiments used both steel walls and absorber plates (LEU-COMP-THERM-013). Some circular, triangular-pitched lattices with pitches of 2.4, 1.8, or 1.6 cm were used to measure the effect of gadolinium dissolved in the water (LEU-COMP-THERM-005).

This evaluation documents nine water-reflected experiments, performed in February-March, 1982. Each experiment was a nearly rectangular array of U(4.31)O_2 rods completely submerged in water or borated water in a Plexiglas tank, or box, surrounded by a water reflector. The pitch of the rods for five experiments was 1.890 cm and was 1.715 cm for four experiments. Moderator-to-fuel volume ratios were 1.59 and 1.09. The critical number of rods was extrapolated from subcritical configurations. Boron concentration in the moderator ranged from 0 to 2.55 g/liter. The purpose of the experiments was to observe the simultaneous effects of boron concentration and pitch on critical number of rods.

Because the standard uncertainty in k_{eff} for four experiments was greater than 1%, due to the large effect of the uncertainty in boron concentration in the moderator, the four are rejected as benchmark experiments. The other five experiments are judged to be acceptable as benchmark data.

1.2 Description of Experimental Configuration

Information in this section comes from References 1 - 10, which are the original PNL reports of these experiments. References 11 - 13, logbooks, and conversations with experimenters provided supplementary information. The primary reference for this set of experiments is Reference 7.

1.2.1 Experiment Setup – A diagram of the experiment setup, taken from Reference 7, is shown in Figure 1. A photo from the same reference is shown in Figure 2. The experiment tank was a Plexiglas box containing the fuel-rod array in water or borated-water moderator. Outer dimensions of the experiment tank were 79.69 ± 0.15 cm wide by 83.41 ± 0.15 cm long by 119.4 ± 0.2 cm high. The inner height of the tank was 116.8 ± 0.2 cm. Side walls were 1.905 cm thick. No uncertainty in tank wall thickness was given. The bottom was 2.6 cm thick, derived from dimensions in the diagram (Figure 1). The tank sat on a 15.2-cm-thick Plexiglas slab which rested on the bottom of the reflector tank.

As shown in Figure 1, the moderator level was at 15.2 cm above the tops of the fuel rods. Reference 7 (p. 2) says, "Water was progressively removed from inside the container as more fuel was added to keep the water level inside constant as shown in [the figure]."

The surroundings and the water reflector are not described other than to say, "The container was surrounded on all four sides by a full water reflector."

Diagrams in the logbook show a control blade on one side of the Plexiglas experiment tank and a safety blade on the other side, similar to the safety blades in the large carbon-steel tank in which other experiments of this series were performed. Logbook data indicate that both blades were "out" for counts used to determine the critical number of rods. A safety blade above and to one side of the array can also be seen in Figure 2. In the photograph, the hardware supporting the experiment-tank edges appears similar to the aluminum angles described and shown in the six earlier references (References 1-6). The six references are all included in the reference list of Reference 7. This set of experiments is described by the authors as "the seventh in a series of criticality experiments."

Figure 1 shows two polypropylene lattice plates, or templates, to hold the rods in place. The one on the bottom of the tank is 2.54 cm thick. The upper lattice plate is 1.27 cm thick. As shown in Figure 1, the top surface of the upper template is 25.4 cm below the top ends of the fuel rods. The templates were "securely fastened inside" the Plexiglas container. An array of holes that was 40 holes wide filled the template for the experiments at the larger pitch. For the smaller pitch, the array was 44 holes wide.

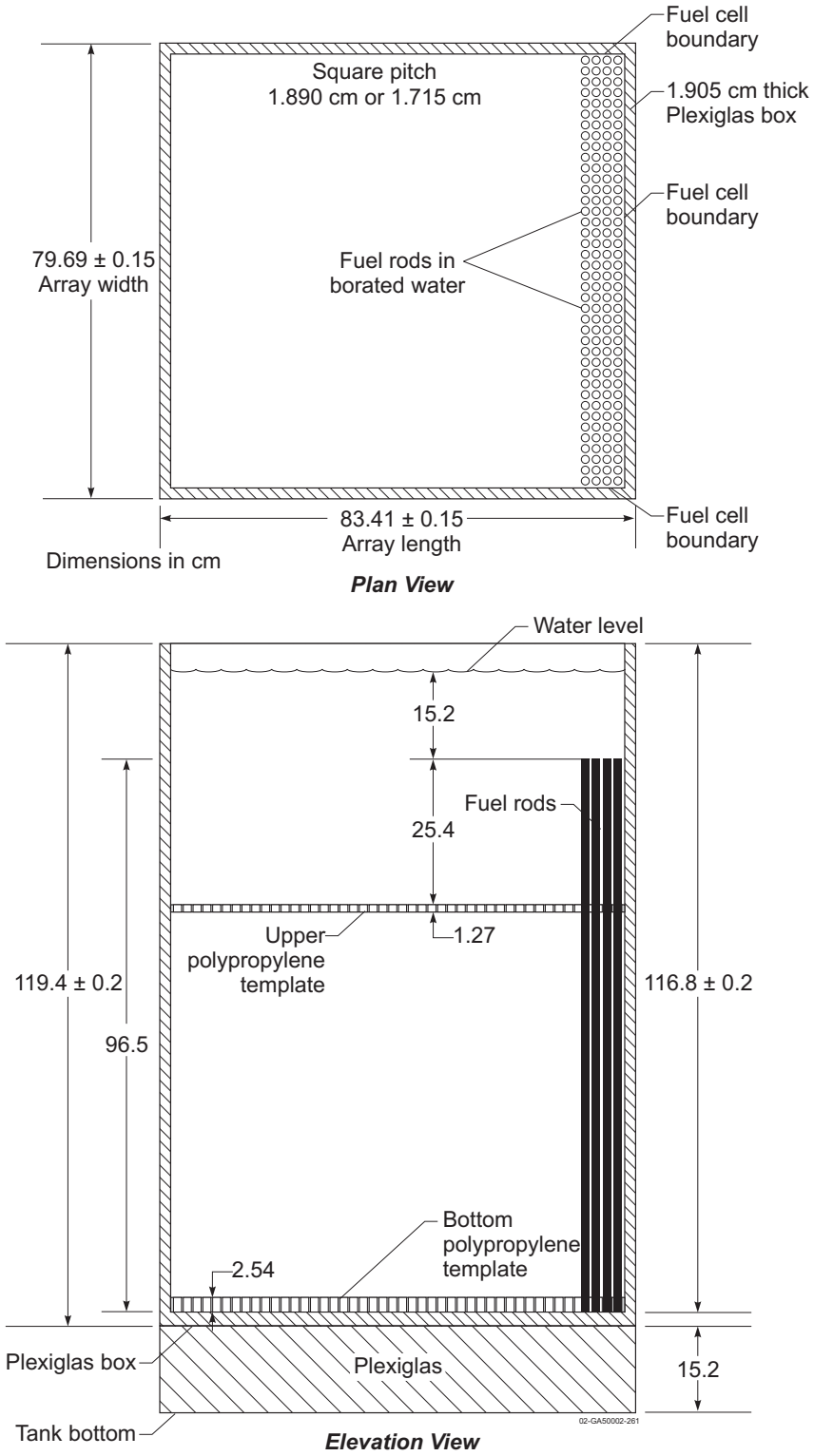


Figure 1. Experiment Setup, from Reference 7.

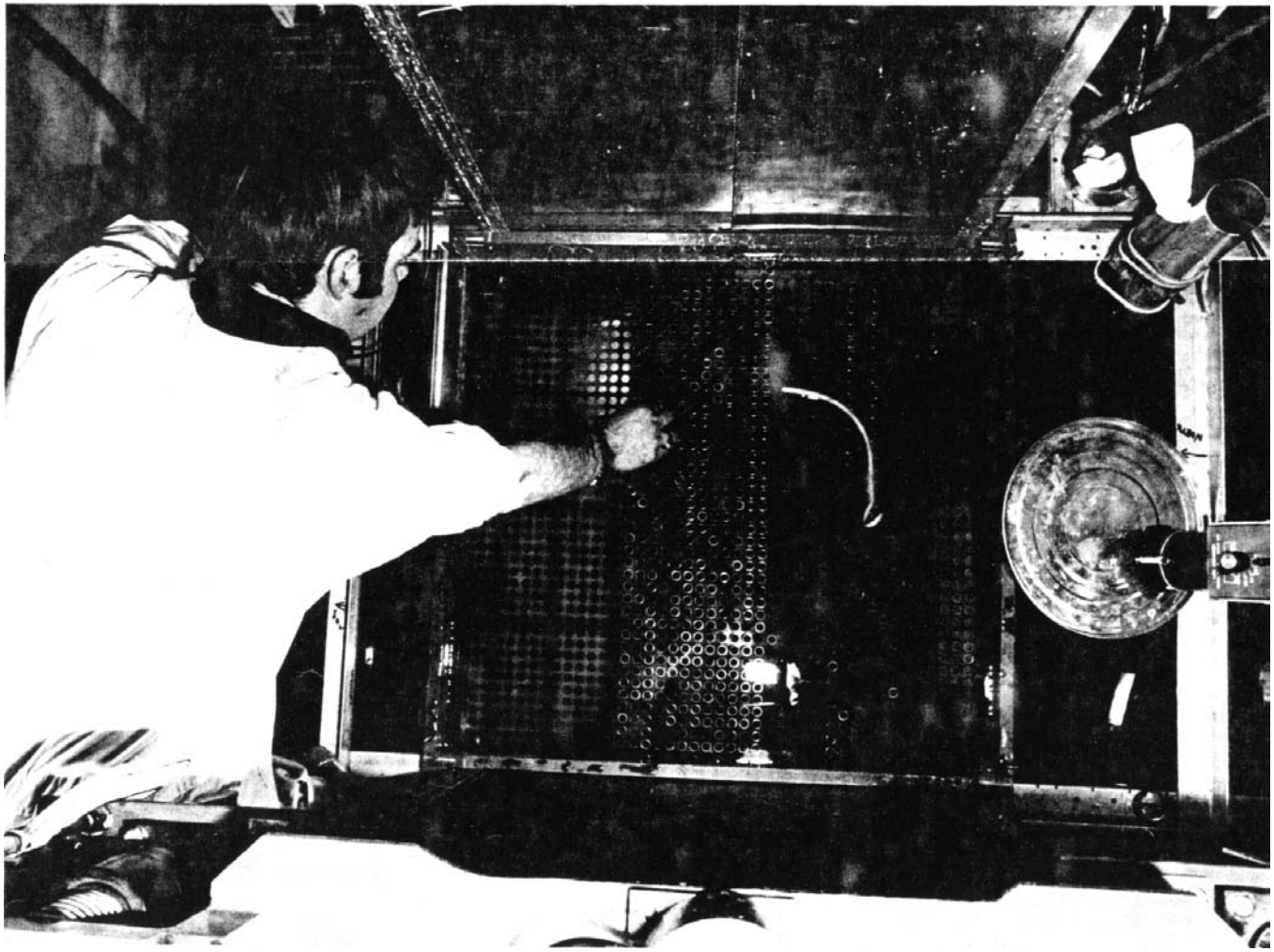


Figure 2. Assembling the Lattice.

1.2.2 Fuel Rods – The same fuel rods, called either 4.29%-enriched or 4.31%-enriched, were used in all experiments of this experimental program. Fuel-rod dimensions are given in diagrams in References 3-10. According to the experimentalist, fuel characterization improved in the later reports.[a]

Figure 3 is a reproduction of the diagram of the fuel rod 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)

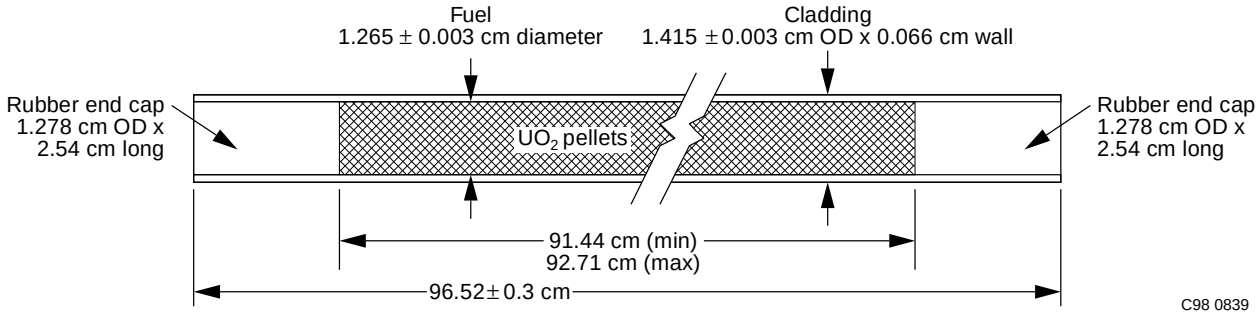


Figure 3. U(4.31)O_2 Fuel Rod.

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.

An experimentalist recalled that the total length of rods (96.52 cm) was actually the length of the aluminum tubing, as shown in the diagrams in later reports. He also remembered that the rubber plugs were carefully inserted in the bottoms of the rods, before filling, so that the rubber plugs 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 thickness was 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 U(4.31)O_2 fuel rods are summarized in Table 1.

[a] Private communication, Sid Bierman, April, 1994.

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
Clad (6061 Al)	96.52 ± 0.3	1.283 ± 0.003 ID [(a)] 1.415 ± 0.003 OD (0.066 cm thick)

(a) derived from clad outer diameter and wall thickness (0.066 cm).

1.2.3 Critical Configurations – The 9 reported critical configurations are listed in Table 2. Note that the array length is not an integral number of rods. Reference 7 states, "This has the same interpretation as all experiments performed before in this program. A fraction of a row is a row which extends full width but is thinner in length. This is the best interpretation for computer modeling. The cell boundary of the first fuel row is next to the Plexiglas wall of the box. The error in critical rod number is <0.5%."

Table 2. Critical Configurations (Reference 7, p. 8).

Case	Date in [(a)] 1982	Pitch (cm)	Boron Concentration, g/liter	Array Width, rods	Array Length, number of rows[(b)]	Critical Number of Rods
1	2/18	1.890 ± 0.002	0.0	40	8.92 (8, 8.5)	357
2	2/19	1.890 ± 0.002	0.49 ±0.06	40	10.72 (10, 10.5)	429
3	2/19	1.890 ± 0.002	1.25 ± 0.21	40	14.05 (13, 13.5)	562
4	2/22	1.890 ± 0.002	2.15 ± 0.35	40	23.07 (22, 23)	923
5	2/23	1.890 ± 0.002	2.55 ± 0.07	40	30.92 (30, 30.5)	1237
6	2/26	1.715 ± 0.005	0.0	44	11.57 (11, 11.5)	509
7	3/1	1.715 ± 0.005	1.03 ± 0.05	44	16.75 (16, 16.5)	737
8	3/2	1.715 ± 0.005	1.82 ± 0.30	44	20.84 (20, 20.5)	917
9	3/3	1.715 ± 0.005	2.55 ± 0.21	44	27.09 (26, 27)	1192

(a) From the logbook.
(b) The number of rows in the two most reactive subcritical configurations from which the critical number of rods was extrapolated is given in parentheses. This information is from the logbook.

1.2.4 Experimental Method for Determining the Critical Configuration - The arrays were built next to one wall of the tank. Logbook data[a] indicate that the critical number of rods was determined in the following manner, illustrated in Figure 4:

Arrays were built starting with the row against the north wall of the tank (right side in Figure 1). Boral control blades were next to the east and west sides of the tank. The largest subcritical array with complete rows was built and counter pulses were counted, first with one of the control blades 'in', then with both control blades 'out', i.e., raised above the core. With both control blades out, five 80-second counts were recorded and averaged.

Then half a row of rods was added to one side (e.g., the control-blade side) of the next row and counts taken, first with one control blade out, then with both blades out. Then the half row of rods was moved to the other side of the row (e.g., the safety-blade side) and a second series of counts was taken.

The reciprocals of these three count rates, with both control blades out, and after subtracting background, were calculated. The slopes of the two straight-line graphs of number of rods vs reciprocal of counts between the configuration with only complete rows and each of the two configurations with an additional half row were calculated and averaged. The average slope was used to extrapolate to a reciprocal count rate of zero and critical number of rods.

The calculation was repeated using counts from a second counter. Counts from a third counter were recorded but were not used to determine criticality, probably because of the low number of counts relative to the first two counters. The standard deviation was also calculated.

It appears, from logbook data, that critical number of rods was calculated from both the reciprocal count rates and reciprocal count rates multiplied by number of rods (i.e., reciprocal of counts per rod). The average was taken as the final value. The two values that were averaged were the same to within one or two rods. The experimentalist said,[b] "We would use rods over inverse count rate as typically it overestimated the true critical point, while inverse count rate gave a slightly non-conservative estimation. At critical, they always converged to one another."

Figure 4 is an example taken from the logbook (Case 2) of the three subcritical configurations used to extrapolate to critical.

[a] Logbooks are stored at the Los Alamos National Laboratory Archives (experiments SSC-4.3-000-173 through 181; stored as A-93-049, 34-1).

[b] Personal communication, B. M. Durst, July, 2002.

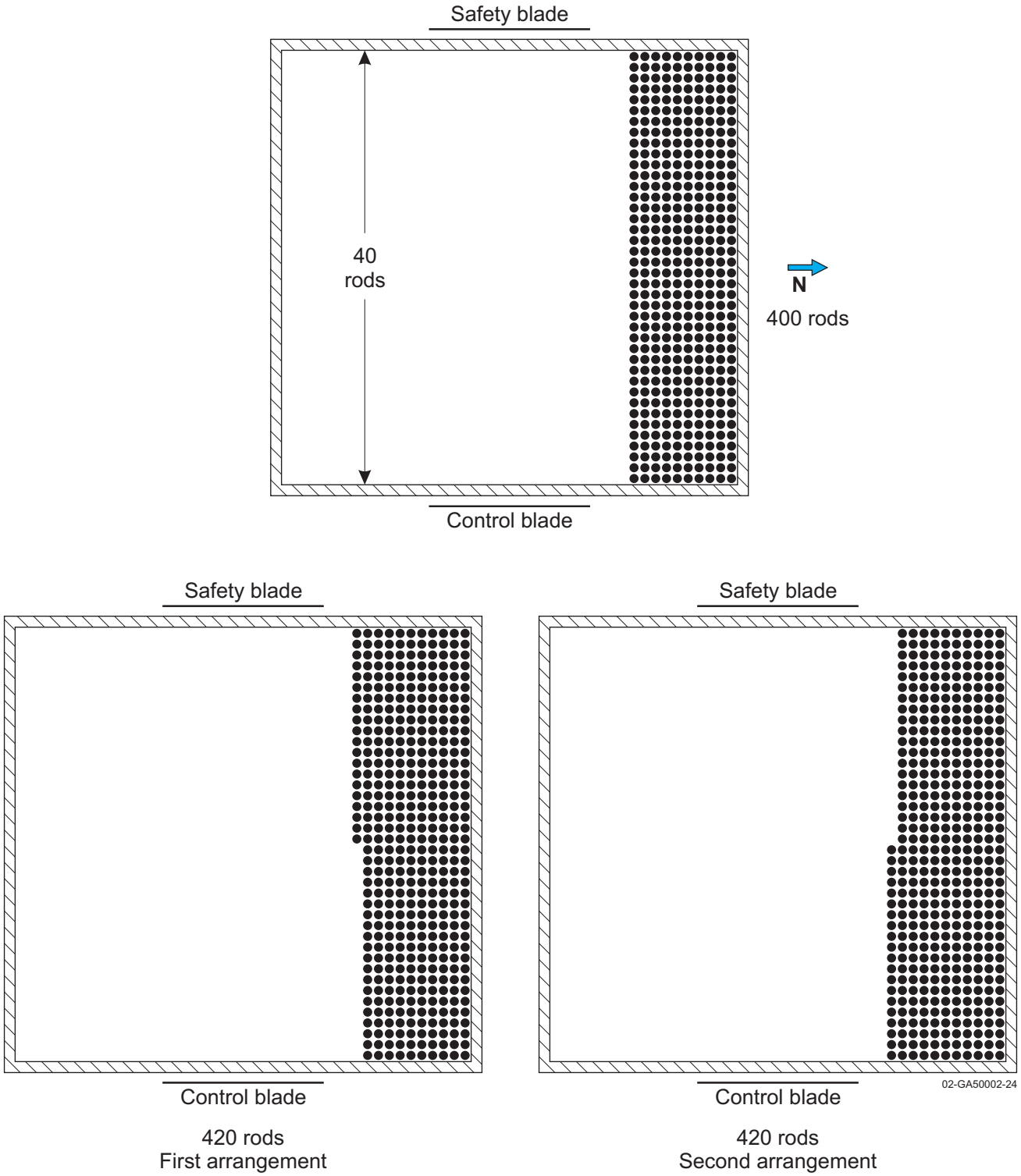


Figure 4. Example of Variations of Number of Rods and Rod Placement Used to Extrapolate to Critical Number of Rods.

1.3 Description of Material Data

1.3.1 Fuel Rod - Over the course of performing the series of experiments, the experimenters improved their analyses of the fuel rods. In Reference 5, pg. x, the experimenters state

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

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

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

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

Although no tests of reproducibility of measurement data were described for this specific set of experiments, tests had been performed earlier with configurations without boron. Reference 2 says (p. 19)

> During the course of the measurements, 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. All of the measurement data thus checked were reproduced to within a one sigma limit of 0.3%.[a] (Some of the data given [in the tables] show larger deviations than 0.3% on the critical separation [between arrays of rods]. Because of scatter in the approach to critical data, better accuracy could not be claimed for these measurements.)

[a] Although not specifically stated, the term "measurement data" seems to refer to such things as number of fuel rods or distance between rectangular arrays of rods to give a particular multiplication. As mentioned, larger deviations than 0.3% are shown for some extrapolated critical data.

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

Reference 10 gives rubber end-cap data (p. 2.3) and data about the 6061-aluminum tubing used for cladding (p. A.2). The rubber end-cap composition is the same as reported in Reference 7. The 6061-aluminum data in Reference 10 includes the ASTM Standard chemical composition[a] and the density "measured by volume displacement." Compositions and densities are given in Table 4.

[a] Also found in the *Alcoa Aluminum Handbook*, Aluminum Company of America, pp. 46-50, 1967.

Table 4. Rubber End-Cap and 6061-Aluminum Clad Data (Reference 10).

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, density 2.69 g/cm^3	
Si	0.40-0.80 (0.6 nominal)
Fe	0.7 (maximum)
Cu	0.15-0.40 (0.25 nominal)
Mn	0.15 (maximum)
Mg	0.8-1.2 (1.0 nominal)
Cr	0.04-0.35 (0.2 nominal)
Zn	0.25 (maximum)
Ti	0.15 (maximum)
Al	remainder (96.00-98.61)

1.3.2 Lattice Plates – According to Reference 7, the material density of the two polypropylene lattice templates was 0.904 g/cm^3. No composition data were given, however the chemical composition of polypropylene is CH_2.[a] The impurity analysis on polypropylene lattice plates in later experiments probably does not apply to these experiments.[b]

1.3.3 Experiment Tank and Support Platform – No information was given about the material of the experiment tank (box) and tank support platform other than that it was Plexiglas. In Reference 12, acrylic lattice plates were described as "an acrylic $(C_5H_8O_2)_n$ material (Plexiglas) having about the same density (1.18 g/cm^3) and neutron moderating characteristics as water."

1.3.4 Borated-Water Moderator and Water Reflector – Laboratory analysis of the water before addition of boron is given in Table 5.

[a] R.T. Morrison and R.N. Boyd, *Organic Chemistry*, second edition, Allyn and Bacon, Inc., 1966, p. 265.

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

Table 5. Water Impurities (Reference 7, p. 6).

Component	Concentration (ppm)
Cl	≤5
NO_3^-	0.02
Cr^{+6}	<0.01
Zn	16
Mn	<0.01
Pb	<0.005
F	0.18
Fe	24
Cu	<0.01
Cd	0.001
SO_3	14.5
Dissolved Solids	61 ± 3

According to Reference 7 (p. 2), the moderator was

> poisoned with varying amounts of boric acid (H_3BO_3). ... The soluble absorber was restricted to the water within the container, while the outside reflector region was left unpoisoned. ... An experiment was performed at one boric acid concentration, poisoned water samples were taken and then additional boric acid was added prior to the next fuel loading.

Boron concentrations of the moderator inside the Plexiglas box are given in Table 2. According to the experimenter,[a] the reported uncertainties in boron concentration "are 1σ as measured analytically by chemists at PNNL." No solution densities were reported.

As indicated in records of the Hanford Environmental Health Foundation (HEHF) analytical laboratory, the boron concentration was measured by atomic absorption. The method, as explained by the director of the laboratory at the time, is the following: Light from a glowing boron filament shines through a mist of the sample heated by a flame. The attenuation of the characteristic wavelengths of boron as the light shines through the sprayed, heated sample is measured electronically. This is done both with calibrated standards, for which a curve of concentration vs attenuation is plotted, and with the samples to be measured. The concentration of the sample is determined from the curve.[b]

Details and discussion of the sample analyses are given in Appendix E.

[a] Personal communication, B. M. Durst, July, 2002.

[b] Personal communication, Maureen Hamilton, HEHF Laboratory Director (retired), July, 2002.

Water temperatures were recorded in logbooks for approximately ten percent of experiments of the entire series reported in the references (References 1-12).[a] Recorded temperatures ranged from 18 to 26 °C, with most values between 20 °C and 25 °C. However, no temperature values were found in the logbook pages for this particular set of experiments.

1.4 Supplemental Experimental Measurements

No supplemental experimental measurements were reported.

[a] This estimate was made by the evaluator in August, 1993, while perusing the logbooks at the Los Alamos National Laboratory Archives.

2.0 EVALUATION OF EXPERIMENTAL DATA

Data in Reference 7, the description of this particular set of experiments, is presented concisely, with minimal additional description. The authors of Reference 7 state (p. vii) that this set of experiments is seventh in a series. References 1-6 (see Section 5), which they also authored, are included in the reference list of Reference 7. The diagram of the fuel rod and information about it is similar to the other references. Therefore, it is assumed that fuel-rod data is the same and experimental conditions are similar to those of other experiments in this series. In particular, it is assumed that full water reflection means the same as previous experiments, namely 30 cm or more of water outside the four sides of the Plexiglas tank.

It was not specified in the report whether uncertainties represented standard deviations or the entire ranges of variables. More information was provided by the experimentalist[a] who said that all uncertainties specified with ± were 1σ uncertainties. In earlier reports of the series, uncertainties were often specified as standard deviations. Computer printouts in the logbooks showed "sigma" of various quantities and "standard deviation." Therefore, it is assumed that all reported uncertainties are standard deviations.

Sensitivity studies described in Sections 2.1 through 2.5 used ONEDANT models with ENDF/B-V 44-group cross sections. The basic model is a slab of a homogeneous mixture of fuel rods and moderator (created by XSDRNPM and CSASIX of SCALE4.4) with 15 cm of borated water on one side, and the Plexiglas tank wall (1.905 cm thick) followed by ~15 cm of water on the other side. The buckling height is 94 cm, the approximate fuel length. The buckling width is 76 cm, the approximate length of each row of rods. The thickness of the slab was adjusted to obtain a k_{eff} of 1.00. The calculations were P_1, S_8, with a convergence criterion of 10^{-6}. (See sample input in Appendix B.) Sensitivity studies described in Section 2.6 used TWODANT with ENDF/B-IV 27-group cross sections.

Results show that the effects of uncertainties are sensitive to boron concentration. Therefore, effects were calculated for all nine cases. Trends in the effects depend on boron concentration and pitch, but the "shape" of the trend depends on the nature of the uncertainty, as can be seen in the tables.

2.1 Tank and Array Dimensions

Tables 6.a and 6.b summarize the effects on k_{eff} of uncertainty in tank and array dimensions.

Critical number of rods - The uncertainty in critical number of rods (indicated as the standard deviation in the logbook) is 0.5%. This uncertainty is modelled as an additional 0.5% thickness of the homogenized fuel-rod slab. The calculated effect on k_{eff} varies from 0.07 to 0.16%.

Pitch - The reported uncertainties in pitch were ±0.002 cm for 1.890 cm pitch and ±0.005 cm for 1.715 cm pitch. The two pitch values recorded in the logbook were 0.744 in. (1.88976 cm) and 0.676 in. (1.71704 cm), which are within the uncertainties. Because the two pitch values were given

[a] Personal communication, B. M. Durst, July, 2002.

as "1.890cm ± .002" and "1.715cm ± .005," and because uncertainties were said to be 1σ uncertainties,[a] it is assumed that the reported pitch uncertainties are the standard uncertainties of the average pitch, not the random spacing uncertainty. The pitch was increased by 0.002 cm for Cases 1-5 and by 0.005 cm for Cases 6-9 in the CSASIX input files that produce cross sections for the homogenized slab. Slab thickness and slab width were also increased by the factor 1.892/1.89 for Cases 1-5 and by 1.720/1.715 for Cases 6-9, to conserve number of rods. Calculated effects of increasing the pitch by the pitch uncertainty are positive in all cases except the two cases at 1.89-cm pitch with the highest boron concentration. The magnitude of the effect of pitch uncertainty varies from 0.02 to 0.29%.

Table 6.a. Effects of Array Standard Uncertainties.

Case	Pitch (cm)	Boron Conc (g/l)	Δk_{eff} (%), Critical Number of Rods (±0.5%)	Δk_{eff} (%), Pitch[(a)]	Combined Δk_{eff} (%) [(b)]
1	1.89	0.0	0.161	0.075	**0.178**
2	1.89	0.49	0.155	0.056	**0.165**
3	1.89	1.251	0.128	0.023	**0.130**
4	1.89	2.15	0.086	-0.015	**0.087**
5	1.89	2.55	0.066	-0.032	**0.073**
6	1.715	0.0	0.143	0.293	**0.326**
7	1.715	1.03	0.132	0.204	**0.243**
8	1.715	1.82	0.110	0.126	**0.167**
9	1.715	2.55	0.088	0.055	**0.104**

(a) Pitch variations are +0.002 cm for Cases 1-5 and +0.005 cm for Cases 6-9.
(b) Square root of sum of squares

Gap between tank wall and array - According to Figure 1, the inside horizontal dimensions of the Plexiglas experiment tank are 75.88 by 79.6 cm. Figure 1 shows the fuel-rod cell boundaries at the inside surfaces of the tank. However, the exact position of the array depends on placement of the polypropylene templates. For holes at pitch 1.89 cm, the distances between the outer cell boundaries of a 40x42-hole array are 75.6 cm and 79.38 cm. These dimensions are 0.28 cm and 0.22 cm less than the tank inner dimensions. Similarly, for holes at pitch 1.715 cm, the distances between the outer cell boundaries of a 44x46-hole array are 75.46 cm and 78.89 cm. These dimensions are 0.42 cm and 0.71 cm less than the tank inner dimensions. The most likely position of the polyethylene templates holding the fuel rods is assumed to be centered in the tank. Therefore gaps equal to half these values are included between the outer cell boundaries and Plexiglas tank walls in the benchmark model.

To estimate the gap standard uncertainty, the full range of the gap is assumed to be the difference between tank inner width and the width, between outer cell boundaries, of the array of holes in the templates. This is because the template may be pushed against one side or the other of the inner tank wall. It is also possible that the outer edges of the template were within the outer cell boundaries of

[a] Personal communication, B. M. Durst, July, 2002.

the arrays of holes. Therefore, the complete ranges of the gap for the two array sizes are taken as 0.22 cm and 0.71 cm. The standard uncertainty of the gap between the right wall of the inner tank and the cell boundary is $0.22/\sqrt{12} = 0.064$ cm for Cases 1 - 5 and is $0.71\sqrt{12} = 0.205$ cm for Cases 6 - 9. The effects of the gap uncertainty were calculated by increasing the gap by 0.5 cm. The effects of the standard uncertainty varied from 0.001% to 0.06% for Cases 1-5 and from 0.002% to 0.2% for Cases 6-9, as shown in Table 6.b.

Tank wall thickness - The uncertainty in the 1.905-cm (3/4-inch) thickness of the Plexiglas experiment tank was not given. The probability distribution for the thickness is assumed to be uniform between bounds equal to 5/8 inches and 7/8 inches. These values are chosen because it is assumed that the wall thickness would have been given as 5/8 or 7/8 inches, if the measurement had been closer to either of those two dimensions. To be sure that the uncertainty is bounding, those values are taken as the extent of the range. (This range is larger than expected, but the effect is small.) Therefore the standard uncertainty is $(7/8\text{-}5/8)/\sqrt{12}$ inches = 0.072 cm. The average change in k_{eff} from increasing and decreasing Plexiglas thickness by 0.072 cm is given in Table 6.b. The effect ranges from 0.006 to 0.02%. Replacing the Plexiglas tank wall with water, which is also shown in Table 6.b, is a negative effect for all cases. The effect on k_{eff} ranges from 0.1% to 0.5%.

Tank wall density - The Plexiglas density was not given. Reference 12 gives 1.18 g/cm^3 as the density of other Plexiglas (acrylic lattice plates). A measured density of common Plexiglas was reported in HEU-SOL-THERM-003 as 1.186 g/cm^3. HEU-MET-FAST-004 reports that the nominal Plexiglas density from the Batelle Pacific Laboratory "Criticality Safety Analysis Sourcebook," (Aug 1977) is of 1.2 g/cm^3. Some MSDS's for various types of Plexiglas[a] gave "Specific Gravity (water=1)" of 1.19 for Plexiglas G, SG, and MC, 1.1 to 1.2 for Plexiglas Q and T, and 1.15 to 1.19 for Plexiglas V, DR, HFI, and MI. A caution given under a Plexiglas description said, "When acrylic sheet is heated to 325 °F it will shrink 2.2%." Considering all this, the complete range is assumed to be from 1.1 to 1.19 g/cm^3. So the standard uncertainty in Plexiglas density is $0.09/\sqrt{12} = 0.026$ g/cm^3. The effects, shown in Table 6.b, are small, <0.02%.

[a] Rohm and Haas chemical company website (~1997).

Table 6.b. Effects of Tank Standard Uncertainties.

Case	Pitch (cm)	Boron Conc (g/l)	Δk_{eff} (%), Gap[(a)]	Δk_{eff} (%), Plexiglas Tank Wall Thickness [(b)] (±0.072 cm)	Δk_{eff} (%), Plexiglas Density Reduced by -0.026/cm^3	Combined Δk_{eff} (%)[(c)]	Δk_{eff} (%), Replace Plexiglas Wall with Water
1	1.89	0.0	-0.001	0.021 (0.020, 0.022)	-0.018	**0.028**	-0.521
2	1.89	0.49	-0.044	0.016 (0.016, 0.015)	-0.014	**0.049**	-0.433
3	1.89	1.251	-0.061	0.013 (0.011, 0.014)	-0.009	**0.063**	-0.296
4	1.89	2.15	-0.042	0.006 (0.006, 0.007)	-0.005	**0.043**	-0.149
5	1.89	2.55	-0.029	0.005 (0.004, 0.007)	-0.003	**0.030**	-0.094
6	1.715	0.0	0.002	0.019 (0.017, 0.022)	-0.016	**0.025**	-0.445
7	1.715	1.03	-0.194	0.012 (0.012, 0.012)	-0.011	**0.195**	-0.330
8	1.715	1.82	-0.204	0.008 (0.009, 0.007)	-0.008	**0.204**	-0.233
9	1.715	2.55	-0.167	0.007 (0.006, 0.007)	-0.005	**0.167**	-0.157

(a) Effect of increasing the gap between fuel-rod cell boundaries and tank wall by the standard uncertainty, 0.064 cm for Cases 1-5 at 1.89-cm pitch and 0.205 cm for Cases 6-9 at 1.715-cm pitch.

(b) The two values in parentheses are the effect of 0.072 cm calculated by two methods: 1) replacing the entire tank wall by water (multiply effect of entire wall by 0.072/1.905), and 2) increasing and decreasing the wall thickness by 0.005 cm (multiply difference by 0.072/0.01). The two values are averaged to give the effect of the standard uncertainty. The two values are different because the effect is not linear over the entire wall thickness, the second value is affected by small mesh differences, and the effect is small compared to the convergence criteria, 10^{-6}.

(c) Square root of sum of squares of the three individual uncertainty effects. (Effect of replacing the tank wall with water is not included.)

2.2 Boron Concentration

The borated water used as moderator in the experiment tank was made by adding H_3BO_3 to water. No impurity analysis of the H_3BO_3 was reported. However the experimentalist said that "the chemical composition of the boric acid was very pure."[a] The boron concentrations in the logbook, which were slightly different from the published values, were shown as only approximate (e.g., "~.4 g/l Boron," "~2.57 g/l B"). Reference 7 says "poisoned water samples were taken." The final boron concentrations were from chemical analyses of the solutions, as confirmed by the lead experimenter and by the former director of the analytical laboratory (see Section 1.3.4). The experimenter also noted that if the boric acid had not been well mixed with the water, they would have observed erratic count rates, "which we did not."[a]

The relative standard deviations of boron concentrations (Table 2) range from 3% to 17%. It is possible that the inconsistency in relative uncertainty might indicate low reliability of the boron analysis. When the experimenter was asked about this and whether he thought that this large a difference in relative uncertainties was reasonable, he replied, "It may be if their chemistry standards were this uncertain. Recall, at that time, they utilized standards, probably with photo-sensitive analytical techniques. If the calibration standards over the ranges measured were this uncertain, it is possible. But, in general, I would have expected all of the calibration standards to have been

[a] Personal communication, B. M. Durst, July, 2002.

prepared with a high degree of accuracy. ... The error bars are as stated by the laboratory which performed the boron analysis. ... If there is an error bar for chemical analysis, it was provided - I didn't calculate it."

Without being able to check the records of the details of the analysis, which were not readily available, the director of the analytical laboratory at that time said that she could not make a definitive judgment about the uncertainties, but she did comment that they "did not seem to be out of line." The analysis of these relatively large concentrations of boron would have been a "special request," which the laboratory received at times from the experimentalists. Multiple measurements or statement of uncertainties may have been part of the special request. She said that the detailed records may still be available in the laboratory archives.[a] (See Appendix E.)

Formula for calculating atom densities - Formula 2.6 in Section 2.3 of LEU-COMP-THERM-015 gives the density of borated water at 22 °C if Cb, the mass of H_3BO_3 added to each liter of water, is known. The formula can be used to derive the borated-water density from the measured boron concentration. (See Appendix C.) Atom densities of the moderator in the benchmark model are calculated from this formula. The differences in atom densities and in k_{eff}'s between using this formula and assuming that the moderator is water at 0.99777 g/cm^3 plus boron at the reported concentrations are shown in Table 7. The effects are small (<0.02%), indicating that lack of knowledge of the correct formula for solution density is probably not significant for this set of experiments. The small differences are used here as estimates of the standard uncertainty in the solution density, which was not measured.

Table 7. Effect of Assuming Constant Water Density with Only Boron Added (Uncertain Moderator Density).

Case	Pitch (cm)	Boron Conc (g/l)	Change in H Atom Density (%)	Change in O Atom Density (%)	Δk_{eff} (%) if density formula[(a)] is not used
1	1.89	0.0	0.00	0.00	—
2	1.89	0.49	-0.02	0.10	**0.004**
3	1.89	1.251	-0.06	0.25	**0.006**
4	1.89	2.15	-0.10	0.43	**0.010**
5	1.89	2.55	-0.12	0.52	**0.011**
6	1.715	0.0	0.00	0.00	—
7	1.715	1.03	-0.05	0.21	**0.009**
8	1.715	1.82	-0.09	0.37	**0.015**
9	1.715	2.55	-0.12	0.52	**0.019**

(a) See Appendix C.

[a] Personal communication, Maureen Hamilton, July, 2002.

Boron concentration and isotopic content - The calculated effects of the reported uncertainties in boron concentration are shown in Table 8. Besides uncertainty in the reported concentration, there is uncertainty in the isotopic content of the boron, which was not measured.[a] The nominal ^{10}B content of boron is 19.9 at.%, with natural variations from 19.1 at.% to 20.3 at.%.[b] Assuming this is the entire range of variation (with uniform distribution, since the actual distribution is unknown[c]), the effect of ±1.2 at.% ^{10}B divided by $\sqrt{12}$ is also given in Table 8, as the uncertainty in isotopic composition of the boron. The total effects on k_{eff} of boron uncertainties are large, varying from 0.4% for Case 7 to 3.0% for Case 4.

Table 8. Effects of Uncertainties in Boron.

Case	Boron Concentration in Moderator ± 1σ (g/liter)	Δk_{eff} (%), Boron Concentration[(a)]	Δk_{eff} (%), Boron Isotopics (±0.6 at.% $^{10}B/\sqrt{3}$)	Total Δk_{eff} (%) from Boron Uncertainties
1	0.0	—	—	—
2	0.49 ±0.06	0.741	0.107	**0.749**
3	1.25 ± 0.21	2.079	0.219	**2.090**
4	2.15 ± 0.35	2.995	0.325	**3.013**
5	2.55 ± 0.07	0.567	0.367	**0.676**
6	0.0	—	—	—
7	1.03 ± 0.05	0.363	0.133	**0.387**
8	1.82 ± 0.30	1.896	0.204	**1.907**
9	2.55 ± 0.21	1.214	0.262	**1.242**

(a) Average of effects of adding and subtracting the uncertainty amount to the nominal value.

[a] Experimentalist Sid Bierman said that if isotopic content of boron had been measured, it would have been reported. (Personal communication, July, 1993)

[b] Nuclides and Isotopes, 14th edition, General Electric Company, 1989, p. 8.

[c] Because the assumed 19.9 at.% ^{10}B is not the midpoint of the range, a unifrom distribution over the entire range is impossible. However this is used as an approximation.

2.3 Fuel-Rod Data

A maximum fuel length of 92.71 cm and a minimum fuel length of 91.44 cm were reported. Using the average of the reported maximum and minimum lengths (92.075 cm), the reported fuel diameter, and the reported average mass of UO_2 per rod, a calculation of density does give the reported average UO_2 density of 10.40 g/cm^3. A sensitivity study that increased the buckling height by half the difference of maximum and minimum lengths (0.635 cm) without changing fuel density shows only a small effect (≤0.03%). The standard uncertainty is this effect divided by √3, assuming a uniform distribution between maximum and minimum lengths. Because fuel length is expected to vary randomly among fuel rods, a better estimate of the random effect is obtained by dividing by √n. Therefore the effect is negligible.

End-plug dimensions and density were reported for uncompressed plugs. A sensitivity study reported in LEU-COMP-THERM-004, used compressed plugs that exactly filled the clad on both ends of the centered fuel region, thereby decreasing the length and increasing the density by ~12%. The calculated effect was 0.01%. This is used as an estimate of the effect of uncertainty in plug density and size.

The uncertainty in fuel diameter was ±0.003 cm, assumed to be 1σ. Increasing the fuel diameter by this amount, with a corresponding change in UO_2 density, gave effects less than 0.01%.

Uncertainties in isotopics of the uranium were 0.013 wt.% for ^{235}U, 0.002 wt.% for ^{234}U and ^{236}U, and 0.017 wt.% for ^{238}U. Because wt.%'s of the uranium isotopes sum to exactly 100% and uncertainty in ^{238}U equals the sum of uncertainties of the other isotopes, it is surmised that ^{238}U was not measured but was taken as balance, with its uncertainty assigned to be the sum of the uncertainties in the other isotopes. When varying enrichment, uranium mass was maintained, with a compensating change in ^{238}U weight percent; the oxygen atom density did not change, although the O:U atom ratio decreased very slightly. Effects of uncertainties in ^{234}U and ^{236}U are assumed to be negligible. The calculated k_{eff} effects of the 0.013-wt.% enrichment uncertainty (1σ) varied from 0.05 to 0.09%.

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.%), all assumed to be 1σ uncertainties. Average mass of UO_2 per rod was increased while maintaining uranium density; therefore only the oxygen in the fuel increased. Similarly, when the amount of uranium per rod was increased, the O:U atom ratio was set to 2, so that the UO_2 density would be minimally increased. (The O:U atom ratio of the benchmark model is 2.017, obtained from using the reported uranium and UO_2 mass per rod.) The effects varied from 0.02 to 0.08% in k_{eff}.

Calculated effects for each of these changes for all cases are given in Table 9.a.

Table 9.a. Effect of Uncertainties in Fuel-Rod Characterization, Δk_{eff} (%).

Quantity (Variation)→ Case ↓	Fuel Length[a] (+0.635cm/√3)	End-Plug Density, Size	Fuel [b] Diameter (+0.003 cm)	Enrichment (+0.013 wt.%) [c]	UO_2 Mass Per Rod [d] (+4.12 g)	U Mass Per Rod (+4.80 g)[e]	Combined Effect [f]
1	0.014	0.01	-0.005	0.046	0.042	0.025	**0.069**
2	0.014	0.01	-0.004	0.056	0.043	0.039	**0.083**
3	0.014	0.01	0.002	0.067	0.042	0.058	**0.100**
4	0.015	0.01	0.007	0.080	0.030	0.074	**0.115**
5	0.015	0.01	0.008	0.088	0.021	0.082	**0.124**
6	0.016	0.01	-0.009	0.042	0.047	0.014	**0.068**
7	0.016	0.01	-0.004	0.057	0.051	0.034	**0.086**
8	0.016	0.01	-0.001	0.066	0.044	0.047	**0.094**
9	0.017	0.01	0	0.073	0.035	0.058	**0.102**

(a) Fuel density is constant. (These values are overestimates, since the variation is probably random among rods.)
(b) Fuel mass is constant.
(c) Constant uranium and oxygen mass.
(d) Constant uranium mass, therefore only oxygen increases.
(e) O:U = 2 (rather than 2.017); therefore minimal density increase.
(f) Square root of sum of squares of individual effects.

For comparison, the UO_2 mass uncertainty was also calculated by keeping UO_2 density and O:U ratio constant and varying first the fuel-pellet diameter and then fuel length. In these calculations, the uranium mass varies along with UO_2 mass, implying a correlation between UO_2 mass and uranium mass uncertainties. Results, which are similar to those in Table 9.a, are shown in Table 9.b for mass of fuel in each fuel pin increased by 4.12 g. Because the O:U ratio and the correlation between UO_2 mass and uranium mass uncertainties are not known, the calculated effect of UO_2 mass uncertainty in Table 9.a, where other reported quantities are kept constant, is used to determine the total uncertainty.

Table 9.b. Effect of +4.12-g/rod UO_2 Mass Increase, Calculated by Increasing Fuel Length or Pellet Diameter.

Case	Δk_{eff} (%) Fuel Length (+0.315cm)	Δk_{eff} (%) Fuel Diameter (+0.0022 cm)
1	0.014	0.027
2	0.014	0.037
3	0.014	0.054
4	0.015	0.068
5	0.015	0.073
6	0.016	0.014
7	0.016	0.033
8	0.016	0.044
9	0.017	0.052

2.4 Reflectors

The stated thickness of the top reflector, which was continuous with the moderator, was 15.2 cm above the ends of the rods. Plugs in the ends of the rods were 2.54 cm long. Therefore the surface of the top reflector was 17.74 cm above the fuel region.

ONEDANT calculations were performed for a slab fuel region with moderator water on one side and the Plexiglas tank followed by a water reflector on the other side. The difference in k_{eff} between 24-cm-thick reflectors and 16-cm-thick ones was less than 0.0001 for the five cases calculated (Cases 1, 3, 5, 6, and 9). This indicates that 17 cm of moderator above the fuel and 20-cm-thick side water reflectors provide essentially full reflection.

Water impurities measured before boron addition to the moderator are given in Table 5. Measured values were small. Water impurity sensitivity studies described in Appendix C of LEU-COMP-THERM-004 indicate that only gadolinium and boron impurities significantly affect k_{eff}. No gadolinium impurity is reported for the water used in this set of experiments. It is assumed that impurities in the reflectors and moderator have negligible effect.

2.5 Temperature

Water temperatures were recorded in logbooks for approximately ten percent of all the experiments of the series described in the references listed in Section 5. Measured temperatures ranged from 18 °C to 26 °C. Effects were calculated for all cases for a 4 °C increase in temperature of cross sections as well as reduction in water density from the density at 22 °C to the density at 26 °C (0.99679 g/cm^3). Two sets of calculations were done, one set with no change in boron atom densities and one set with changes in boron atom densities proportional to the water density change.

The larger effect was for no change in boron, which gave Δk_{eff}'s less than 0.0004. The larger effect is used as the uncertainty, to cover the possibility that the boron analysis was at the experimental temperature, but the experimental temperature was not 22 °C. Since the calculated effect for ±4 °C is assumed to represent the complete range of possible temperatures, the results are divided by √3 to give the standard uncertainty due to uncertain temperature. Results are shown in Table 10.

Table 10. Effect of Standard Uncertainty in Temperature.

Case	Pitch (cm)	Boron Conc (g/l)	Δk_{eff} (%), +4 °C (water only)	Δk_{eff} (%), +4 °C (water and B)	Δk_{eff} (%), Standard Temperature Uncertainty (±4 °C/√3)
1	1.89	0.0	-0.024	-0.024	**0.014**
2	1.89	0.49	-0.032	-0.027	**0.018**
3	1.89	1.251	-0.032	-0.020	**0.018**
4	1.89	2.15	-0.026	-0.007	**0.015**
5	1.89	2.55	-0.023	-0.005	**0.013**
6	1.715	0.0	-0.031	-0.031	**0.018**
7	1.715	1.03	-0.038	-0.030	**0.022**
8	1.715	1.82	-0.037	-0.026	**0.021**
9	1.715	2.55	-0.035	-0.020	**0.020**

2.6 Polypropylene Templates and Plugs

Sensitivity studies described in this section used TWODANT models, with CSASIX ENDF/B-IV 27-group cross sections. (See sample inputs in Appendix B.) A homogeneous mixture, with macroscopic cross sections which are resonance-corrected and cell-weighted by CSASIX to account for fuel diameter, clad thickness, and fuel-rod pitch in the particular moderator, was used to model fuel-rod arrays. The TWODANT calculations were P_1, S_8, with a convergence criterion of 10^{-6}.

A description of the base case is the following: Above the homogenized fuel-rod region is 2.5 cm of plug homogenized with Al clad and moderator, followed by 15.2 cm of moderator. The Plexiglas tank wall is on one side of the rod-array region. Outside the tank wall is 18 cm of water. On the other side of the rod array is 15 cm of moderator water. Below the fuel region is 2.54 cm of plug homogenized with Al clad and polypropylene. Beneath the moderator reflector is polypropylene homogenized with moderator. Plexiglas of thickness 17.8 cm is below the two polypropylene template regions.

Plexiglas slab – It is possible that the Plexiglas slab supporting the experimental tank extended sideways beyond the edges of the experimental tank. This is probably not the case because the diagram in Reference 7 shows the slab only directly beneath the tank, and the wording indicates that the slab is "beneath the container." Nevertheless, the effect of the Plexiglas slab extending into the water reflector was calculated. The calculated effect was <0.002%.

Lower polypropylene template – The effect of the composition of this region is investigated by replacing the homogenized mixture of end-plug and polypropylene 1) with polypropylene, 2) with the end-plug in polypropylene with a small amount of moderator equivalent to the contents of a 0.006-cm gap between plug and template, and 3) with the end plug homogenized with moderator replacing the polypropylene. Results are shown in Table 11. The effect of the 0.006-cm gap, although negligible, is included as the standard uncertainty of the size of holes in the templates. Replacing the bottom end-plug region with pure polypropylene in the model produces a small negative bias in k_{eff}, -0.0001 (-0.0002 for Case 9).

The effect of replacing the lower polypropylene template outside the array region with moderator was negligible (≤0.001%).

Because the lower template was 2.54 cm thick, but the compressed lower end plugs may be less than 2.54 cm long, the effect of a small length of fuel (0.34 cm) extending into the bottom template, with total fuel length constant, is included as an estimate of the standard uncertainty of this possibility. The effect is <0.03%.

The benchmark model includes 0.006-cm gaps between rods and template, so that the diameter of holes in the templates is 1.427 cm. This is similar to holes in grid plates of other experiments of this series, which were no more than 5 mils (0.0127 cm) larger than the rods.[a]

Table 11. Effects of Composition and Uncertainties of Lower Template.

Case	Pitch (cm)	Boron Conc (g/l)	Δk_{eff} (%), 0.006-cm Gap between Template and Rod	Δk_{eff} (%), 0.34-cm Fuel within Lower Template	Combined Δk_{eff} (%)	Δk_{eff} (%), No Lower Template (Plugs and Moderator Only)	Δk_{eff} (%), Lower Template Region Solid Polypropylene
1	1.89	0.0	0.000	0.002	**0.002**	-0.002	-0.005
2	1.89	0.49	0.000	0.007	**0.007**	-0.028	-0.006
3	1.89	1.251	-0.001	0.015	**0.015**	-0.059	-0.009
4	1.89	2.15	-0.002	0.024	**0.024**	-0.084	-0.012
5	1.89	2.55	-0.002	0.028	**0.028**	-0.092	-0.013
6	1.715	0.0	0.000	0.001	**0.001**	-0.002	-0.009
7	1.715	1.03	-0.001	0.012	**0.012**	-0.057	-0.011
8	1.715	1.82	-0.003	0.020	**0.020**	-0.084	-0.014
9	1.715	2.55	-0.004	0.026	**0.026**	-0.103	-0.017

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

Upper polypropylene template – The effect of the upper template is calculated by including a region of fuel rods homogenized, by CSASIX, with polypropylene, rather than with moderator, for a vertical length of 1.27 cm beginning at 67.3 cm above the bottom of the fuel. The calculated effect is relatively large, varying from 0.09 to 0.45% as boron content of the moderator varies from zero to the largest amounts. (See Table 12.) Therefore, the upper polypropylene template is included in the benchmark model.

The effect of a 0.006-cm gap between template and plugs (estimated by assuming the same fraction of the effect of no template as calculated for the lower template) is included in the combined uncertainty. The effect is ≤0.01%.

The effect of extending the upper template into the moderator region next to the array was also ≤0.01%. Therefore, it is not necessary to model the entire upper template.

Effect of top plugs – The effect of replacing the region of the top plugs with moderator was calculated. Results, which were <0.04%, are shown in Table 12. The end plugs are included in the benchmark model.

Table 12. Effects of Upper Template and Top Plugs.

Case	Pitch (cm)	Boron Conc (g/l)	Δk_{eff} (%), Add Upper Template	Δk_{eff} (%), 0.006-cm Gap between Template and Rod	Δk_{eff} (%), Replace Top Plugs with Moderator
1	1.89	0.0	0.094	**0.004**	-0.006
2	1.89	0.49	0.181	**0.003**	-0.017
3	1.89	1.251	0.292	**0.005**	-0.022
4	1.89	2.15	0.404	**0.010**	-0.024
5	1.89	2.55	0.450	**0.012**	-0.025
6	1.715	0.0	0.089	**0.004**	-0.010
7	1.715	1.03	0.207	**0.005**	-0.032
8	1.715	1.82	0.276	**0.008**	-0.035
9	1.715	2.55	0.335	**0.011**	-0.036

2.7 Total Combined Uncertainties and Conclusions of Acceptability

The combined calculated effects on k_{eff} of material and geometrical standard uncertainties are summarized in Table 13.

Table 13. Summary of Δk_{eff} (%) Effects of Material and Geometrical Uncertainties.

Case→ Type of Uncertainty↓	1	2	3	4	5	6	7	8	9
Array	0.178	0.165	0.130	0.087	0.073	0.326	0.243	0.167	0.104
Tank	0.028	0.049	0.063	0.043	0.030	0.025	0.195	0.204	0.167
Moderator Density	—	0.004	0.006	0.010	0.011	—	0.009	0.015	0.019
Boron Conc, Isotopics	—	0.749	2.090	3.013	0.676	—	0.387	1.907	1.242
Fuel Rod	0.069	0.083	0.100	0.115	0.124	0.068	0.086	0.094	0.102
Temperature	0.014	0.018	0.018	0.015	0.013	0.018	0.022	0.021	0.020
Fuel in Lower Template	0.002	0.007	0.015	0.024	0.028	0.001	0.012	0.020	0.026
Gaps in Upper Template	0.004	0.003	0.005	0.010	0.012	0.004	0.005	0.008	0.011
Total Combined Uncertainty	**0.194**	**0.773**	**2.098**	**3.017**	**0.693**	**0.334**	**0.505**	**1.928**	**1.262**

The combined k_{eff} uncertainties of the seven cases with borated water are dominated by the uncertainty in boron concentration. The total combined k_{eff} uncertainties for four cases are especially large, 1-3%. The total k_{eff} uncertainties of the remaining three cases with borated-water are 0.5-0.8%. As can be seen in Table 13, these large uncertainties are due almost entirely to the uncertainty in the amount of ^{10}B in the moderator.

The effect of the boron uncertainty on k_{eff} is not linear over the range of the uncertainty. This is seen by comparing the effect of adding the amount of the uncertainty in boron concentration with the effect of subtracting it for each case. The calculated effects are given in Table 14. Because of the large contribution of the boron uncertainty and because its effect on k_{eff} is not linear, the distribution of k_{eff} for parameter values within their standard uncertainties is not expected to be normal. Therefore, the level of confidence of the 1σ uncertainty in k_{eff} cannot be reliably estimated and may deviate significantly from 68%.

Table 14. Comparison of the Effects of Adding and Subtracting the Uncertainty in Boron Concentration, Δk_{eff} (%).

Case	Δk_{eff} (%) for Adding the Uncertainty in B Conc.	Δk_{eff} (%) for Subtracting the Uncertainty in B Conc.
1	—	—
2	-0.497	0.986
3	-1.863	2.284
4	-2.798	3.168
5	-0.516	0.613
6	—	—
7	-0.203	0.525
8	-1.733	2.049
9	-1.122	1.301

The experiments are good candidates for benchmarks because they were carefully performed, all required experimental data and uncertainties were measured and recorded, and uncertainties for all cases are well-characterized and can be calculated. However, because of the large effect (1-3%) of the 1σ boron concentration on k_{eff} for Cases 3, 4, 8 and 9, these four cases are rejected as benchmark experiments. The other five cases (Cases 1, 2, 5, 6, and 7) may be used as benchmark experiments. However, the user should note that the uncertainties in k_{eff} for the three cases with borated-water moderator are dominated by the boron uncertainty, and the effect of the boron uncertainty on k_{eff} is not linear over its range.

3.0 BENCHMARK SPECIFICATIONS

3.1 Description of Model

The models of the accepted Cases 1, 2, 5, 6, and 7 consist of square-pitched, aluminum-clad cylindrical fuel rods completely submerged in moderator (water or borated water). The fuel rods are arranged in rows inside a Plexiglas tank, which is on a Plexiglas slab. The rows of rods are next to one side of the tank. The last row, farthest from the tank wall, is only partially filled with rods. Beyond the last partial row, only 20 cm of the moderator inside the tank is included; therefore only one side and parts of two sides of the Plexiglas tank are modeled. Outside the tank walls, on 3 sides, is the water reflector.

The polypropylene templates (grid plates), with a 0.006-cm gap between fuel rod and template, are included in the benchmark model only to the outer edge of the last row of pins. Sensitivity studies in Section 2.6 showed that limiting the templates to the fuel-rod region has negligible effect on k_{eff}.

Positions of rods in the last, incomplete row of each model are arbitrary in the sense that critical configurations with these partial rows were not actually built. The number of rods in the last row is extrapolated from configurations containing either full rows or rows that were half filled from one end. Therefore, it may be assumed that the average importance of a rod in the last row is equal to the average importance of a rod in a row filled or half-filled (from one end) with rods. (The average importance of a rod is assumed to be approximately the same for these two cases.) Therefore, in the models the rods in the last row are spread out evenly so that the average importance of a rod is approximately equal to the average importance of a rod in a filled or half-filled row. It is judged that the effect of the small difference between average importance of rods in the last partial row as modeled and average importance of rods in a last filled of half-filled row is negligible.

In other evaluations with these fuel rods (see Section 1.1), the end plugs were shorter in the model than their nominal lengths of 2.54 cm. This was done in order to preserve the total length of the fuel rod and to use the average of the minimum and maximum reported fuel lengths. It was assumed that the end plugs were, therefore, compressed in the ends of the fuel tubes, as was likely true in fact. However, because the lower template thickness is 2.54 cm, in this evaluation the nominal 2.54-cm length of plug is used, with corresponding reduction of density of the compressed plug used in the other benchmark models, by a factor of 2.2225/2.54 = 0.875, where 2.2225 cm is the length of the compressed plug. Because end effects are small, the effect of this modification is estimated to be negligible.

Results of calculations (Section 2.4) showed that 20 cm of reflector on the sides provided essentially full reflection. Because of the thick water reflector on three sides and borated water (moderator) on one side and above the arrays, and the Plexiglas beneath, nothing outside the reflectors is included in the benchmark model. The effect of this simplification is judged to be negligible.

3.2 Dimensions

Fuel-rod dimensions are shown in Figure 5. The rod has an outer diameter of 1.415 cm and is 97.155 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 inner diameter of the clad is 1.283 cm, and the gap between UO_2 and clad is 0.009 cm. The rubber end plugs are 2.54 cm long with a diameter of 1.283 cm, to fit exactly within the ends of the fuel rod.

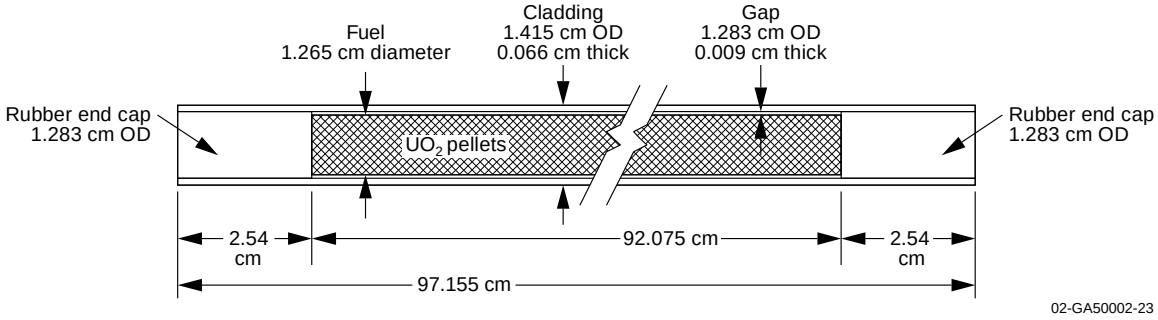


Figure 5. Fuel-Rod Model.

Configuration characteristics of the five accepted benchmark models are given in Table 15 and are shown in Figures 6-9.[a] Each configuration is a square-pitched array inside the Plexiglas tank. The last, partial row is the one farthest from the tank wall, next to the moderator-reflector. The arrays are placed next to one side of the tank. Two other sides of the array are also next to tank walls. The three tank walls are 1.905 cm thick.

Table 15. Critical Configurations.

Case	Pitch (cm)	Boron in Moderator (g/liter)	Width of Rows (rods)	Number of Complete Rows	Number of Rods in Last, Incomplete Row
1	1.890	0.0	40	8	37
2	1.890	0.49	40	10	29
5	1.890	2.55	40	30	37
6	1.715	0.0	44	11	25
7	1.715	1.03	44	16	33

[a] Configuration characteristics for rejected Cases 3, 4, 8, and 9 are given in a table and figure in Appendix D.

The reflector below the fuel rods is 17.8 cm of Plexiglas (acrylic). The Plexiglas extends horizontally to the outer edges of the Plexiglas tank on three sides, and to the outer edge of the moderator-reflector on the remaining side.

The lower polypropylene template rests on the Plexiglas. Bottom plugs of the fuel rods are completely enclosed within the 2.54-cm-thick lower template. The upper template is 1.27 cm thick and is 67.3 cm above the lower one. The edges of the upper and lower templates coincide with the outer cell boundaries of the array. Small gaps are between the templates and the Plexiglas tank walls, as shown in the magnifications in Figures 7 and 8. The two templates do not extend past the last, partial row of the array. Holes in the templates are 0.012 cm larger in diameter than the fuel rods.

The top of the model is the top surface of the upper reflector (water or borated water inside the tank), which is 15.2 cm above the top plugs of the fuel rods. Outside the three tank walls is the water reflector. The top level of the water reflector and tank walls is the same as the top surface of the moderator. The thickness of the water reflector and the moderator (water or borated water) reflector inside the tank is 20 cm.

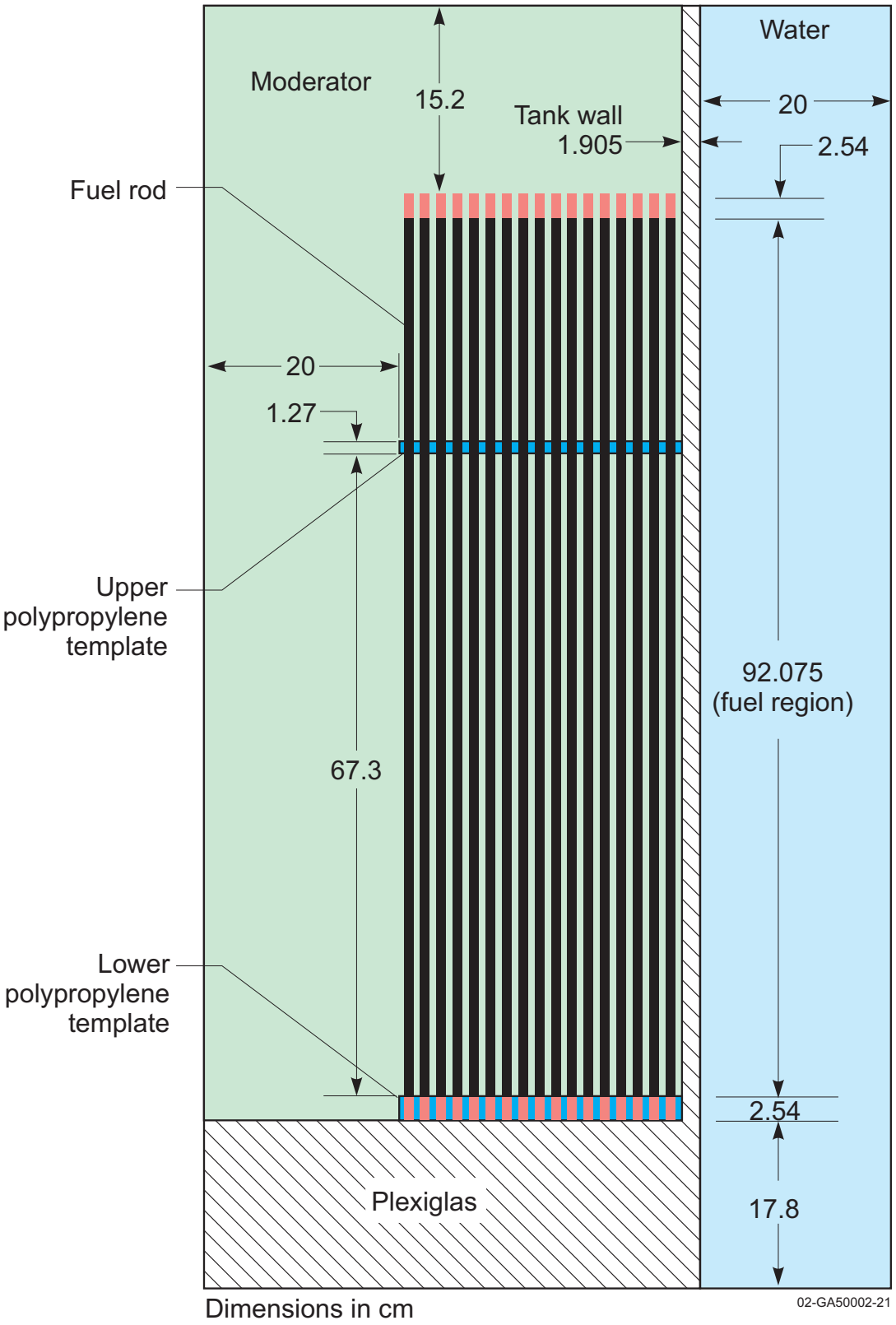


Figure 6. Benchmark Model.

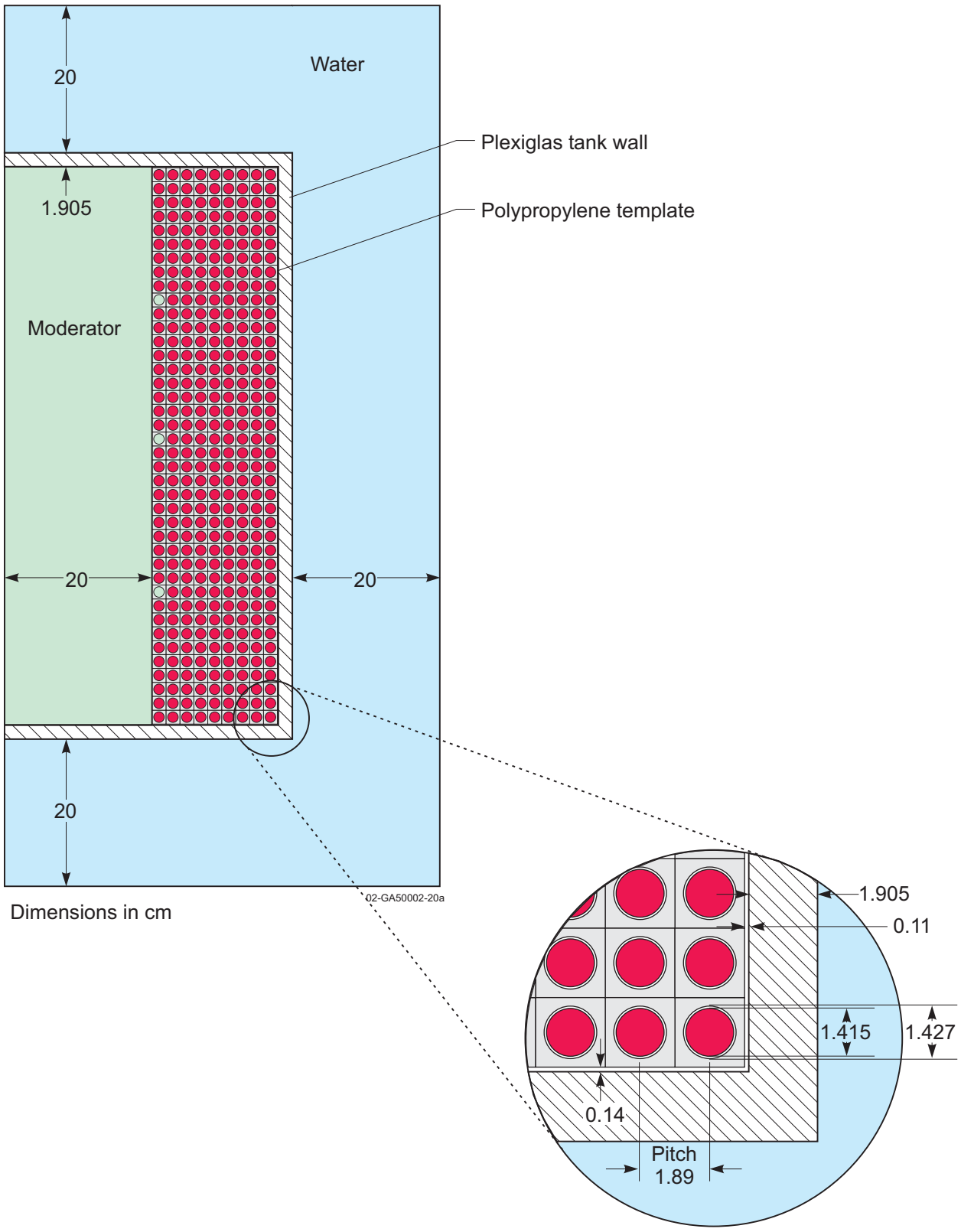


Figure 7. Benchmark Model, Case 1.
(also applies to Cases 2 and 5)

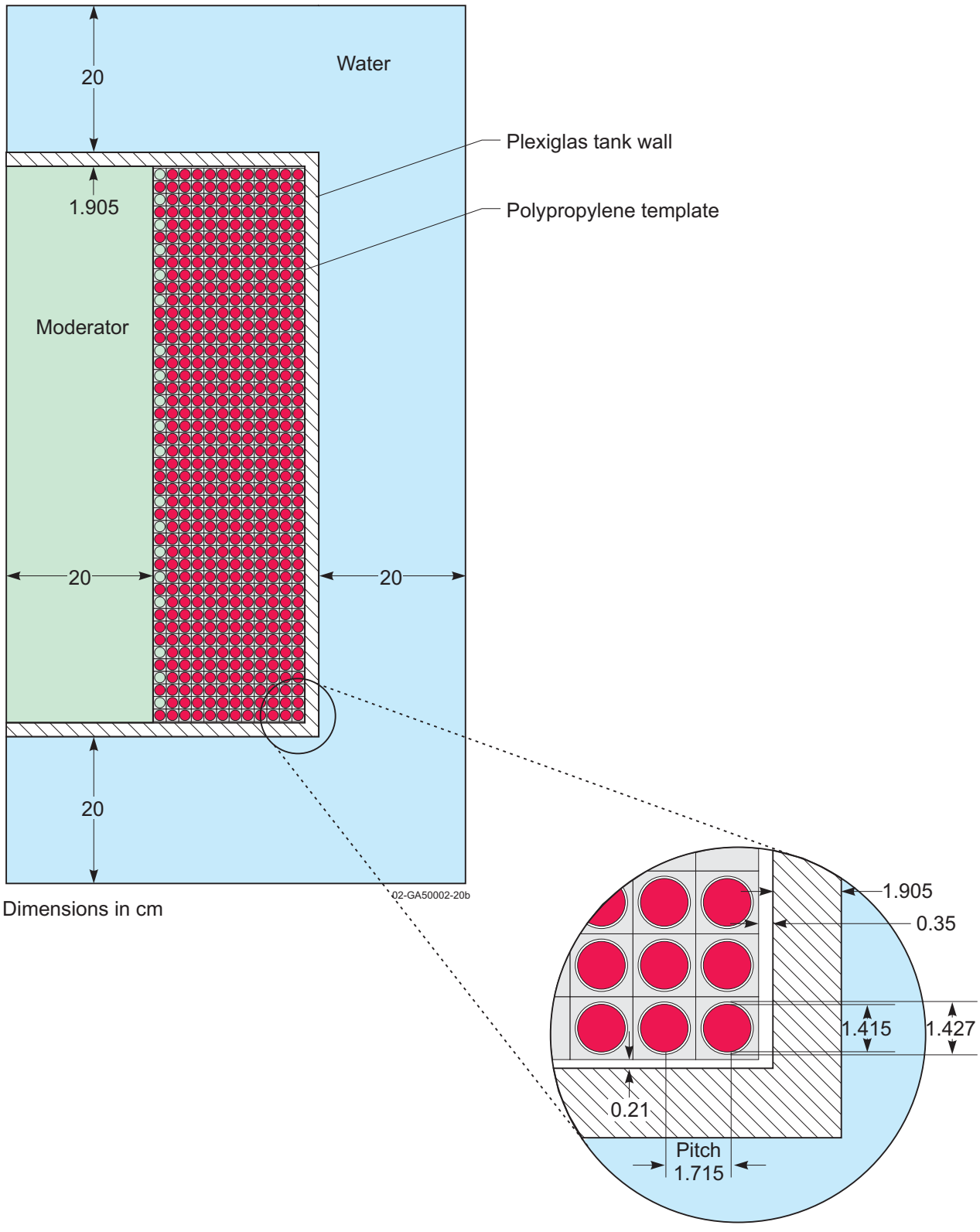


Figure 8. Benchmark Model, Case 6.
(also applies to Case 7)

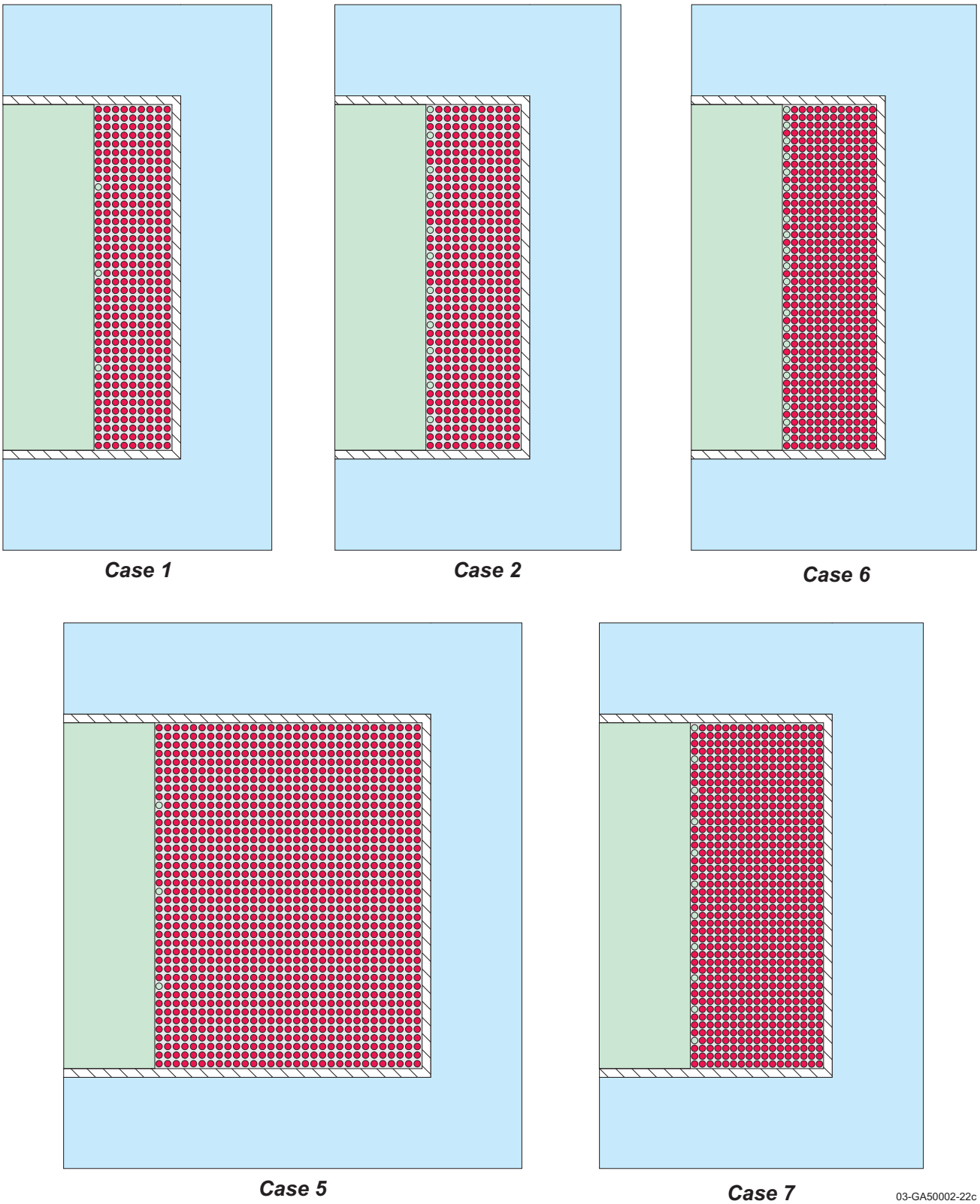


Figure 9. Array Configurations Showing Placement of Rods in Last, Partial Row.

3.3 Material Data

Fuel Rods - The fuel region in each fuel rod 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 (average, nominal composition) and rubber end plugs within the clad. Atom densities are given in Table 16.

Table 16. Fuel-Rod Atom Densities.

Material	Isotope	Atom Density $(barn\text{-}cm)^{-1}$
$U(4.306)O_2$ Fuel	^{234}U	5.1835×10^{-6}
	^{235}U	1.0102×10^{-3}
	^{236}U	5.1395×10^{-6}
	^{238}U	2.2157×10^{-2}
	O	4.6753×10^{-2}
6061-Aluminum Clad ($2.69\ g/cm^3$)	Al	5.8433×10^{-2}
	Cr	6.2310×10^{-5}
	Cu	6.3731×10^{-5}
	Mg	6.6651×10^{-4}
	Mn	2.2115×10^{-5}
	Ti	2.5375×10^{-5}
	Zn	3.0967×10^{-5}
	Si	3.4607×10^{-4}
	Fe	1.0152×10^{-4}
Rubber End Plug ($1.321\ g/cm^3$)	C	3.8415×10^{-2}
	H	5.1303×10^{-2}
	Ca	2.2628×10^{-3}
	S	4.2170×10^{-4}
	Si	8.4975×10^{-5}
	O	1.0989×10^{-2}

Moderator (Borated Water) – Atom densities of the moderator for each case are given in Table 17.[a] Derivation of the densities of the constituents of borated water is given in Appendix C.

[a] Atom densities for the moderator of rejected Cases 3, 4, 8, and 9 are given in Table D.2 in Appendix D.

Table 17. Moderator Atom Densities (atoms/barn-cm).

Case	Boron, g/l	H	O	^{10}B	^{11}B
1	0	6.6706E-02	3.3353E-02	0.0	0.0
2	0.49	6.6691E-02	3.3386E-02	5.4316E-06	2.1863E-05
5	2.55	6.6626E-02	3.3526E-02	2.8267E-05	1.1378E-04
6	0	6.6706E-02	3.3353E-02	0.0	0.0
7	1.03	6.6674E-02	3.3423E-02	1.1418E-05	4.5957E-05

Reflectors and Templates - The Plexiglas (tank wall and slab beneath the tank) has a density of 1.18 g/cm^3. The reflector on three sides outside the tank is water at a temperature of 22 °C. This corresponds to a density of 0.997766 g/cm^3.[a] The reported density of the polypropylene templates is 0.904 g/cm^3. Atom densities are given in Table 18.

Table 18. Template and Reflector Atom Densities.

Material	Isotope	Atom Density (barn-cm)$^{-1}$
Water	H	6.6706×10^{-2}
	O	3.3353×10^{-2}
Plexiglas	H	5.6782×10^{-2}
	C	3.5489×10^{-2}
	O	1.4196×10^{-2}
Polypropylene	C	3.8811×10^{-2}
	H	7.7623×10^{-2}

3.4 Temperature Data

Temperature data were not given. Logbook records for other experiments of the series give temperature data for approximately every tenth experiment. Recorded values vary between 18 °C and 26 °C, with most values between 20 °C and 25 °C. An approximate temperature of 22 °C was used in the model. The effect of uncertain temperature (≤0.02%) is included in the total combined uncertainty of the benchmark-model k_{eff}.

[a] Interpolated between densities at 20 and 25°C, CRC Handbook of Chemistry and Physics, 68th Edition, p. F-10.

3.5 Experimental and Benchmark-Model k_{eff}

The reported configurations were extrapolations from subcritical configurations. Therefore the experimental k_{eff} was 1.000.

Some model simplifications were judged to have negligible effect on k_{eff} (Section 3.1). Experimental uncertainties (Section 2.7, Table 13) contribute to the estimated standard uncertainty in the benchmark-model k_{eff}. Because the total uncertainties of Cases 2, 5, and 7, with borated-water moderator, are dominated by the asymmetric uncertainties in boron concentration (see Section 2.7), the level of confidence for the 1σ benchmark-model uncertainties for Cases 2, 5, and 7 cannot be estimated.

Benchmark-model k_{eff}'s and uncertainties for the five accepted cases are listed in Table 20.

Table 20. Benchmark-Model k_{eff}'s.

Case	Benchmark-Model k_{eff} and Uncertainties
1	1.0000 ± 0.0019
2	1.0000 ± 0.0077
5	1.0000 ± 0.0069
6	1.0000 ± 0.0033
7	1.0000 ± 0.0051

4.0 RESULTS OF SAMPLE CALCULATIONS

Results of calculations of the benchmark models of the five critical configurations with KENO and MCNP are presented in Table 21.[a] Two results, for Case 2, are more than 1% lower than expected. The six results shown in bold font are outside the 1σ uncertainty range, leaving 9 results (60%) within 1σ of the predicted value of 1.000 for k_{eff} of the benchmark models.

The calculated k_{eff} values for two MONK code/cross section combinations are given in Table 21.b. As seen in the U.S. code results, an under-prediction is seen in Case 2. One result, for Case 6, is more than 1% high.

Sample input listings are provided in Appendix A.

Table 21.a. Sample Calculation Results (United States).

Code (Cross Section Set) → Case ↓	KENO (44-Group ENDF/B-V)	KENO (238-Group ENDF/B-V)	MCNP (Continuous Energy ENDF/B-V)
1	**0.9969** ± 0.0005	**0.9938** ± 0.0005	0.9994 ± 0.0003
2	0.9949 ± 0.0005	**0.9812** ± 0.0005	**0.9878** ± 0.0003
5	1.0031 ± 0.0004	0.9997 ± 0.0004	1.0044 ± 0.0004
6	**1.0046** ± 0.0005	0.9981 ± 0.0005	**1.0045** ± 0.0004
7	1.0018 ± 0.0004	0.9962 ± 0.0005	1.0029 ± 0.0004

Table 21.b. Sample Calculation Results (United Kingdom).[(a)]

Code (Cross Section Set) → Case ↓	MONK8B (Continuous Energy JEF2.2)	MONK8B (Continuous Energy ENDFB/VI.3)
1	1.0026 ± 0.0010	0.9940 ± 0.0010
2	0.9907 ± 0.0010	0.9841 ± 0.0010
5	1.0076 ± 0.0010	1.0022 ± 0.0010
6	1.0112 ± 0.0010	0.9997 ± 0.0010
7	1.0061 ± 0.0010	0.9990 ± 0.0010

(a) Results provided by David Hanlon, Serco Assurance.

[a] Tables of calculated results for models of unacceptable Cases 3, 4, 8, and 9 is in Appendix D.

5.0 REFERENCES

1. S. R. Bierman, E. D. Clayton, B. M. Durst, "Critical Separation Between Subcritical Clusters of 2.35 Wt% ^{235}U Enriched UO_2 Rods in Water with Fixed Neutron Poisons," PNL-2438, Batelle Pacific Northwest Laboratories, Richland, Washington, October 1977.

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

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

4. S. R. Bierman, E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 Wt% and 4.31 Wt% ^{235}U Enriched UO_2 Rods in Water at a Water-to-Fuel Volume Ratio of 1.6," NUREG/CR-1547, PNL-3314, Batelle Pacific Northwest Laboratories, Richland, Washington, July 1980.

5. S. R. Bierman, E. D. Clayton, "Criticality Experiments with Subcritical Clusters of 2.35 Wt% and 4.31 Wt% ^{235}U Enriched UO_2 Rods in Water with Steel Reflecting Walls," NUREG/CR-1784, PNL-3602, Batelle Pacific Northwest Laboratories, Richland, Washington, April 1981.

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

7. B. M. Durst, S. R. Bierman, E. D. Clayton, "Critical Experiments with 4.31 Wt% ^{235}U Enriched UO_2 Rods in Highly Borated Water Lattices," NUREG/CR-2709, PNL-4267, Batelle Pacific Northwest Laboratories, Richland, Washington, August 1982.

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

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

10. S. R. Bierman, Criticality Experiments with Neutron Flux Traps Containing Voids," PNL-7167, TTC-0969, UC-722, Batelle Pacific Northwest Laboratories, Richland, Washington, April 1990.

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

12. 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., Vol. **54**, August 1981.

13. 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., Vol. **47**, January 1980.

APPENDIX A: TYPICAL INPUT LISTINGS

A.1 KENO Input Listings

The version of KENO V.a used was SCALE4.4. Results were for 3 million neutron histories (1250 active generations of 2400 neutrons each, after skipping 100 generations).

The following input listings are for the 44-group library.

```
KENO V.a Input Listing for Case 2 of Table 21.a (44-Energy Group
SCALE Cross Sections)

=CSAS25     PARM=SIZE=4500000
CASE 2, 1.89-CM PITCH, 0.49 GB/LITER, 11 ROWS, 29 RODS IN LAST ROW
44GROUPNDF5 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
' BORATED WATER
H  2 0  6.6691E-02 295 END
O    2 0  3.3386E-02 295 END
B-10 2 0  5.4316E-06 295 END
B-11 2 0  2.1863E-05 295 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  3.8117-2 295 END
H-POLY   4 0  5.0906-2 295 END
CA  4 0  2.2453-3 295 END
S   4 0  4.1843-4 295 END
SI  4 0  8.4315-5 295 END
O   4 0  1.0903-2 295 END
' ACRYLIC
H-POLY   5 0  5.6706-2 295 END
C   5 0  3.5489-2 295 END
O   5 0  1.4196-2 295 END
' POLYPROPYLENE
C   6 0  8.9346-6 295 END
H-POLY   6 0  5.6706-2 295 END
'  WATER
H  7 0  6.6706-2 295 END
O  7 0  3.3353-2 295 END
' BORATED WATER
H  8 0  6.6691E-02 295 END
O     8 0  3.3386E-02 295 END
B-10  8 0  5.4316E-06 295 END
B-11  8 0  2.1863E-05 295 END
END COMP
SQUAREPITCH 1.89 1.265 1 2 1.415 3 1.283 0 END
CASE 2, 1.89-CM PITCH, 0.49 GB/LITER, 11 ROWS, 29 RODS IN LAST ROW
READ PARA TME=200 GEN=1350 NPG=2400 NSK=100 NUB=YES XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
```

KENO V.a Input Listing for Case 2 of Table 21.a (44-Energy Group SCALE Cross Sections) (cont'd)

```
 COM=* BOTTOM PLUG IN LOWER TEMPLATE *
 CYLINDER  4 1  0.6415 0 -2.54
 CYLINDER  3 1  0.7075 0 -2.54
 CYLINDER  2 1  0.7135 0 -2.54
 CUBOID    6 1  4P0.945 0 -2.54
UNIT 2
 COM=* FUEL ROD ABOVE LOWER TEMPLATE *
 CYLINDER  1 1  0.6325 67.3 0.0
 CYLINDER  0 1  0.6415 67.3 0.0
 CYLINDER  3 1  0.7075 67.3 0.0
 CUBOID    2 1  4P0.945 67.3 0.0
UNIT 3
 COM=* FUEL ROD WITHIN UPPER TEMPLATE *
 CYLINDER  1 1  0.6325 1.27 0.0
 CYLINDER  0 1  0.6415 1.27 0.0
 CYLINDER  3 1  0.7075 1.27 0.0
 CYLINDER  2 1  0.7135 1.27 0.0
 CUBOID    6 1  4P0.945 1.27 0.0
UNIT 4
 COM=* FUEL ROD ABOVE UPPER TEMPLATE *
 CYLINDER  1 1  0.6325 23.505 0.0
 CYLINDER  0 1  0.6415 23.505 0.0
 CYLINDER  3 1  0.7075 23.505 0.0
 CUBOID    2 1  4P0.945 23.505 0.0
UNIT 5
 COM=* TOP PLUG IN MODERATOR *
 CYLINDER  4 1  0.6415 0 -2.54
 CYLINDER  3 1  0.7075 0 -2.54
 CUBOID    2 1  4P0.945 0 -2.54
UNIT 6
 COM=* FUEL ROD *
 ARRAY 1 3R0
UNIT 7
 COM=* HOLE IN LOWER TEMPLATE, MODERATOR ABOVE *
 CYLINDER  2 1  0.7135 0 -2.54
 CUBOID    6 1  4P0.945 0 -2.54
 CUBOID    2 1  4P0.945 67.3 -2.54
UNIT 8
 COM=* HOLE IN UPPER TEMPLATE, MODERATOR ABOVE, TO TOP OF PLUG *
 CYLINDER  2 1  0.7135 0 -1.27
 CUBOID    6 1  4P0.945 0 -1.27
 CUBOID    2 1  4P0.945 26.045 -1.27
UNIT 9
 COM=* VACANT POSITION IN ARRAY *
 ARRAY 2 3R0
UNIT 10
 COM=* FUEL-ROD ARRAY, COMPLETE ROWS *
 ARRAY 3 3R0
UNIT 11
 COM=* FUEL-ROD ARRAY, PARTIAL ROW *
 ARRAY 4 3R0
GLOBAL
UNIT 12
 COM=* FUEL-ROD ARRAY, MODERATOR, TANK, WATER REFLECTOR *
 ARRAY 5 3R0
 REPLICATE 8 1  0.11 20 0.14 0.14 15.2 0  1
 REPLICATE 5 1  1.905 0 1.905 1.905 0 17.8  1
 REPLICATE 7 1  20 0 20 20 0 0  1
END GEOM
READ ARRAY  ARA=1 NUZ=5  FILL 1 2 3 4 5 END FILL
            ARA=2 NUZ=2 FILL  7 8  END FILL
            ARA=3 NUX=10 NUY=40 FILL 400R6 END FILL
            ARA=4 NUY=40 FILL6 6 6 9 6 6 6 9 6 6 6 9 6 6 6 9 6 6 6
                  9 6 6 6 9 6 6 9 6 6 6 9 6 6 9 6 6 6 9 6 6 9 END FILL
            ARA=5 NUX=2 FILL 11 10 END FILL
END ARRAY
READ PLOT
  XUL=-2 YUL=78 ZUL=70 XLR=66 YLR=-2
  ZLR=70  UAX=1  VDN=-1 NAX=1200 END
END PLOT
END DATA
END
```

```
KENO V.a Input Listing for Case 6 of Table 21.a (44-Energy Group
SCALE Cross Sections)

=CSAS25     PARM=SIZE=4500000
CASE 6, 1.715-CM PITCH, 0 GB/LITER, 12 ROWS, 25 RODS IN LAST ROW
44GROUPNDF5 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
' BORATED WATER
H  2 0  6.6706-2 295 END
O  2 0  3.3353-2 295 END
'B-10 2 0  4.9384-6 295 END
'B-11 2 0  1.9878-5 295 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  3.8117-2 295 END
H-POLY   4 0  5.0906-2 295 END
CA  4 0  2.2453-3 295 END
S   4 0  4.1843-4 295 END
SI  4 0  8.4315-5 295 END
O   4 0  1.0903-2 295 END
' ACRYLIC
H-POLY   5 0  5.6706-2 295 END
C   5 0  3.5489-2 295 END
O   5 0  1.4196-2 295 END
' POLYPROPYLENE
C   6 0  8.9346-6 295 END
H-POLY   6 0  5.6706-2 295 END
'  WATER
H  7 0  6.6706-2 295 END
O  7 0  3.3353-2 295 END
' BORATED WATER
H  8 0  6.6706-2 295 END
O  8 0  3.3353-2 295 END
'B-10 8 0  4.9384-6 295 END
'B-11 8 0  1.9878-5 295 END
END COMP
SQUAREPITCH 1.715 1.265 1 2 1.415 3 1.283 0 END
CASE 6, 1.715-CM PITCH, 0 GB/LITER, 12 ROWS, 25 RODS IN LAST ROW
READ PARA TME=200 GEN=1350 NPG=2400 NSK=100 NUB=YES XS1=YES RUN=YES
END PARA
READ GEOM
UNIT 1
 COM=* BOTTOM PLUG IN LOWER TEMPLATE *
 CYLINDER  4 1  0.6415 0 -2.54
 CYLINDER  3 1  0.7075 0 -2.54
 CYLINDER  2 1  0.7135 0 -2.54
 CUBOID    6 1  4P0.8575 0 -2.54
UNIT 2
 COM=* FUEL ROD ABOVE LOWER TEMPLATE *
 CYLINDER  1 1  0.6325 67.3 0.0
 CYLINDER  0 1  0.6415 67.3 0.0
 CYLINDER  3 1  0.7075 67.3 0.0
 CUBOID    2 1  4P0.8575 67.3 0.0
UNIT 3
 COM=* FUEL ROD WITHIN UPPER TEMPLATE *
 CYLINDER  1 1  0.6325 1.27 0.0
 CYLINDER  0 1  0.6415 1.27 0.0
 CYLINDER  3 1  0.7075 1.27 0.0
 CYLINDER  2 1  0.7135 1.27 0.0
```

KENO V.a Input Listing for Case 6 of Table 21.a (44-Energy Group SCALE Cross Sections) (cont'd)

```
 CUBOID    6 1  4P0.8575 1.27 0.0
UNIT 4
 COM=* FUEL ROD ABOVE UPPER TEMPLATE *
 CYLINDER  1 1  0.6325 23.505 0.0
 CYLINDER  0 1  0.6415 23.505 0.0
 CYLINDER  3 1  0.7075 23.505 0.0
 CUBOID    2 1  4P0.8575 23.505 0.0
UNIT 5
 COM=* TOP PLUG IN MODERATOR *
 CYLINDER  4 1  0.6415 0 -2.54
 CYLINDER  3 1  0.7075 0 -2.54
 CUBOID    2 1  4P0.8575 0 -2.54
UNIT 6
 COM=* FUEL ROD *
 ARRAY 1 3R0
UNIT 7
 COM=* HOLE IN LOWER TEMPLATE, MODERATOR ABOVE *
 CYLINDER  2 1  0.7135 0 -2.54
 CUBOID    6 1  4P0.8575 0 -2.54
 CUBOID    2 1  4P0.8575 67.3 -2.54
UNIT 8
 COM=* HOLE IN UPPER TEMPLATE, MODERATOR ABOVE, TO TOP OF PLUG *
 CYLINDER  2 1  0.7135 0 -1.27
 CUBOID    6 1  4P0.8575 0 -1.27
 CUBOID    2 1  4P0.8575 26.045 -1.27
UNIT 9
 COM=* VACANT POSITION IN ARRAY *
 ARRAY 2 3R0
UNIT 10
 COM=* FUEL-ROD ARRAY, COMPLETE ROWS *
 ARRAY 3 3R0
UNIT 11
 COM=* FUEL-ROD ARRAY, PARTIAL ROW *
 ARRAY 4 3R0
GLOBAL
UNIT 12
 COM=* FUEL-ROD ARRAY, MODERATOR, TANK, WATER REFLECTOR *
 ARRAY 5 3R0
 REPLICATE 8 1  0.35 20 0.21 0.21 15.2 0  1
 REPLICATE 5 1  1.905 0 1.905 1.905 0 17.8  1
 REPLICATE 7 1  20 0 20 20 0 0  1
END GEOM
READ ARRAY  ARA=1 NUZ=5  FILL 1 2 3 4 5 END FILL
            ARA=2 NUZ=2 FILL  7 8  END FILL
            ARA=3 NUX=11 NUY=44 FILL 484R6 END FILL
            ARA=4 NUY=44 FILL 6 9 6 9 6 9 6 6 6 9 6 9 6 9 6 9 6
            9 6 6 6 9 6 9 6 9 6 9 6 9 6 6 6 9 6 9 6 9 6 9 6 9 6 9 END FILL
            ARA=5 NUX=2 FILL 11 10 END FILL
END ARRAY
READ PLOT
  XUL=-2 YUL=78 ZUL=70 XLR=66 YLR=-2
  ZLR=70  UAX=1  VDN=-1 NAX=1200 END
END PLOT
END DATA
END
```

A.2 MCNP Input Listings

MCNP4c was used. MCNP k_{eff} calculations used 2300 generations of 1300 neutrons each (2500 neutrons each for Cases 1-3) after skipping 100 generations.

Cu replaces Zn in the clad, due to nonavailability of Zn cross sections.

Input listings for 2 cases with ENDF/B-V continuous-energy cross sections are given below.

```
MCNP Input Listing for Case 2 (ENDF/B-V) of Table 21.a

LCT14-2, 40x10+29 rod cluster, 0.49 gB/liter, 1.89-cm pitch, LCT15 formula
1   1 0.069930423 1 -6 -44    u=1 $ fuel
2   0 1 -6 44 -45             u=1 $ gap
3   3 0.059751655  45 -46     u=1 $ clad
4   4 0.10267347 6 -45        u=1 $ top plug
5   4 0.10267347 -1 -45       u=1 $ bottom plug
6   2 0.10010462644 46 1 -50      u=1 $ water between grids
7   2 0.10010462644 46 51         u=1 $ water above upper grid
8   2 0.10010462644 46 -47 50 -51 u=1 $ water within upper grid
9   5 0.116434 47 50 -51      u=1 $ upper grid
10  2 0.10010462644 46 -47 -1     u=1 $ water within lower grid
11  5 0.116434 47 -1          u=1 $ lower grid
12  2 0.10010462644 -40 41 42 -43 lat=1 u=2 fill=1:40 1:11 0:0
              1 399r 1 1 1 5 1 1 1 5 1 1 1 5 1 1 5 1 1 1 5 1
                     1 1 5 1 1 5 1 1 1 5 1 1 5 1 1 1 5 1 1 5 $ **
13  0 -10 11 30 -31 2 -7 fill=2 $ rod array
14  5 0.116434 47         u=3 $ polypropylene
15  2 0.10010462644 -47      u=3 $ water-filled hole in polypropylene
16  0 -40 41 42 -43 lat=1  u=4 fill=3  $ polypropylene grid
17  2 0.10010462644 1 -50  u=5 $ water between grids, no rod
18  2 0.10010462644 51     u=5 $ water above upper grid, no rod
19  0 50 -51 fill=4    u=5    $ upper grid, in array, no rod
20  0 -1     fill=4    u=5    $ lower grid, in array, no rod
21  6 0.1064666 -2 3 12 -21 34 -35 $ Plexiglas slab
24  2 0.10010462644 2 -8 32 -33 12 -20 #13   $ borated water
25  6 0.1064666 34 -32 12 -21 2 -8 $ tank wall (-y)
26  6 0.1064666 33 -35 12 -21 2 -8 $ tank wall (+y)
27  6 0.1064666 32 -33 20 -21 2 -8 $ tank wall (+x)
29  7 0.100059 3 -8 36 -34 12 -22   $ water refl (-y)
30  7 0.100059 3 -8 35 -37 12 -22   $ water refl (+y)
31  7 0.100059 3 -8 34 -35 21 -22   $ water refl (+x)
35  0 -12:22:-3:8:-36:37  $ outside

1    pz 0.0      $ bottom of fuel, top of bot plug and template
2    pz -2.54  $ bottom of bottom plug, polypropylene grid, inside of tank
3    pz -20.34 $ bottom of box+Plexiglas slab, water refl
6    pz 92.075   $ top of fuel
7    pz 94.615  $ top of top plug
8    pz 109.815 $ top of water, moderator, tank
10   px 0.0      $ right edge of cluster (cell boundary)
11   px -20.79   $ left edge of cluster, including partial rows **
12   px -40.79   $ side of borated water, left edge of model **
20   px 0.11     $ inner surface of experiment tank
21   px 2.015    $ outer surface of experiment tank
22   px 22.015   $ side of water reflector
30   py 0.0      $ edge of cluster
31   py 75.6     $ edge of cluster
32   py -0.14    $ inner surface of experiment tank
33   py 75.74    $ inner surface of experiment tank
34   py -2.045   $ outer surface of experiment tank
35   py 77.645   $ outer surface of experiment tank
36   py -22.045  $ side of water reflector
37   py 97.645   $ side of water reflector
40   py 0.0      $ cell boundary
41   py -1.89    $ cell boundary
```

MCNP Input Listing for Case 2 (ENDF/B-V) of Table 21.a (cont'd)

```
42   px 0.0      $ cell boundary
43   px 1.89     $ cell boundary
44   c/z  0.945 -0.945 0.6325  $ fuel
45   c/z  0.945 -0.945 0.6415  $ gap
46   c/z  0.945 -0.945 0.7075  $ clad
47   c/z  0.945 -0.945 0.7135 $ hole in grid
50   pz  67.3 $ bottom surface of upper grid
51   pz  68.57 $ top surface of upper grid

imp:n  1 33r 0
kcode  2500 1 100 2400 500000
ksrc  -10.395 38.745 46
c   m1 is U(4.31)O2 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 borated water, B is 0.49 g/liter
m2    8016.50c 3.3386e-2  1001.50c 6.6691e-2
      5010.50c 5.4316E-06 5011.50c 2.1863E-05
mt2   lwtr.01t
c   m3 is 6061 aluminum clad of fuel rods
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 is replaced with Cu, due to no Zn cross sections
      29000.50c 3.0967e-5  14000.50c  3.4607e-4
      26000.50c  1.0152e-4
c   m4 is rubber plug
m4    6000.50c 3.8117e-2  1001.50c 5.0906e-2
      20000.50c 2.2453e-3  16032.50c 4.1843e-4
      14000.50c 8.4315e-5  8016.50c 1.0903e-2
mt4   poly.01t
c   m5 is polypropylene
m5    6000.50c 3.8811e-2  1001.50c 7.7623e-2
mt5   poly.01t
c   m6 is Plexiglas (acrylic)
m6    1001.50c 5.6782e-2  6000.50c 3.5489e-2
      8016.50c 1.4196e-2
mt6   poly.01t
c   m7 is reflector water
m7    8016.50c 3.3353e-2  1001.50c 6.6706e-2
mt7   lwtr.01t
print
```

A.3 ONEDANT/TWODANT Input Listings

Because the benchmark model is 3-dimensional ONEDANT and TWODANT models cannot be provided.

CSASIX, ONEDANT and TWODANT input listings for sensitivity studies are given in Appendix B.

A.4 MONK Input Listings

Each MONK8B calculation, using its standard JEF2.2-based cross section library, employed 1000 superhistories per stage and was run to achieve a precision of 0.0010.

```
MONK Input Listing for Case 1 of Table 21.b

COLUMNS 1 132
* LEU-COMP-THERM-014 Case 1

BEGIN MATERIAL SPECIFICATION
TYPE DICE

NUMBER DENSITY
MATERIAL Fuel
U234 5.1835E-6
U235 1.0102E-3
U236 5.1395E-6
U238 2.2157E-2
O    4.6753E-2

NUMBER DENSITY
MATERIAL Clad
AL   5.8433E-2
CR   6.2310E-5
CU   6.3731E-5
MG   6.6651E-4
MN   2.2115E-5
TI   2.5375E-5
ZN   3.0967E-5
SI   3.4607E-4
FE   1.0152E-4

NUMBER DENSITY
MATERIAL Rubber
C    3.8117E-2
H1   5.0906E-2
CA   2.2453E-3
S    4.1843E-4
SI   8.4315E-5
O    1.0903E-2

NUMBER DENSITY
MATERIAL Moderator
H1   6.6706E-2
O    3.3353E-2

NUMBER DENSITY
MATERIAL Reflector
H1   6.6706E-2
O    3.3353E-2

NUMBER DENSITY
MATERIAL Plexiglas
H1   5.6782E-2
C    3.5489E-2
O    1.4196E-2

NUMBER DENSITY
MATERIAL Polypropylene
C    3.8811E-2
H1   7.7623E-2

USE H1INCH2 FOR H1 IN MATERIAL Plexiglas
USE H1INCH2 FOR H1 IN MATERIAL Polypropylene

END

BEGIN MATERIAL GEOMETRY
@comp_rows=8
```

MONK Input Listing for Case 1 of Table 21.b (cont'd)

```
@width=40
@pitch=1.89

PART 1 NEST
BOX BH2
    [20.0+@pitch] 0.14 0.0
    [@comp_rows*@pitch] [@width*@pitch] 97.155
BOX BH4
    20.0 0.14 0.0
    [(@comp_rows+1)*@pitch] [@width*@pitch] 97.155
BOX M Moderator
    0.0 0.0 0.0
    [20.0+((@comp_rows+1)*@pitch)+0.11] [(@width*@pitch)+(2*0.14)] 112.355
BOX M Plexiglas
    0.0 -1.905 -17.8
    [20.0+((@comp_rows+1)*@pitch)+0.11+1.905] [(@width*@pitch)+(2*(0.14+1.905))] 130.155
BOX M Reflector
    0.0 -21.905 -17.8
    [20.0+((@comp_rows+1)*@pitch)+0.11+1.905+20.0] [40.0+(@width*@pitch)+(2*(0.14+1.905))]
130.155

END

BEGIN HOLE DATA

HOLE 1 ! Fuel Pin
RZMESH
3
0.6325 0.6415 0.7075
3
0.0 2.54 94.615 97.155
3 3 2
1 0 2
3 3 2
4

HOLE 2 ! Square Array
SQUARE
@pitch
[@pitch/2] [@pitch/2]
0.7075 0.7135
-1  4  -3

HOLE 3 !  Lattice Plates
PLATE
0 0 1
4
0.0   7
2.54  4
69.84 7
71.11 4
4

HOLE 4 ! Incomplete Row
LATTICE
1 @width
@pitch
[-@pitch/2] [-@pitch/2]
PINS
0.7075 0.7135
(-1)*9 4 (-1)*10 4 (-1)*9 4 (-1)*9
4
-3

END

BEGIN CONTROL DATA

STAGES -10 1000 1000
STDV 0.0010

END
```

MONK Input Listing for Case 1 of Table 21.b (cont'd)

```
BEGIN SOURCE GEOMETRY

ZONEMAT
ZONE 1 PART 1 / MATERIAL 1
ZONE 2 PART 1 / MATERIAL 1

END
```

```
MONK Input Listing for Case 7 of Table 21.b

COLUMNS 1 132
* LEU-COMP-THERM-014 Case 7

BEGIN MATERIAL SPECIFICATION
TYPE DICE

NUMBER DENSITY
MATERIAL Fuel
U234 5.1835E-6
U235 1.0102E-3
U236 5.1395E-6
U238 2.2157E-2
O    4.6753E-2

NUMBER DENSITY
MATERIAL Clad
AL   5.8433E-2
CR   6.2310E-5
CU   6.3731E-5
MG   6.6651E-4
MN   2.2115E-5
TI   2.5375E-5
ZN   3.0967E-5
SI   3.4607E-4
FE   1.0152E-4

NUMBER DENSITY
MATERIAL Rubber
C    3.8117E-2
H1   5.0906E-2
CA   2.2453E-3
S    4.1843E-4
SI   8.4315E-5
O    1.0903E-2

NUMBER DENSITY
MATERIAL Moderator
H1   6.6674E-2
O    3.3423E-2
B10  1.1418E-5
B11  4.5957E-5

NUMBER DENSITY
MATERIAL Reflector
H1   6.6706E-2
O    3.3353E-2

NUMBER DENSITY
MATERIAL Plexiglas
H1   5.6782E-2
C    3.5489E-2
O    1.4196E-2

NUMBER DENSITY
MATERIAL Polypropylene
C    3.8811E-2
H1   7.7623E-2

USE H1INCH2 FOR H1 IN MATERIAL Plexiglas
USE H1INCH2 FOR H1 IN MATERIAL Polypropylene

END

BEGIN MATERIAL GEOMETRY
@comp_rows=16
@width=44
@pitch=1.715

PART 1 NEST
BOX BH2
    [20.0+@pitch] 0.21 0.0
    [@comp_rows*@pitch] [@width*@pitch] 97.155
```

MONK Input Listing for Case 7 of Table 21.b (cont'd)

```
BOX BH4
    20.0 0.21 0.0
    [(@comp_rows+1)*@pitch] [@width*@pitch] 97.155
BOX M Moderator
    0.0 0.0 0.0
    [20.0+((@comp_rows+1)*@pitch)+0.35] [(@width*@pitch)+(2*0.21)] 112.355
BOX M Plexiglas
    0.0 -1.905 -17.8
    [20.0+((@comp_rows+1)*@pitch)+0.35+1.905] [(@width*@pitch)+(2*(0.21+1.905))] 130.155
BOX M Reflector
    0.0 -21.905 -17.8
    [20.0+((@comp_rows+1)*@pitch)+0.35+1.905+20.0] [40.0+(@width*@pitch)+(2*(0.21+1.905))]
130.155

END

BEGIN HOLE DATA

HOLE 1 ! Fuel Pin
RZMESH
3
0.6325 0.6415 0.7075
3
0.0 2.54 94.615 97.155
3 3 2
1 0 2
3 3 2
4

HOLE 2 ! Square Array
SQUARE
@pitch
[@pitch/2] [@pitch/2]
0.7075 0.7135
-1  4  -3

HOLE 3 !  Lattice Plates
PLATE
0 0 1
4
0.0   7
2.54  4
69.84 7
71.11 4
4

HOLE 4 ! Incomplete Row
LATTICE
1 @width
@pitch
[-@pitch/2] [-@pitch/2]
PINS
0.7075 0.7135
(-1 -1 -1 4)*11
4
-3

END

BEGIN CONTROL DATA

STAGES -10 1000 1000
STDV 0.0010

END

BEGIN SOURCE GEOMETRY

ZONEMAT
ZONE 1 PART 1 / MATERIAL 1
ZONE 2 PART 1 / MATERIAL 1

END
```

APPENDIX B: SAMPLE CSASIX, ONEDANT, AND TWODANT INPUTS FOR SENSITIVITY STUDIES USING HOMOGENIZED FUEL-ROD REGION

B.1 Sample CSASIX and TWODANT Input Listings for Sensitivity Studies

Typical input listings for sensitivity studies reported in Section 2 are given below. Note that in all CSASIX calculations, an outer diameter of the fuel pin's clad of 1.4105 cm, rather than 1.415 cm, was used. This difference is not expected to significantly affect any of the Δk_{eff}'s from the calculations. Several sensitivities were redone. The largest difference in Δk_{eff} was 0.00015 for a large effect, namely, a 2% boron-concentration uncertainty for a case with the smaller pitch.

CSASIX

```
=CSASIX       PARM=SIZE=45000000
LCT14 Case 3
27GR LATTICECELL
' Fuel - U(4.31)02
U-234  1 0  5.1835-6 END
U-235  1 0  1.0102-3 END
U-236  1 0  5.1395-6 END
U-238  1 0  2.2157-2 END
O  1 0  4.6753-2 END
'Case  (boron in borated water)
'2      B-10    5.4316E-06      0.49    g/liter
'       B-11    2.1863E-05
'3      B-10    1.3856E-05      1.25    g/liter
'       B-11    5.5773E-05
'4      B-10    2.3833E-05      2.15    g/liter
'       B-11    9.5930E-05
'5, 9   B-10    2.8267E-05      2.55    g/liter
'       B-11    1.1378E-04
'7      B-10    1.1418E-05      1.03    g/liter
'       B-11    4.5957E-05
'8      B-10    2.0175E-05      1.82    g/liter
'       B-11    8.1205E-05
' Borated water  1.25   gB/liter
H  2 0  6.6706-2 END
O  2 0  3.3353-2 END
B-10 2 0   1.3856E-05 END
B-11 2 0   5.5773E-05 END
' Clad  -  6061 Al
AL  3 0  5.8433-2 END
CR  3 0  6.2310-5 END
CU  3 0  6.3731-5 END
MG  3 0  6.6651-4 END
MN  3 0  2.2115-5 END
TI  3 0  2.5375-5 END
'        (Zn replaced by Cu)
CU  3 0  3.0967-5 END
SI  3 0  3.4607-4 END
FE  3 0  1.0152-4 END
'Plug in borated water
C       4       0       1.5766E-02      END
H       4       0       5.8374E-02      END
Ca      4       0       9.2870E-04      END
S       4       0       1.7307E-04      END
Si      4       0       6.1974E-05      END
O       4       0       2.3228E-02      END
Al      4       0       4.5755E-03      END
Cr      4       0       4.8791E-06      END
Cu      4       0       4.9904E-06      END
Mg      4       0       5.2190E-05      END
Mn      4       0       1.7317E-06      END
Ti      4       0       1.9870E-06      END
'Zn     4       0       2.4248E-06      END
Fe      4       0       7.9494E-06      END
B-10    4       0       7.7563E-06      END
B-11    4       0       3.1220E-05      END
' Borated water  1.25   gB/liter
```

```
H  5 0  6.6706-2 END
O  5 0  3.3353-2 END
B-10 5 0   1.3856E-05 END
B-11 5 0   5.5773E-05 END
' Acrylic (Plexiglas)
H   6 0  5.6782-2 END
C   6 0  3.5489-2 END
O   6 0  1.4196-2 END
' Water reflector  (0.997766 g/cc)
H  7 0  6.6706-2 END
O  7 0  3.3353-2 END
' Polypropylene (CH2) plate
C   8 0  3.8811E-02 END
H   8 0  7.7623E-02 END
'Plug in polypropylene (no gap)
C       9       0       3.7492E-02      END
H       9       0       6.4507E-02      END
Ca      9       0       9.2870E-04      END
S       9       0       1.7307E-04      END
Si      9       0       6.1974E-05      END
O       9       0       4.5100E-03      END
Al      9       0       4.5755E-03      END
Cr      9       0       4.8791E-06      END
Cu      9       0       4.9904E-06      END
Mg      9       0       5.2190E-05      END
Mn      9       0       1.7317E-06      END
Ti      9       0       1.9870E-06      END
'Zn     9       0       2.4248E-06      END
Fe      9       0       7.9494E-06      END
'Polypropylene and moderator
C       10      0       2.1434E-02      END
H       10      0       7.2718E-02      END
O       10      0       1.4971E-02      END
B-10    10      0       6.2038E-06      END
B-11    10      0       2.4971E-05      END
'Plug in polypropylene (gap)
C       11      0       3.7201E-02      END
H       11      0       6.4425E-02      END
Ca      11      0       9.2870E-04      END
S       11      0       1.7307E-04      END
Si      11      0       6.1974E-05      END
O       11      0       4.7607E-03      END
Al      11      0       4.5755E-03      END
Cr      11      0       4.8791E-06      END
Cu      11      0       4.9904E-06      END
Mg      11      0       5.2190E-05      END
Mn      11      0       1.7317E-06      END
Ti      11      0       1.9870E-06      END
'Zn     11      0       2.4248E-06      END
Fe      11      0       7.9494E-06      END
B-10    11      0       1.0390E-07      END
B-11    11      0       4.1821E-07      END
END COMP
SQUAREPITCH 1.89 1.265 1 2 1.4105 3 1.283 0  END
MORE DATA EPS=1.-7 PTC=1.-7 DY=75.6 DZ= 16.86825
AXS=7  END MORE
END
```

TWODANT

```
     1     0     0
LCT14 Case 3 - slab 27 cm wide, no upper template
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r7;
      6r6 2r7;
      2r10 3r9 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
      5r5 6 2r7  t

/ Block 3
 lib=c327.txt savbxs=1
 chivec=.021 .188 .215 .125 .166 .180 .090 .014 .001 18z
 maxord=3 ihm=42 iht=3 ihs=16 ititl=1 ifido=2 i2lp1=1   t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
!eof
     1     0     0
LCT14 Case 3 - slab 27 cm wide, bottom plugs have water gap
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r7;
      6r6 2r7;
      2r10 3r11 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
      5r5 6 2r7  t

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

/ Block 4
```

```
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
!eof
     1     0     0
LCT14 Case 3 - slab 27 cm wide, bottom template solid polypropylene
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r7;
      6r6 2r7;
      2r8 3r8 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
      5r5 6 2r7  t

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

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
!eof
     1     0     0
LCT14 Case 3 - slab 27 cm wide, add Plexiglas slab next to tank
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r6;
      6r6 2r6;
      2r10 3r9 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
```

```
      5r5 6 2r7  t

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

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
!eof
     1     0     0
LCT14 Case 3 - slab 27 cm wide, add upper template
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r7;
      6r6 2r7;
      2r10 3r9 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r10 3r13 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
      5r5 6 2r7  t

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

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

/ Block 6
 edoutf=3
 pted=1 zned=0  t
!eof
     1     0     0
LCT14 Case 3 - slab 27 cm wide, add upper template but not in moderator
/  Block 1
igeom=6 ngroup=27 isn=8 niso=13 mt=13 nzone=13
      im=8 it=84 jm=13 jt=187  maxscm=560000 maxlcm=450000000 t

/  Block 2
xmesh=-14 -1 0 1 26 27 28.905 29.905 46.905
xints=14 4  4 34 4  8  4 12
ymesh=-20.34 -3.54 -2.54 0 1 66.3 67.3 68.57
       69.57 90.47 91.47 93.97 94.97 109.17
yints=17 4 10 4 90 4 10 4 18 4 6 2 14
zones=6r6 2r7;
      6r6 2r7;
      2r10 3r9 6 2r7;
      2r5 3r12 6 2r7;
```

```
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r13 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r12 6 2r7;
      2r5 3r4 6 2r7;
      5r5 6 2r7;
      5r5 6 2r7  t

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

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0 ibt=0 ibb=0
 epsi=0.000001 iitm=60 influx=0 oitm=40 bhgt=76  t

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

B.2 Sample CSASIX and ONEDANT Input Listings for Sensitivity Studies

CSASIX

```
=CSASIX       PARM=SIZE=45000000
LCT14 Case 9
44GR LATTICECELL
' Fuel - U(4.31)02
U-234  1 0  5.1835-6 END
U-235  1 0  1.0102-3 END
U-236  1 0  5.1395-6 END
U-238  1 0  2.2157-2 END
O  1 0  4.6753-2 END
'Case  (boron in borated water)
'2      B-10    5.4316E-06      0.49    g/liter
'       B-11    2.1863E-05
'3      B-10    1.3856E-05      1.25    g/liter
'       B-11    5.5773E-05
'4      B-10    2.3833E-05      2.15    g/liter
'       B-11    9.5930E-05
'5, 9   B-10    2.8267E-05      2.55    g/liter
'       B-11    1.1378E-04
'7      B-10    1.1418E-05      1.03    g/liter
'       B-11    4.5957E-05
'8      B-10    2.0175E-05      1.82    g/liter
'       B-11    8.1205E-05
' Borated water  2.55   gB/liter
H  2 0  6.6706-2 END
O  2 0  3.3353-2 END
B-10 2 0   2.8267E-05 END
B-11 2 0   1.1378E-04 END
' Clad  -  6061 Al
AL  3 0  5.8433-2 END
CR  3 0  6.2310-5 END
CU  3 0  6.3731-5 END
MG  3 0  6.6651-4 END
MN  3 0  2.2115-5 END
TI  3 0  2.5375-5 END
'        (Zn replaced by Cu)
CU  3 0  3.0967-5 END
SI  3 0  3.4607-4 END
FE  3 0  1.0152-4 END
'  Rubber end plug
C  4 0   4.3562-2 END
H   4 0  5.8178-2 END
CA  4 0  2.5660-3 END
S   4 0  4.7820-4 END
SI  4 0  9.6360-5 END
O   4 0  1.2461-2 END
' Borated water  2.55   gB/liter
H  5 0  6.6706-2 END
O  5 0  3.3353-2 END
B-10 5 0   2.8267E-05 END
B-11 5 0   1.1378E-04 END
' Acrylic (Plexiglas)
H   6 0  5.6782-2 END
C   6 0  3.5489-2 END
O   6 0  1.4196-2 END
' Water reflector  (0.997766 g/cc)
H  7 0  6.6706-2 END
O  7 0  3.3353-2 END
' Polypropylene (CH6) plate
H   8 0  1.8088-1 END
C   8 0  3.0147-2 END
END COMP
SQUAREPITCH 1.715 1.265 1 2 1.4105 3 1.283 0  END
MORE DATA EPS=1.-7 PTC=1.-7 DY=75.6 DZ= 16.86825
AXS=7  END MORE
END
```

ONEDANT

```
     1     0     0
lct14 case 9 - base case, slab 41 cm wide
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=150  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.4 41 42.905 43.5 60
xints=20 4  4 80 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=c944.txt savbxs=1
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - add 0.5 cm before Plexiglas
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=9
it=154  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.4 41 41.5 43.405 44 60.5
xints=20 4  4 80 4 4 4  4 30
zones=5 5 9 9 9 5 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - replace Plexiglas with water
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=150  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.4 41 42.905 43.5 60
xints=20 4  4 80 4  4  4 30
zones=5 5 9 9 9 7 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t
```

```
/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - reduce Plexiglas thickness by 0.005 cm
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=150  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.4 41 42.9 43.5 60
xints=20 4  4 80 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - increase Plexiglas thickness by 0.005 cm
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=150  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.4 41 42.91 43.5 60
xints=20 4  4 80 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - increase rods by 0.5%
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=151  maxscm=560000 maxlcm=4500000 t
```

```
/  Block 2
xmesh=-15 -.6 0 0.6 40.6 41.205 43.11 43.7 60.2
xints=20 4  4 81 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - decrease rods by 0.5%
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=150  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-15 -.6 0 0.6 40.2 40.795 42.7 43.3 60
xints=20 4  4 80 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - slab 41 cm wide, 16 cm reflectors
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=152  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-16 -.6 0 0.6 40.4 41 42.905 43.5 58.905
xints=22 4  4 80 4  4  4 30
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t
```

```
/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - slab 41 cm wide, 20 cm reflectors
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=165  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-20 -.6 0 0.6 40.4 41 42.905 43.5 62.905
xints=27 4  4 80 4  4  4 38
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
     1     0     0
lct14 case 9 - slab 41 cm wide, 24 cm reflectors
/  Block 1
igeom=1 ngroup=44 isn=8 niso=9 mt=9 nzone=9 im=8
it=176  maxscm=560000 maxlcm=4500000 t

/  Block 2
xmesh=-24 -.6 0 0.6 40.4 41 42.905 43.5 66.905
xints=32 4  4 80 4  4  4 44
zones=5 5 9 9 9 6 7 7  t

/ Block 3
 lib=bxslib
 chivec=0.005028 0.013931 0.043798 0.152637 0.085317 0.024143 0.114918
        0.126722 0.164684 0.172660 0.082688 0.011741 0.000758 0.000902
        0.000067 0.000006 28z
 maxord=3 ihm=68 iht=3 ihs=25 ititl=1 ifido=2 i2lp1=1 t

/ Block 4
 matls=isos  assign=matls   t

/ Block 5
 ievt=1  isct=1 ith=0 ibl=0 ibr=0
 epsi=0.000001  oitm=50 bhgt=94 bwth=76 t

/ Block 6
 edoutf=0
 pted=0 zned=0  t
!eof
```

APPENDIX C: DERIVATION OF BORATED-WATER DENSITY

From LEU-COMP-THERM-015, the density of borated water made by adding Cb grams of H_3BO_3 to 1 liter of water at 22 °C is $\rho_{bw} = \frac{0.99777 + Cb/1000}{1 + Cb/1920}$ g/cm^3, where 0.99777 g/cm^3 is the density of pure water at 22 °C. This formula can be derived by assuming that the water and H_3BO_3 are "volume-additive" [a] and maintain their "characteristic specific volumes" when mixed. The characteristic specific volume of a substance may be defined as its volume, relative to 1 cm^3 of water at 22 °C, that is maintained when dissolved in water. In this sense, the characteristic specific volume (cm^3/g) of H_3BO_3 is 1/1.92. The numerator of the expression is the mass of 1 cm^3 of water plus the H_3BO_3 added to it, and the denominator is its volume.

The H_3BO_3 concentration in the solution is then its mass divided by volume, or $\frac{Cb/1000}{1 + Cb/1920}$, and the boron concentration is the H_3BO_3 concentration multiplied by R=$\frac{A_{w,B}}{M_{w,H3BO3}}$, the ratio of atomic weight of boron divided by the molecular weight of H_3BO_3.

Let x = Cb/1000, the amount of H_3BO_3 added to 1 cm^3 of water, and let b = the boron concentration, g/cm^3, in the solution (which, for these experiments, has been measured and reported). Then $b = \frac{R\,x}{1 + \frac{x}{1.92}}$, which can be solved for x to obtain $x = \frac{b}{R - \frac{b}{1.92}}$. Substituting this expression for x in the original formula, which, in terms of x is $\rho_{bw} = \frac{0.99777 + x}{1 + x/1.92}$, or $\rho_{bw} = \frac{\rho_w + x}{1 + x/1.92}$, yields an expression for ρ_{bw} in terms of ρ_w, b, and R. That expression is

$$\rho_{bw} = \rho_w - \rho_w \frac{b}{1.92\,R} + \frac{b}{R}.$$

Assuming that the boron is 19.9 at.% ^{10}B, R = 0.174842. This can be used to find the atom densities of solution constituents.

Another way to interpret this result is the following: Since the boron density is b, the H_3BO_3 density is b/R. Since the water and H_3BO_3 maintain their respective specific volumes when mixed, the density of water in the solution (i.e., the mass of water in one cm^3 of solution) is then

$$\rho_w\left(1 - \frac{b}{R} \cdot \frac{1}{1.92}\right).$$

[a] Personal communication, Curtis Jordan, February, 1997.

APPENDIX D: MODEL DESCRIPTION FOR CASES REJECTED AS BENCHMARK MODELS (CASES 3, 4, 8, AND 9)

Recommended models of Cases 3, 4, 8, and 9, are summarized in Table D.1. The models are basically the same as the benchmark models described in Section 3 for cases with the same pitch. Figure 7 applies to Cases 3 and 4. Figure 8 applies to Cases 8 and 9. Individual configurations of the four rejected cases are shown in Figure D.1.

Table D.1. Critical Configurations of Rejected Cases.

Case	Pitch (cm)	Boron in Moderator (g/liter)	Width of Rows (rods)	Number of Complete Rows	Number of Rods in Last, Incomplete Row
3	1.890	1.25	40	14	2
4	1.890	2.15	40	23	3
8	1.715	1.82	44	20	37
9	1.715	2.55	44	27	4

Atom densities for all materials are the same as the benchmark models except for the moderator. Moderator atom densities for these four cases are given in Table D.2.

Table D.2. Moderator Atom Densities (atoms/barn-cm) for Rejected Cases.

Case	Boron, g/l	H	O	^{10}B	^{11}B
3	1.25	6.6667E-02	3.3438E-02	1.3856E-05	5.5773E-05
4	2.15	6.6638E-02	3.3499E-02	2.3833E-05	9.5930E-05
8	1.82	6.6649E-02	3.3477E-02	2.0175E-05	8.1205E-05
9	2.55	6.6626E-02	3.3526E-02	2.8267E-05	1.1378E-04

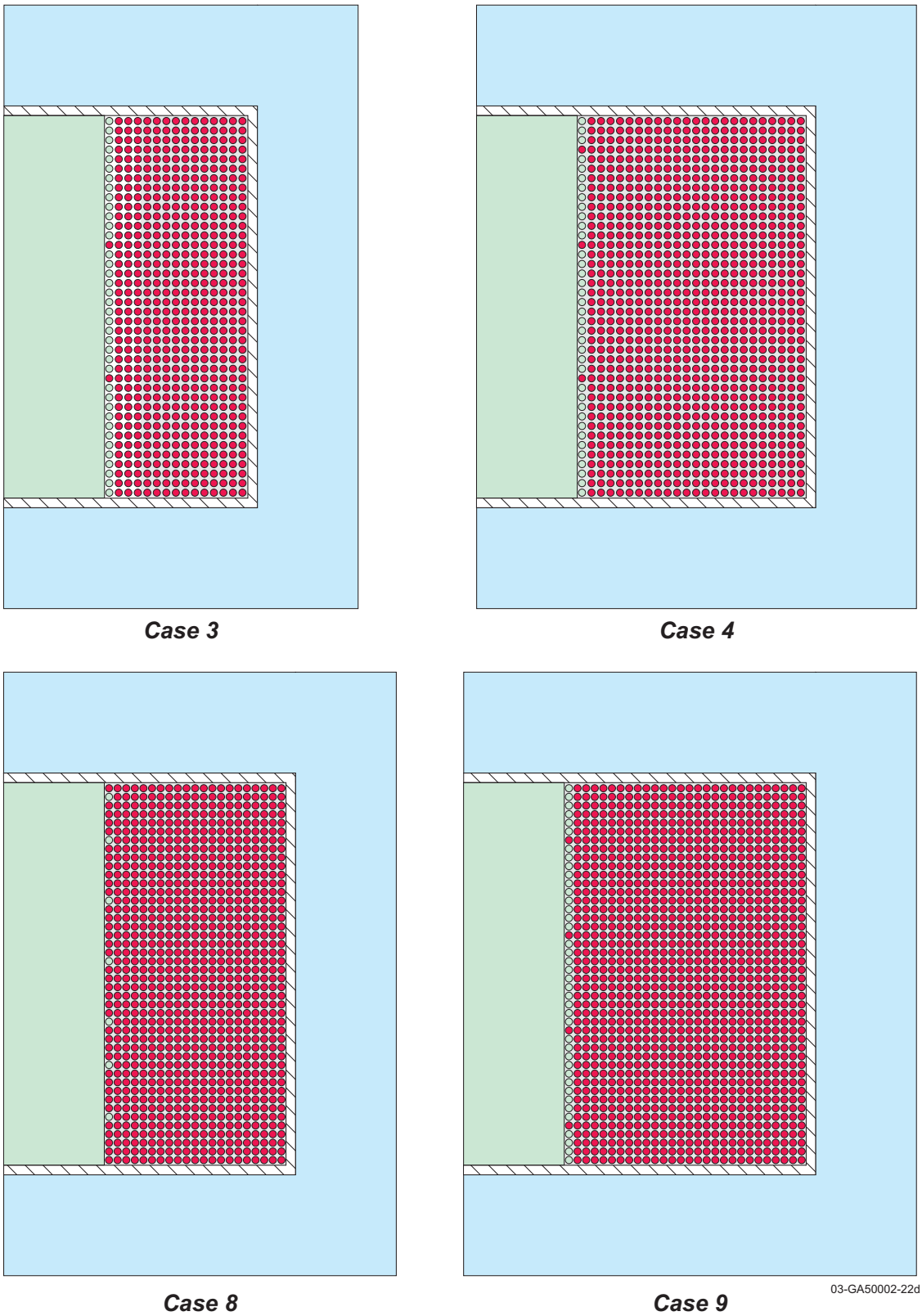


Figure D.1. Array Configurations for Unacceptable Cases, Showing Placement of Rods in Last, Partial Row.

The expected k_{eff} for models of the four rejected cases is 1.000. The combined standard k_{eff} uncertainties, which are greater than 1% (see Section 2), are given in Table D.3. As noted in Section 2.7, k_{eff} is not linear with boron concentration over the range of the uncertainty. Therefore the level of confidence of the uncertainty interval is unknown.

Table D.3. Expected k_{eff}'s and Uncertainties for the Models of Cases with Unacceptably High Uncertainties.

Case	Benchmark-Model k_{eff} and Uncertainty
3	1.0000 ± 0.0210
4	1.0000 ± 0.0302
8	1.0000 ± 0.0193
9	1.0000 ± 0.0126

Sample calculation results for the 4 rejected cases are shown in Tables D.4 and D.5. Note that the result for Case 3 is lower than expected by approximately 2.5%, which is outside its 1σ range of ±2.1%. The reason is not known. The experimenter commented,[a] "It does appear that the third experiment case is low for some reason. Either the boron is misquoted (too high relative to what was actually there), or something else strange is going on. The fact that it seems to appear in several international calculational-result comparisons seems to imply that the error is real. I find it hard to believe that all of the cross-section results could lead to the same low bias." Results for other cases are within 1% of the expected k_{eff}, 1.000.

Table D.4. Sample Calculation Results (United States).

Code (Cross Section Set) → Case ↓	KENO (44-Group ENDF/B-V)	KENO (238-Group ENDF/B-V)	MCNP (Continuous Energy ENDF/B-V)
3	0.9770 ± 0.0005	0.9738 ± 0.0005	0.9791 ± 0.0003
4	0.9980 ± 0.0005	0.9944 ± 0.0004	0.9998 ± 0.0005
8	0.9958 ± 0.0004	0.9909 ± 0.0004	0.9975 ± 0.0004
9	0.9992 ± 0.0005	0.9943 ± 0.0004	0.9996 ± 0.0004

[a] Personal communication, B. M. Durst, July, 2002.

Table D.5. Sample Calculation Results (United Kingdom).[(a)]

Code (Cross Section Set) → Case ↓	MONK8B (Continuous Energy JEF2.2)	MONK8B (Continuous Energy ENDFB/VI.3)
3	0.9816 ± 0.0010	0.9738 ± 0.0010
4	1.0036 ± 0.0010	0.9963 ± 0.0010
8	1.0016 ± 0.0010	0.9935 ± 0.0010
9	1.0037 ± 0.0010	0.9946 ± 0.0010

(a) Results provided by David Hanlon, Serco Assurance.

APPENDIX E: RECORDS OF LABORATORY ANALYSIS OF BORON

Records containing details of the boron analysis from the Hanford Environmental Health Foundation laboratory are included at the end of this appendix.

Reported results in the letter to Mr. Durst, which are the same as reported boron concentrations in the main reference (Table 2 in Reference 7), are shown as the average of two measurement "runs."

Table E.1 shows boron-concentration results for the seven water samples from both runs and their average, as given in the letter to the experimenters from the laboratory. The measurement uncertainty is not specifically given in this letter. Comparing the run values and averages to the report values, the reported 1-σ uncertainty is 0.7 times the difference between the first and second run results. This is from the definition of standard deviation,

$$s = \sqrt{\frac{1}{n-1}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2} = \sqrt{\frac{\left(x_1 - x_2\right)^2}{2}} \cong 0.7\left|x_1 - x_2\right| \text{ when n = 2.}$$

Table E.1. Boron Analysis Results from HEHF Laboratory, March 26, 1982.

Case	Sample Number	1st Run, mgB/ml	2nd Run, mgB/ml	Average, mgB/ml	Report Values, g/l (Reference 7)
2	29	0.53	0.45	0.490	0.49 ±0.06
3	30	1.1	1.4	1.250	1.25 ± 0.21
4	31	1.9	2.4	2.150	2.15 ± 0.35
5	32	2.5	2.6	2.550	2.55 ± 0.07
7	33	1.0	1.07	1.035	1.03 ± 0.05
8	34	1.6	2.03	1.815	1.82 ± 0.30
9	35	2.4	2.7	2.550	2.55 ± 0.21

The date of the "customer order" to "Analyze 7 water solutions for Boron" is 3-4-82. Under "Date Completed" on the "analyst worksheet" are two dates: 3-12-82 and 3-25-82. The letter to the experimenter reporting the results is dated 3-26-82.

According to the "analyst worksheet," the method used was "AA," atomic absorption. (See Section 1.3.4.) It appears that each run was the average of two measurements. On the worksheet, sample results are on the left and standard results are on the right. It appears that the basic measurements were characteristic heights of the absorption spectrum which were converted to mgB/ml by comparison to results from the standard concentrations: 0, 50, 150, 300, 400, and 500 μg/ml. In order that the samples be comparable to the standards, all except the first sample

were diluted to 1/10 their original concentration, as indicated in the second column of the analyst worksheet, with heading "dil".

The graph showing the absorption curves indicates that the standards were measured before and after the sample measurements. Additionally, the absorption of a standard concentration that was close to the sample's value was measured between the two measurements of the sample. The graph included in the laboratory records appears to be the absorption curves for the first run.

Table E.2 shows the boron-absorption curve heights recorded on the analyst worksheet for both the samples and for the standard concentrations.

Table E.2. Heights of Boron-Absorption Curves.

Case	dilu-tion	Measured B-absorption curve height (a)	Measured B-absorption curve height (a)	Standard Conc (μg/ml)	Measured B-absorption curve heights (a)	Recorded Average B-abs curve height	Calculated Average
First Run - March 12, 1982							
2	-	28.3	29.1	50	4.0, 4.4	4.2	4.2
3	1/10	6.2	6.9	150	8.7, 9.5, 9.7, 9.6	9.4	9.372
4	1/10	12.2	12.0	300	16.9, 17.2, 17.3, 17.2, 17.4	17.2	17.2
5	1/10	15.4	14.9	400	22.4, 21.8, 22.4	22.2	22.2
7	1/10	6.4	6.4	500	26.9, 27.3, 28.2	27.5	27.4667
8	1/10	10.7	9.7				
9	1/10	15	14.7				
Second Run - March 25, 1982							
2	-	26.9	26.9	50	2.8, 3.9	3.3	3.35
3	1/10	7.0	7.8	150	7.0, 11.9	9.4	9.45
4	1/10	13.1	13.4	300	14.2, 19.2	16.7	16.7
5	1/10	14.4	14.9	400	20.7, 24.7	22.7	22.7
7	1/10	4.2	6.9	500	26.0, 32	29	29
8	1/10	11.9	9.5				
9	1/10	15.2	15.4				

(a) Arbitrary units from graph paper of the plot of the boron-absorption curves.

The last graph shows two plots of the average heights of the standard concentrations plotted on different scales. These average heights are the last numbers in the last column of the first page of the analyst worksheet. Curves that each seem to approximate a least-squares fit are drawn through the origin and the points. It appears that the sample concentrations are obtained from the recorded heights of the sample absorptions by using the curves. However, not all sample concentration values on the analyst worksheet could be obtained by use of the curves. It appears that perhaps some other procedure was used to obtain concentrations from absorption-curve heights.

The absorption curves and plots of the average heights of the standard concentrations for the second run are not included in these laboratory records.

Table E.3 shows the 4 boron concentrations recorded on the analyst worksheet, along with their derived average and standard deviation. It appears that, in almost all cases, the two measurements from a single run are correlated. Also note that all measured values except 3 in the second run are higher than both measured values of the same sample in the first run.

Table E.3. Four Values of Boron Concentration (mgB/ml) for Each of the Seven Samples.

Case	1st Run, 1	1st Run, 2	2nd Run, 1	2nd Run, 2	Average of 4 measurements	Standard deviation	Standard deviation of mean [(a)]	Report Values, g/l (Reference 7)
2	0.52	0.535	0.445	0.445	0.48625	0.05	0.042	0.49 ± 0.06
3	1.03	1.17	1.32	1.47	1.2475	0.19	0.164	1.25 ± 0.21
4	1.95	1.92	2.35	2.42	2.16	0.26	0.227	2.15 ± 0.35
5	2.55	2.45	2.60	2.67	2.5675	0.09	0.080	2.55 ± 0.07
7	1.00	1.00	0.82	1.32	1.035	0.21	0.180	1.03 ± 0.05
8	1.70	1.53	2.32	1.75	1.825	0.34	0.297	1.82 ± 0.30
9	2.47	2.40	2.71	2.75	2.5825	0.17	0.150	2.55 ± 0.21

(a) Calculated from the formula $u = \sqrt{\frac{1}{n(n-3)}\sum_{i=1}^{n}\left(x_i - \bar{x}\right)^2}$, with n=4. See ICSBEP Uncertainty Guide.

HANFORD ENVIRONMENTAL
HEALTH FOUNDATION

March 26, 1982 CO 6812

Mr. B. M. Durst
Pacific Northwest Laboratory
209E/200E

BORON ANALYSES

The results of the 7 water samples analyzed for boron are following:

	mg/mL Boron		
Sample	1st Run	2nd Run	Average
SSC-43-00-174	0.53	0.45	0.49
-175	1.1	1.4	1.25
-176	1.9	2.4	2.15
-177	2.5	2.6	2.55
-179	1.0	1.07	1.03
-180	1.6	2.03	1.87
-181	2.4	2.7	2.55

If you have any questions, please contact Environmental Health Sciences.

P. A. Swoboda
Environmental Health Sciences

bis

KADLEC MEDICAL – DENTAL BUILDING / P. O. BOX 100, RICHLAND, WASHINGTON 99352

HANFORD ENVIRONMENTAL HEALTH FOUNDATION

CUSTOMER ORDER

ORDER NO. 6821

DATE 2-4-82 | CONT. PAGE

CUSTOMER PNL

ADDRESS 3745/300E

CONTACT Mike Wust | PHONE 3-5443 | CUSTOMER ORDER NO.

DESCRIPTION OF SERVICES:

Analyze 7 water solutions for Boron

EQUIPMENT USAGE				
DATE	DESCRIPTION	HRS.	RATE	TOTAL

LABOR CHARGES				
DATE	EMPLOYEE	HRS.	RATE	TOTAL
2/12	R H Sorbeta	3.0		

MATERIALS AND SUPPLIES				
DATE	DESCRIPTION	QTY.	PRICE	TOTAL

OTHER COSTS		
DATE	DESCRIPTION	TOTAL

ORDER ACCEPTED BY: | ASSIGNED TO:

COST QUOTATION

BY

BASIS OF QUOTE

JOB COMPLETED (DATE) 2/12

JOB CLOSED BY [illegible signature]

ACCOUNTING USE ONLY	
LABOR	
EQUIPMENT USAGE	
MATERIALS AND SUPPLIES	
OTHER COSTS	
TOTAL	

BD-8800-357 (3-72)

DOE Richland, WA

QC Entered	Y	N
	(NA)	
QC OK	Y	N

ANALYST WORKSHEET

Log Sample Nos.	Received From:	Customer Order:
E82-3-29→35	RHO - ~~[illegible]~~ Mike Durst	6812

Type of Sample:	Desired Analysis:	Method Used:	Date Received
water	Boron	AA	

ANALYTICAL RESULTS:

[illegible]	dil	peak ht	peak ht	μg/ml alig.	total μg/ml	mg/ml
29	–	28.3 29.1		52	520 535	0.53
30	1/10	6.2 6.9		95 103 113	1100	1.1
31		12.2 12.0		195 192	1940	1.9
32		15.4 14.9		255 245	2500	2.5
33		6.4 6.4		100	1000	1.0
34		10.7 9.7		170 153	1615	1.6
35	↓	15 14.7		247 240	2435	2.4

μg/ml	ht					
0	–					
50	4.0	4.4			4.2	
150	8.7	9.5	9.7	9.6	9.1	
300	16.9	17.2	17.3	17.2	17.4	17.2
400	22.4	21.8	22.4		22.2	
500	26.9	27.3		28.2	27.5	

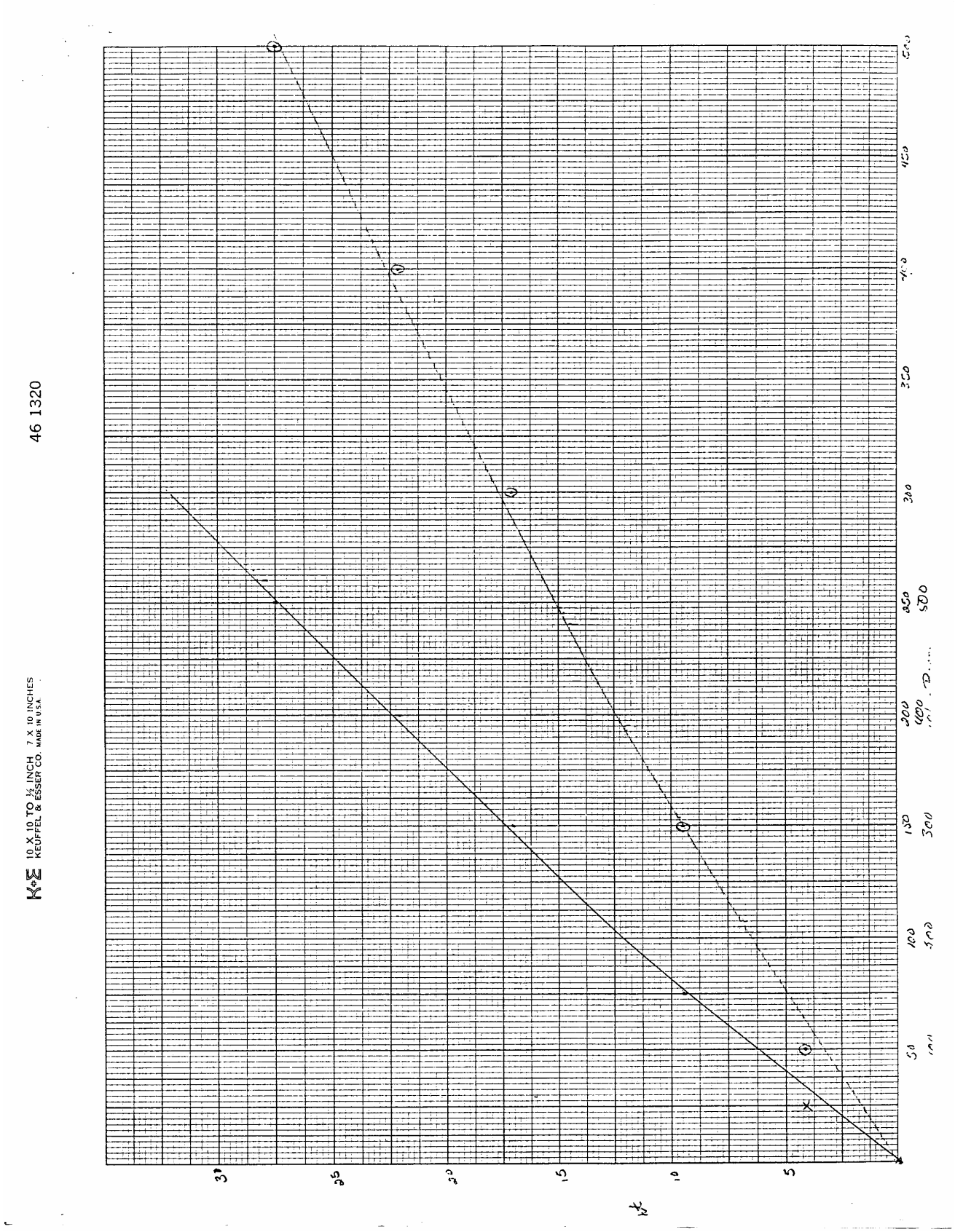
over

Comments:	Date Completed:	Analyst:	Approved By:
	3-12-82 3-25-82	pas	MKH.

Sol. #	dil	ppt	aliq. μg/ml	μg/ml B	std ppt
29	—	24.9 26.9	445	.45	27
30	1/10	2.0 7.8	132 147	1.4	11.8
31	↓	13.1 13.4	235 242	2.4	9.0
32		14.4 14.9	260 267	2.6	19.1
33		4.2 6.9	82 132	1.07	3.9
34		11.9 9.5	332 175	2.03	
35		15.2 15.4	271 275	2.7	9.8

FE
Boron (3ox)

μg/ml	ppt
0	—
50	2.8 3.9
150	7.0 11.9
300	14.2 16.7
400	20.7 24.7 22.7
500	26.0 32 29


46 1320
KE 10 X 10 TO ½ INCH 7 X 10 INCHES
KEUFFEL & ESSER CO. MADE IN U.S.A.