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IDENTIFICATION NUMBER: HEU-SOL-THERM-034 SPECTRA

KEY WORDS: acceptable, acrylic, critical experiment, Lucite®, PMMA, slab, solution, uranium oxyfluoride, uranyl fluoride, uranyl oxyfluoride, water-moderated, water-reflected

1.0 DETAILED DESCRIPTION

1.1 Overview of the Experiment

A series of ten experiments were conducted at the Oak Ridge National Laboratory Critical Experiment Facility in December 1955 and January 1956 in an attempt to determine critical conditions for a slab of infinitely reflected aqueous uranium oxyfluoride (UO_2F_2). These experiments were recorded in an Oak Ridge Critical Experiments Logbook[a] and results were published in a journal of the American Nuclear Society, *Nuclear Science and Engineering*, by J. K. Fox, L. W. Gilley, and J. H. Marable (Reference 1).

The purpose of these experiments was to obtain the minimum critical thickness of an effectively infinite slab of UO_2F_2 solution by extrapolation of experimental data. To do this a slab-tank was manufactured, the slab thickness was varied, and critical solution and water-reflector heights were measured using two different fuel solutions. Of the ten conducted experiments eight of the experiments reached critical conditions but the results of only six of the experiments were published in Reference 1.

All ten experiments were evaluated from which five critical configurations were judged as acceptable criticality safety benchmark experiments. The total uncertainty in the acceptable benchmark experiments is between 0.19 and 0.27 % $\Delta k/k_{eff}$. Evaluations of aqueous solutions of UO_2F_2 fuel for large unreflected spheres are reported in HEU-SOL-THERM-043, reflected spheres in HEU-SOL-THERM-010, HEU-SOL-THERM-011 and HEU-SOL-THERM-012, and aluminum cylinders of UO_2F_2 solution are evaluated in HEU-SOL-THERM-050.

1.2 Description of Experimental Configuration

The ten experiments using aqueous uranium oxyfluoride in a slab configuration were recorded in the logbook as Experiments 103 through 112. During these experiments, UO_2F_2 was introduced incrementally into a 3/4-inch-thick Lucite® or plastic (terms used interchangeably, the registered trademark notation was not used in Reference 1 or the logbook entries) slab tank with nominal inner dimensions of 58-inches across, 71-inches tall, and 2.25-inches wide while varying the height of the water reflector around the box. A safety blade, source, and selsyn motor were referred to in Reference 1 and/or the logbook but no detailed information regarding this equipment was given. The critical level of the solution was measured after each addition or removal of solution and/or reflector material. Because of the continuous change in solution and reflector height and box deformation, critical conditions were met several times during each experiment. In order to vary the slab thickness, Lucite® inserts were placed adjacent to one of the inside surfaces. "In some instances the slab thickness was measured with gauge

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, http://www-rsicc.ornl.gov/rsiccnew/criticallist.htm, (last accessed on June 23, 2010).

blocks" (Reference 1). Liquid height measurements were made using a finely controlled selsyn motor sensor mechanism. Throughout the ten experiments there was a noticeable deformation of the box due to the hydrostatic forces of the water reflector. Changes in experimental setup were made to mitigate this problem.

A schematic of the experimental setup at the beginning and the end of the experimental series can be found in Figure 1.

A critical configuration was achieved in only some of the experiments; however, all experiments are summarized in this section to preserve all aspects of this experimental series. All measurements in Section 1.2 are given in the same form and with the same units as were reported in the logbook or Reference 1 unless noted otherwise. See Section 2.0 for a summary of which experiments achieved critical configurations and were used in this study.

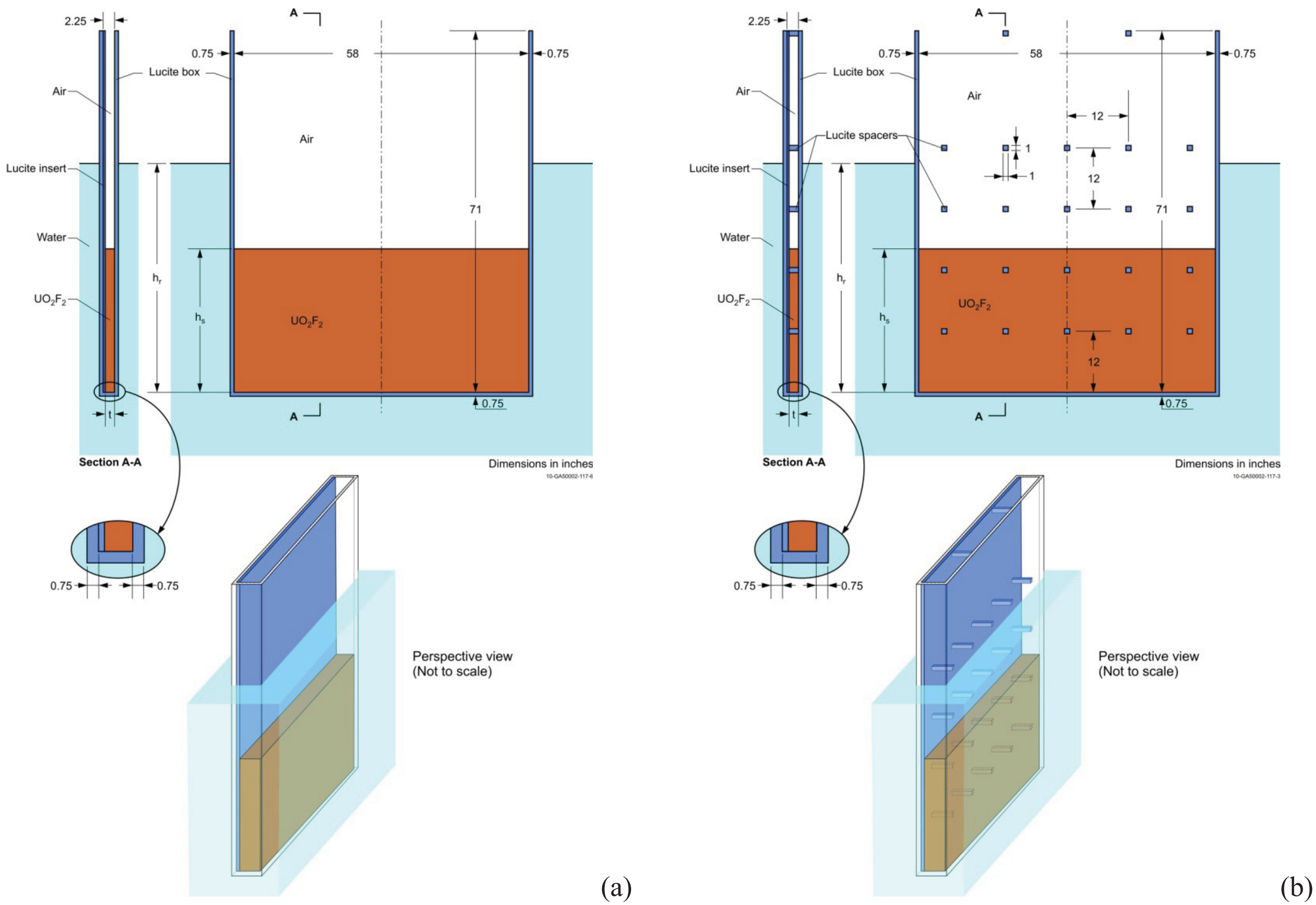

Figure 1. (a) Initial Experimental Setup (b) Final Experimental Setup.

1.2.1 Experiment 103

Experiment 103 was conducted on December 15, 1955, with a slab thickness of 2.25-inches and a reported H/X ratio of 44.7. First, equipment checks were completed and then the selsyn probe zeros were recorded. True fuel height can be obtained by adding 5.47-inches to the selsyn reading and for the true water reflector height 15 3/16 in. or 38.3 cm must be added to the selsyn reading. In later experiments this value is changed to 41 cm. Finally a critical solution height was found while the safety blade was inserted into the solution approximately 5-inches. No description of the safety blade or its position was recorded. Table 1 contains the data obtained during Experiment 103.

Table 1. Experiment 103 Results.

Selsyn Solution Height (in.)	Calculated Solution Height[(a)] (in.)	Experimenter Remarks
23.38	38.57	slightly super
23.34	38.53	" "
23.30	38.49	slightly super
23.29	38.48	just critical
water height	113.7 cm	
Temp.	76 ^{o}F	

(a) Solution heights were calculated by adding 15 3/16 in. to the selsyn solution height.

1.2.2 Experiment 104

Experiment 104 was conducted on December 16, 1955, with a slab thickness of 2 ¼-inches and a reported H/X ratio of 44.7. Instead of finding a critical configuration, counts were measured for various solution heights. Table 2 shows the recorded measurements.

Table 2. Recorded Data from Experiment 104.

Solution Height – selsyn (in)	C_1	C_2
36.24	$5^{\underline{11}}$ x 64	$65^{\underline{9}}$ x 64
36.21	$5^{\underline{48}}$	85
36.21	$4^{\underline{34}}$	$66^{\underline{14}}$
31.49	$5^{\underline{40}}$	$65^{\underline{32}}$ (smudged)
22.16	$4^{\underline{43}}$	$64^{\underline{56}}$ (smudged)

It is unclear from Reference 1 or the logbook what the count measurement notation in Table 2 means. Table 2 was included in this report only to preserve experimental results.

1.2.3 Experiment 105

Experiment 105 was conducted on December 19, 1955, with a slab thickness of ~2 1/8-inches and a solution with a 44.7 H/X ratio. The safety blade was zero at 202.9.[a] The source was out. It is noted at the bottom of logbook page 250 that 41 must be added to the water height to get the correct reading (38.3 had been crossed out and 41 written over).[b] Table 3 contains the results from this experiment.

Table 3. Recorded Data From Experiment 105.

Solution Height (in.)	H_2O Height - sight glass reading (cm)	Experimenter Remarks
28.44-in.	75.6	super
28.30-in.	"	super
28.19-in.	"	slightly super
28.13-in.	"	" sub.
28.18-in.	"	just crit.

1.2.4 Experiment 106

Experiment 106 consists of a solution with a reported H/X ratio of 44.7 in a 2.0-inch thick slab. Counts were measured for various solution heights with the source in the solution. After a few measurements it was found that the counters were too far away to give a true M^{-1} curve. The counters were relocated after which the experiment was continued. The recorded data are given in Table 4.

[a] Units were not reported and are not important for this evaluation.
[b] Units were not reported for the water height correction factor during Experiment 105 but were reported as being in cm during other experiments.

Table 4. Recorded Data from Experiment 106.

Solution Height (in.)	H_2O height reading (cm)	C_4	M^{-1}_4	C_5	M^{-1}_5
46.48		$9^{\underline{13}\ x64}$, $8^{\underline{54}}$	--	$14^{\underline{0}\ x64}$, $14^{\underline{40}}$	--
43.00		$9^{\underline{32}}$	--	$14^{\underline{28}}$	--
37.66		--	--	--	--
29.48		--	--	--	--
20.13	24.5 cm	$24.25^{\ x\ 64}$	--	$62.75^{\ x\ 64}$	--
"	"	23.25	--	62.5	--
25.13	38.2 cm	$33.0^{\ x\ 64}$	0.728	$94.25^{\ x\ 64}$	0.665
"	"	35.25, 36.0	0.676	76.5, 92.15	0.664
33.09	58.7	61.5, 58.25	0.404	163.0, 166.25	0.373
38.05	72.6 cm	116, 117.25	0.206	249, 25.25 (unclear)	0.249
41.77	87.0 cm	180.75, 171.25, 170.25	0.137	347.5, 372.5, 365.75	0.120 (unclear)
43.88	88.0 cm	421, 443	0.0542	760, 810	0.0776 (unclear)
44.02	112.0	152	0.158	360	0.174
44.775	112.0	--	--	--	--
44.90	139.0	$100^{\ x64}$	--	$289^{\ x64}$	--
Temperature by Thermocouple			70 °F		
44.90	139.0	106	0.226	282	0.22
39.97	139.0	$53.25^{\ x64}$ (unclear)	0.46	197.25	0.324
"	"	51.0		190.0	
34.98	"	40.75	0.61	145.75	0.426
"	"	38^{+7}		$148.25^{\ x64}$	

The count results in Table 4 were not used in this study. It is unclear what the superscripts on the count measurements mean. This table was included to preserve the experimenters' results found in the logbook.

During this experiment it was noticed that when the water height was changed from 88 cm to 112 cm the fuel height changed without adding any fuel "indicating that additional pressure of added water [height] pressed the sides of the slab in."[a] This issue was addressed in subsequent experiments.

1.2.5 Experiment 107

Experiment 107 was conducted on December 22, 1955. At the beginning of this experiment it is noted that "3 extra 'spacer bars' were placed along the top edge of plastic shim in addition to [the] six original ones."[b] The experiment was run using a fuel solution with an H/X ratio reported to be 44.7 and a 2 1/16-inch slab thickness. Fuel was added with the source out and the critical level was measured. However

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 253.
[b] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 254.

during the experiment an addition of water reflector caused the fuel height to change even though no fuel had been added indicating that the reflector water was still causing the sides of the slab to be pushed in just as they were in Experiment 108 despite the addition of the spacers. The collected data are given in Table 5.

Table 5. Recorded Data from Experiment 107.

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks	
36.16	80.0	slightly super	
34.04	"	" "	
35.89	"	just critical	← H_2O added while just critical -no solution added
35.91	89.0	slightly sub	
36.17	89.0	just crit.	
Temperature by Thermocouple			72.5 °F

1.2.6 Experiment 108

Experiment 108 was conducted on December 23, 1955, with a "new plate with legs on 12[–inch] centers in each direction [and the] highest row at 48[-inches] up [plus] 2 spacers at the top of tank."[a] A ¼-inch-thick plate and 2.000-inch spacers were used with a fuel solution with a reported H/X ratio of 44.7. Counts were measured with the source inserted. The source was then removed and critical levels were measured. The experiment ended when the system was scrammed by the period meter. Table 6 contains the experiment results. The notation method for recording counts in Table 6 is unclear. They were not used in this study but are included here to preserve all experimental data.

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 255.

Table 6. Recorded Data from Experiment 108.

Solution Height (in.)	H_2O Height Reading (cm)	Two Minute Counts	
		#4	#5
18.565	5	--	--
18.56	28.5 [9 in. above fuel]	4^{+5} x64	$27^{1/4}$ x64
		5^{0}	$27^{1/4}$ x64
24.97	47.7	10.5 x64	66.5 x64
		8.5	65 1/2
		7.5	65 1/2
32.97	47.7	--	--
33.07	67.5	17	193
		16 1/4	191 1/2

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks
37.92	67.5	super (approx. 200 sec)
37.99	76.1	sub
39.15	77.1	super
39.16	78.1	just crit
39.17	79.0	just sub
39.47	79.0	approx. 400 sec period
39.87	80.3	just crit
39.95	83.8	"
40.34	84.8	super
40.36	85.8	super
40.36	86.4	sub (just)
40.77	86.4	super
40.79	88.6	super
40.80	89.7	sub
41.39	89.7	super
41.42	93.5	sub
42.09	93.5	super
42.09	97.5	just crit
43.08	101.9	super
43.08	103.2	just crit
Scrammed by Period Meter		

1.2.7 Experiment 109

Experiment 108, slab thickness of 2.000 inches, was repeated as Experiment 109 on December 27, 1955. The results are summarized in Table 7.

Table 7. Recorded Data from Experiment 109.

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks
45.48"	103.3	slightly super
45.35	105.6	" "
45.38	108.4	just critical
47.21	122.0	barely subcritical
Solution Temp. 75 ^oC [(a)]		
47.25	128.5	subcritical
47.30	121.0	slightly super

(a) This is an error and the experimenter meant Fahrenheit.

At the end of this experiment it is noted that a "2[-inch] gauge block can be moved in the center bay only but with difficulty, (cannot be inserted to bottom)."[a]

1.2.8 Experiment 110

Experiment 110 was run on December 29, 1955, and is a repeat of Experiment 107, slab thickness of 2 1/16 inches, with "more inside spacers and a more uniform plate."[b] Before the experiment had started, it was noted in the logbook that a sample had been taken and the sample requisition number was referenced. The solution analysis results were included on the following page of the logbook. Then it was observed, at 4:20 and 4:25 PM that there was one floating wedge and the sample was taken while draining. The results of the experiment are given in Table 8.

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 258.
[b] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 259.

Table 8. Recorded Data from Experiment 110.

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks
34.99	78.5	slightly super
35.02	94.6	just crit
34.86	86.0	" "
34.91	89	" "
35.64	89	pos. period meas. on chart
Temp 74 °F		

1.2.9 Experiment 111

Experiment 111 was run on January 5, 1956, using a solution with an H/X ratio of 51.5 (~52) and a 3/16-inch spacer. Results are given in Table 9.

Table 9. Recorded Data from Experiment 111.

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks
34.71	67.5	super
34.73	72.0	just crit
35.20	79.2	" "
35.64	86.0	slightly super
"	86.5	just crit
36.66	86.5	pos. period meas.
37.27	94.5	just crit
Solution Temp		66 °F
Water "		74 °F
Repeat at higher solution temperature		
Temperature of solution		71 °F
36.27	94.5	not crit
36.81	"	slightly super
36.73	"	just crit
37.00	105.4	" "
37.54	121	slightly sub
Temp		71.5 °F
37.70	121	slightly super

1.2.10 Experiment 112

Experiment 112 was run on January 6, 1956, as the last uranium oxyfluoride slab with a 2.00-inch slab thickness and a solution with an H/X ratio reported to be 51.5. The following results were obtained (Table 10).

Table 10. Recorded Data from Experiment 112.

Solution Height (in.)	H_2O Height Reading (cm)	Experimenter Remarks
52.09 -in.	139	not critical all solution
51.99	125.4	just crit
51.33	121.3	super crit
51.28	"	just crit
Temp		73.5 ^{o}F

1.2.11 Published Results

Reference 1 is the publication of the experimental results. The experimenters give the following summary of their experimental data (Table 11).

Table 11. Published Results (Reference 1).

Slab thickness (in.)	Critical Solution		Reflector Water Height (in.)	Critical Values			Experiment[(a)]
	Height (in.)	Height $^{-1}$ (in. $^{-1}$)		Volume		Mass	
				(in.^{3})	(liters)	(kg of ^{235}U)	
H: ^{235}U[(b)] = 44.7; 0.532 g of ^{235}U / cm^3							
2.12 ± 0.01	28.18	0.0355	45.7	3465	56.8	30.2	105
2.06 ± 0.01	35.02	0.0286	53.5	4185	68.5	36.4	110
2.06 ± 0.01	34.91	0.0286	51.0	4170	68.3	36.3	110
2.00 ± 0.01	42.09	0.0238	54.5	4885	80.0	42.6	108
2.00 ± 0.01	43.08	0.0232	56.7	5000	81.9	43.6	108
1.995 ± 0.005	45.38	0.0220	59.0	5250	86.0	45.7	109
1.995 ± 0.005	47.20	0.0212	64.0	5460	89.5	47.6	109
H: ^{235}U[(b)] = 51.5; 0.469 g of ^{235}U / cm^3							
2.06 ± 0.01	36.73	0.0272	53.5	4390	71.9	33.7	111
2.06 ± 0.01	37.62	0.0266	64.0	4495	73.7	34.6	111
1.995 ± 0.005	51.99	0.0192	65.5	6015	98.6	46.2	112
1.995 ± 0.005	51.28	0.0195	64.0	5935	97.2	45.6	112

(a) The correlation between the published data and the experiment number was inferred from logbook and published data and was not given by the experimenter.
(b) Atom ratio.

Some of the reported slab thicknesses do not exactly match those recorded in the logbook. The reasons for changes in the slab thickness in the published results was not given by the experimenter but further discussion of the matter can be found in Section 2.3.4. Methods of measuring or calculating critical values and the formulation of the 1/M plots were not given in the published results. An extrapolation to and calculation of the minimum slab thickness were given in the published results.

1.3 Description of Material Data

Reference 1 and the logbook only gave material data for the uranium solutions. Sources for all other material data can be found in Section 2.

1.3.1 Uranium Solutions

As noted in Table 11, Reference 1 reports the use of two solutions with H: ^{235}U ratios of 44.7 and 51.5 and ^{235}U densities of 0.532 and 0.469 g of $^{235}U/cm^3$, respectively. It is not explained how the H: ^{235}U ratio and uranium density were calculated. From the logbook it is clear that one solution is used for Experiments 103-110 (these are the experiments with a reported H/X ratio of 44.7). This solution was then diluted by "adding 14 liters of water to the system"[a] on January 5, 1956. Analysis requisition forms asking for grams uranium per gram total and specific gravity are taped into the logbook for both the initial and diluted solution. (Hereafter the initial solution will be referred to as "Solution 1" and the diluted solution will be "Solution 2.") Table 12 has the values reported for the two solutions.

Table 12. Solution Analysis Results.

	Solution 1	Solution 2
Gram U/gram Total	0.34559	0.31933
Sp. G	1.6526	1.5781

No information was given regarding the solution analysis techniques or the reference temperature for the specific gravity.

The logbook includes calculations for the two published H/X ratios but it is unclear from where the values used in these calculations were obtained. A uranium enrichment of 93.2% is reported in Reference 1, but this value was not recorded in the logbook.

A spectrographic analysis was also completed on January 11. In the logbook, the written year for the solution analysis is not readable, but is likely 1956. The analysis was performed on UNO_3. Table 13 has the results of this analysis. All results are in parts per million (ppm).

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 260.

Table 13. Solution Impurities.

Element	ppm
Be	<.3
Ni	175
Sn	<10
Si	<10
Li	<2
P	<100
Na	<10
Mo	- -
Mn	23
Mg	80
K	<50
Fe	1500
Cu	28
Cr	160
Ca	<50
Ba	<10
B	<1
Al	155
Ag	<1

1.4 Supplemental Experimental Measurements

No supplemental experimental measurements were provided.

2.0 EVALUATION OF EXPERIMENTAL DATA

Of the ten experiments performed, critical conditions were met a total of twenty times during Experiments 103, 105, 107, 108, 109, 110, 111, and 112. During some experiments multiple critical conditions were reported for the same slab thickness due to minor changes in slab thickness caused by hydrostatic forces deforming the tank walls. When multiple critical conditions were reported the condition with the lowest solution and reflector height was used for evaluation because this condition would correspond to the configuration with the least hydrostatic deformation and thus a slab thickness closest to the thickness reported. During Experiment 104 and 106 critical conditions were not recorded.

- **Experiment 103**

  This experiment was preformed with the safety blade in. Since no information about the safety blade was given this experiment cannot be used for a benchmark and is not evaluated further.
- **Experiment 105**

  Critical conditions were reached only once and results can be used for benchmark evaluation.
- **Experiment 107**

  During this experiment it was noted that hydrostatic pressure was causing a fluctuation in the slab thickness and therefore the critical conditions met during this experiment cannot be used and are not evaluated further.
- **Experiment 108**

  Critical conditions were met five times during Experiment 108. The last two of these conditions were reported in the published results but not used in the extrapolation to an infinite height. No reasoning was provided as to why the first three critical conditions were not included in published results. Reference 1 states that "data in which there is greatest confidence have been extrapolated to an infinite height." Because of the experimenters' lack of confidence in Experiment 108 results and the fact that Experiment 109 is a repeat of Experiment 108 it is not considered to be of benchmark quality. Data from Experiment 108 were evaluated and included in Appendix B.
- **Experiment 109**

  This experiment reached critical conditions only once. In Reference 1, however, a second critical condition was reported. The experimenters found this second condition by averaging a sub critical condition with a slightly supercritical condition.
- **Experiment 110**

  Three critical conditions were reached during Experiment 110.
- **Experiment 111**

  During Experiment 111 critical configurations were met six times along with another critical condition reported in Reference 1 which was found by averaging a slightly sub and slightly super critical conditions. Four of these were not used by the experimenters due to a low solution temperature and thus were not considered in this evaluation.
- **Experiment 112**

  The system reached critical conditions twice during Experiment 112.

Table 11 shows slab thicknesses as published by the experimenters in Reference 1. The logbook reports these slab thicknesses with more significant digits or as fractions. Benchmark specifications derived in this evaluation reflect the values reported in the logbook and not Table 11, except for Experiments 109 and 112. A slab thickness of 1.995 inches, as reported in Reference 1, was used for Experiments 109 and 112 instead of the 2.00 inch value reported in the logbook. The reasons for this selection are explained in Section 2.3.4. Table 14 summarizes the slab thicknesses used in this evaluation. It should also be noted for the purpose of this study, all measurements were converted into centimeters. As many significant figures were kept as required to allow for an accurate conversion of values back into inches. The additional significant figures on measurements were not meant to imply improved accuracy.

Table 14 summarizes the critical solution and reflector heights from each experiment which were acceptable for evaluation.

Table 14. Evaluated Critical Conditions.

Experiment	Slab Thickness[(a)] (cm)	Solution Used	Solution Height (cm)	Reflector Height	
				Reading (cm)	Actual (cm)
105	5.39750	1	71.5772	75.6	116.6
109	5.06730	1	115.2652	108.4	149.4
110	5.23875	1	88.5444	86.0	127.0
111	5.23875	2	93.2942	94.5	135.5
112	5.06730	2	130.2512	121.3	162.3

(a) The slab length was 147.32 cm for all experiments.

Uncertainty calculations were performed for all measured values using MCNP5[a] and ENDF/B-VI.8 nuclear data. Hydrogen in light water thermal scattering treatment was used for the fuel solution, water reflector, and the Lucite® box and spacers (see Appendix F). The statistical uncertainty of the MCNP5 calculations was ~0.00005 for all cases. In cases where the Δk_{eff} value was less than the statistical uncertainty the variable parameter was increased and then Δk_{eff} value was scaled to correspond to a 1σ uncertainty. When the variable parameter could not be increased the uncertainty of that parameter was simply considered insignificant. For uncertainties that were established as bounding uncertainties with a uniform distribution 1σ values are obtained by including division by √3 as a component of the scaling factor given in the applicable Section 2 tables. Uncertainty effects smaller than 0.0001 are considered negligible and not included in the calculation of the overall uncertainty.

2.1 Uncertainty in Solution Properties

Reference 1 reports $H/^{235}U$ and ^{235}U densities for both solutions. Calculations using the measured solution properties given in the logbook do not, however, give the same $H/^{235}U$ values. Calculated $H/^{235}U$ ratios were 44.5 rather than 44.7 and 51.2 rather than 51.5. Calculations used to obtain the published values were shown in the log book, but it is unclear from where some of the numbers used in the calculations were derived. The measured solution specific gravity and uranium weight fraction were used

[a] F. B. Brown, et al., "MCNP Version 5," LA-UR-02-3935, Los Alamos National Laboratory (2002).

to calculate atom density in this evaluation. Calculations were not based on the published H/^{235}U and ^{235}U densities.

No information was given regarding uranium isotopic compositions beyond fuel enrichment. As with other benchmarks involving uranium oxyfluoride solution at Oak Ridge National Laboratory in the 1950's a historically accepted, standard Oak Ridge National Laboratory ^{234}U/^{235}U atom ratio of 0.012284 was used (HEU-SOL-THERM-050). Reference 1 and the logbook make no reference to ^{236}U and it is assumed to not be present in this evaluation.[a] Using this method and the ^{235}U enrichment of 93.2 wt.% given in Reference 1 a ^{234}U and ^{238}U isotopic content of 1.14 and 5.66 wt.% was calculated. These compositions agree with the uranium oxyfluoride compositions reported by J. K. Fox et al. in a 1958 annual progress report.[b] Hugh Clark, in determining subcritical limits for ^{235}U systems, used the same series of experiments to find subcritical limits for uranium oxyfluoride slabs. In his study a uranium composition of 1.1% ^{234}U, 93.13% ^{235}U, 0.5% ^{236}U, and 5.27% ^{238}U was used.[c] This composition was obtained in much the same way (review of typical solutions given in progress reports from about the same period), but it is unclear why the two compositions do not match. Clark's composition was not used in this evaluation because he used a ^{235}U enrichment of 93.13% which conflicts with the published value of 93.2% and the reference he cited for his composition does not actually give the composition.[d] However, as can be seen in Sections 2.1.4, 2.1.5, and 2.1.6, it was ensured that the uncertainty perturbations encompassed the composition used by Clark.

No information was given regarding the storage of the solution used. It is assumed that the solution was stored in climate-controlled solution storage rooms in stainless steel tanks to reduce the amount of breakdown or evaporation of the fuel.[e]

Methods for calculating atom densities from the solution specific gravity and uranium weight fraction and the uranium enrichment can be found in Appendix C.

2.1.1 Uranium Weight Fraction

The logbook contains gram uranium per total gram of solution values for the two solutions (see Table 12). No uncertainty in these measurements was reported so an uncertainty of 1.0% was chosen based on other uranium oxyfluoride experiments by the same experimenters during the same timeframe.[f] This uncertainty was determined to be bounding based on the high precision of the reported uranium weight fraction values. Table 15 contains the Δk_{eff} values for the uncertainty in uranium weight fraction.

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[a] Personal Communication with Calvin M. Hopper of Oak Ridge National Laboratory on May 5, 2010
[b] J. K. Fox, L. W. Gilley, R. Gwin, and J. T. Thomas, "Critical parameters of Uranium Solutions in Simple Geometry," *Neutron Physics Division Annual progress Report for Period Ending September 1, 1958* (ORNL-2609).
[c] Hugh K. Clark, "Subcritical Limits for Uranium-235 Systems", Nuc. Sci. and Eng., Vol. 81, Num. 3, 1982.
[d] J. K. Fox, L. W. Gilley, and D. Callihand, "Critical Mass Studies, Part IW Aqueous ^{235}U Solutions," ORNL-2367, Oak Ridge National Laboratory (1958).
[e] Personal Email Communication with Calvin M. Hopper of Oak Ridge National Laboratory of Jun 2, 2010.
[f] J. K. Fox, L. W. Gilley and D. Callihan, "Critical Mass Studies, Part IX Aqueous U^{235} Solutions," ORNL-2367, Oak Ridge National Laboraoty, 1958, pp. 1.

Table 15. Δk_{eff} Results Due to Uncertainties in Uranium Weight Fraction.

Experi-ment	U Weight Fraction (g U/g sol.)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	0.34559	+ 0.00173	-0.00108	±	0.00007	√3/2	-0.00125	±	0.00008
	0.34559	- 0.00173	0.00097	±	0.00007	√3/2	0.00112	±	0.00008
109	0.34559	+ 0.00173	-0.00088	±	0.00007	√3/2	-0.00102	±	0.00008
	0.34559	- 0.00173	0.00101	±	0.00007	√3/2	0.00117	±	0.00008
110	0.34559	+ 0.00173	-0.00100	±	0.00007	√3/2	-0.00115	±	0.00008
	0.34559	- 0.00173	0.00101	±	0.00007	√3/2	0.00117	±	0.00008
111	0.31933	+ 0.00160	-0.00078	±	0.00007	√3/2	-0.00090	±	0.00008
	0.31933	- 0.00160	0.00093	±	0.00007	√3/2	0.00107	±	0.00008
112	0.31933	+ 0.00160	-0.00074	±	0.00007	√3/2	-0.00085	±	0.00008
	0.31933	- 0.00160	0.00078	±	0.00007	√3/2	0.00090	±	0.00008

In Table 15 the Δk_{eff} effect of increased uranium mass density is opposite of what one would expect when adding more uranium to a system. This is due to the decrease in the amount of moderator that occurs when the uranium mass density of the system is increased. This decrease in moderator decreases the reactivity of the system. Alternatively, with a decreased uranium mass density more moderator is present in the system and the reactivity is increased.

2.1.2 Solution Specific Gravity

The specific gravity of both solutions was given; however, no uncertainty in the measurements was indicated in the logbook or Reference 1. Using similar reasoning as in Section 2.1.1 a uniform bounding uncertainty of 1.0% was chosen. The temperature of the solution when the specific gravity was measured and the reference temperature of the specific gravity were not given. The uncertainty associated with this lack of information is well within the 1.0% bounded uncertainty.[a] Table 16 contains the Δk_{eff} values due to uncertainty in specific gravity.

[a] Personal communication with David H. Meikrantz of Idaho National Laboratory on June 15, 2010.

Table 16. Δk_{eff} Results Due to Uncertainties in Specific Gravity.

Experiment	Specific Gravity		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	1.6526	+ 0.0083	0.00185	±	0.00007	√3/2	0.00214	±	0.00008
	1.6526	- 0.0083	-0.00198	±	0.00007	√3/2	-0.00229	±	0.00008
109	1.6526	+ 0.0083	0.00186	±	0.00007	√3/2	0.00215	±	0.00008
	1.6526	- 0.0083	-0.00175	±	0.00007	√3/2	-0.00202	±	0.00008
110	1.6526	+ 0.0083	0.00182	±	0.00007	√3/2	0.00210	±	0.00008
	1.6526	- 0.0083	-0.00184	±	0.00007	√3/2	-0.00212	±	0.00008
111	1.5781	+ 0.0079	0.00186	±	0.00007	√3/2	0.00215	±	0.00008
	1.5781	- 0.0079	-0.00185	±	0.00007	√3/2	-0.00214	±	0.00008
112	1.5781	+ 0.0079	0.00172	±	0.00007	√3/2	0.00199	±	0.00008
	1.5781	- 0.0079	-0.00183	±	0.00007	√3/2	-0.00211	±	0.00008

In Section 2.1.1 it was seen that an increase in the uranium mass density of the solution led to a less reactive system. In Table 16 it is seen that the trend for changes in specific gravity is opposite that of changes in uranium mass density. This difference is because a change in specific gravity changes both the uranium and moderator contents whereas, a change in uranium mass density leads to inversely related changes in the uranium and moderator content.

The uranium weight fraction and the specific gravity of the solution are not independent of one another. The correlation of these uncertainties is addressed in Section 2.4 and used in the calculation of the overall uncertainty. The correlation coefficient is derived in Appendix G.

2.1.3 Temperature

Reference 1 gives a temperature range of 72-75 ^{o}F. The middle of this range, 73.5 ^{o}F, was used for all of the experiments. However, one experiment had a solution temperature of 71.5 ^{o}F. Because of this a 1σ uncertainty of 3.0 ^{o}F was used. Temperature affects both the solution and the reflector since both calculations are based on the standard density of water.[a] To find the Δk_{eff} values listed in Table 17 the densities of the solution and reflector were varied in accordance with the variation of the temperature. The temperature of the neutron cross section data was not changed, as the temperature difference is quite small and would have had a negligible effect on k_{eff}.

[a] Standard water densities at various temperatures from: *The CRC Handbook of Chemistry and Physics, 89th ed. (Internet version 2009)*.

Table 17. k_{eff} Results Due to Uncertainties in Temperature.

Experiment	Temperature (^{o}F)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	73.5	+15 ˚F	-0.00088	±	0.00007	5	-0.00018	±	0.00001
	73.5	-15 ˚F	0.00060	±	0.00007	5	0.00012	±	0.00001
109	73.5	+15 ˚F	-0.00079	±	0.00007	5	-0.00016	±	0.00001
	73.5	-15 ˚F	0.00063	±	0.00007	5	0.00013	±	0.00001
110	73.5	+15 ˚F	-0.00084	±	0.00007	5	-0.00017	±	0.00001
	73.5	-15 ˚F	0.00061	±	0.00007	5	0.00012	±	0.00001
111	73.5	+15 ˚F	-0.00082	±	0.00007	5	-0.00016	±	0.00001
	73.5	-15 ˚F	0.00072	±	0.00007	5	0.00014	±	0.00001
112	73.5	+15 ˚F	-0.00082	±	0.00007	5	-0.00016	±	0.00001
	73.5	-15 ˚F	0.00064	±	0.00007	5	0.00013	±	0.00001

2.1.4 Enrichment

No information was given regarding the uncertainty in the uranium enrichment thus a ± 0.1 wt.% 1σ uncertainty was chosen based on the least significant reported digit. This uncertainty is similar to that used in other ^{235}U experiments at Oak Ridge National Laboratory. In order to ensure the Δk_{eff} value was well above the statistical uncertainty of the MCNP calculation the 1σ uncertainty was scaled by a factor of three. While varying the ^{235}U content the $^{234}U/^{235}U$ ratio was held constant and the ^{238}U was adjusted to maintain a mass balance. Results are in Table 18.

Table 18. Δk_{eff} Results Due to Uncertainties in Enrichment.

Experiment	Enrichment ^{235}U wt.%		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	93.2	+0.3	0.00038	±	0.00007	3	0.00013	±	0.00002
	93.2	-0.3	-0.00053	±	0.00007	3	-0.00018	±	0.00002
109	93.2	+0.3	0.00042	±	0.00007	3	0.00014	±	0.00002
	93.2	-0.3	-0.00047	±	0.00007	3	-0.00016	±	0.00002
110	93.2	+0.3	0.00053	±	0.00007	3	0.00018	±	0.00002
	93.2	-0.3	-0.00041	±	0.00007	3	-0.00014	±	0.00002
111	93.2	+0.3	0.00049	±	0.00007	3	0.00016	±	0.00002
	93.2	-0.3	-0.00045	±	0.00007	3	-0.00015	±	0.00002
112	93.2	+0.3	0.00046	±	0.00007	3	0.00015	±	0.00002
	93.2	-0.3	-0.00043	±	0.00007	3	-0.00014	±	0.00002

2.1.5 U-234 Concentration

By the method discussed in Section 2.1 the enrichment of ^{234}U in the uranium was found to be 1.14%. As no information regarding the uranium isotopic composition was given the ^{234}U composition was initially varied by ± 1.14%. The percentage of ^{238}U was adjusted to maintain a total of 100%. This yielded a rather high uncertainty; in order to get a better idea of the uncertainty in ^{234}U the average of the ^{234}U content used in all U.S. highly enriched uranium benchmarks except three (two evaluations which had no ^{234}U information and one with specialized fuel) was found. It was found that the average ^{234}U content was 0.9945 wt.% with a standard deviation of 0.085 %.[a] This gave a better idea of typical ^{234}U content and justified reducing the uncertainty by a factor of ten. This is reflected by the scaling factor of 10 in Table 19. This uncertainty encompasses the difference between the ^{234}U composition used in this study and the composition used by Hugh Clark. Table 19 contains the results of this analysis.

Table 19. Δ k_{eff} Results Due to Uncertainties in ^{234}U Content.

Experiment	^{234}U Conc. (wt.% ^{234}U)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	1.14%	+ 1.14%	0.00308	±	0.00007	10	0.00031	±	0.00001
	1.14%	- 1.14%	-0.00366	±	0.00007	10	-0.00037	±	0.00001
109	1.14%	+ 1.14%	0.00295	±	0.00007	10	0.00030	±	0.00001
	1.14%	- 1.14%	-0.00373	±	0.00007	10	-0.00037	±	0.00001
110	1.14%	+ 1.14%	0.00310	±	0.00007	10	0.00031	±	0.00001
	1.14%	- 1.14%	-0.00382	±	0.00007	10	-0.00038	±	0.00001
111	1.14%	+ 1.14%	0.00304	±	0.00007	10	0.00030	±	0.00001
	1.14%	- 1.14%	-0.00352	±	0.00006	10	-0.00035	±	0.00001
112	1.14%	+ 1.14%	0.00290	±	0.00007	10	0.00029	±	0.00001
	1.14%	- 1.14%	-0.00359	±	0.00007	10	-0.00036	±	0.00001

2.1.6 U-236 Concentration

Reference 1 and the corresponding logbook makes no reference to ^{236}U being present nor was it assumed to be present for this evaluation. However, Hugh Clark used ^{236}U in his evaluation thus the effect 0.05 wt.% ^{236}U investigated. The ^{234}U and ^{235}U content was held constant and the ^{238}U was adjusted with the ^{236}U to maintain a mass balance. It was determined that the 0.05 wt.% of ^{234}U was negligible.

2.1.7 Impurities

The logbook contains impurity results from a N.C. spectrographic test run while the uranium was in UNO_3 form.[b] Table 13 contains the results from this test. Because the impurity analysis was completed on the fuel while it was in the form of UNO_3 the impurity concentration could have changed during the conversions process. In order to determine if the impurities listed in Table 13 represent UO_2F_2 impurities other experiments performed at Oak Ridge National Laboratory using UO_2F_2 were studied.

[a] Data compiled from the 2009 ed. of the International Criticality Safety Benchmark Evaluation Project Handbook.
[b] Table of results taped to Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 260.

HEU-SOL-THERM-009 and HEU-SOL-THERM-050 both report solution impurities found by sample analysis. HEU-SOL-THERM-010, HEU-SOL-THERM-011, and HEU-SOL-THERM-012 all use results from a previous experiment and scale the impurities based on the uranium content of the solution. In these experiments only iron, nickel, chromium, and aluminum impurities were reported. If a similar scaling method is used the calculated concentration for the major impurities is approximately the same as those reported in Table 13. Because of this and the wide range of impurity concentrations reported in HEU-SOL-THERM-009 and HEU-SOL-THERM-050 it was determined that the impurity concentrations in Table 13 are appropriate for this evaluation.

For impurities whose concentration was given by a maximum value (i.e. concentration is '<' a number), a concentration of one half the maximum value was included in the detailed model. For impurities with exact concentrations given, the specified concentrations were used in the detailed model. However the following method in determining uncertainty was used to ensure that the highly variable values of the range of concentrations are accounted for. For the uncertainty analysis of the range of impurity concentrations, the range was assumed to be at their maximum concentration and at a concentration of zero. All other impurities were varied by the commonly accepted ±20% for impurities over 10 µg/g. The uncertainty is considered to be bounding and the values uniformly distributed. Table 20 shows how each impurity concentration was varied. Table 21 contains the Δk_{eff} value results due to uncertainty in impurity concentrations.

Table 20. Solution Impurity Concentrations.

Element	Given (ppm)	Detailed Model (ppm)	±	Deviation (1σ)
Be	<.3	0.15	±	0.15
Ni	175	175	±	35
Sn	<10	5	±	5
Si	<10	5	±	5
Li	<2	1	±	1
P	<100	50	±	50
Na	<10	5	±	5
Mo	- -	--	±	--
Mn	23	23	±	4.6
Mg	80	80	±	16
K	<50	25	±	25
Fe	1500	1500	±	300
Cu	28	28	±	5.6
Cr	160	160	±	32
Ca	<50	25	±	25
Ba	<10	5	±	5
B	<1	0.5	±	0.5
Al	155	155	±	31
Ag	<1	0.5	±	0.5

Table 21. Δk_{eff} Results Due to Uncertainty in Impurities.[(a)]

Experiment	Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	-0.00056	±	0.00007	√3	-0.00032	±	0.00004
	0.00042	±	0.00007	√3	0.00024	±	0.00004
109	-0.00048	±	0.00007	√3	-0.00028	±	0.00004
	0.00053	±	0.00007	√3	0.00031	±	0.00004
110	-0.00046	±	0.00007	√3	-0.00027	±	0.00004
	0.00052	±	0.00007	√3	0.00030	±	0.00004
111	-0.00051	±	0.00007	√3	-0.00029	±	0.00004
	0.00049	±	0.00007	√3	0.00028	±	0.00004
112	-0.00046	±	0.00007	√3	-0.00027	±	0.00004
	0.00059	±	0.00007	√3	0.00034	±	0.00004

(a) Additive concentration deviation corresponds with top value. The low range of concentration corresponds to lower value.

2.1.8 Compounds Formed in the UO_2F_2 Solution

It is presumed that no hydrated solids are in the solution because the H/U ratio is sufficiently above the saturation H/U ratio of 16.[a]

Iron complexes, FeF_2, FeF_3, and FeF_5, can form in the presence of iron and uranium oxyfluoride.[b] Effects of iron compounds in the solution were analyzed by assuming all iron impurity forms FeF_3 complexes with fluoride. This analysis was preformed separately from the impurity uncertainty analysis to account for each individually. This led to a one-sided, bounding uncertainty and thus a scaling factor of 2√3 was used to get a 1σ-uncertainty. It was assumed that the fluoride bonded with the iron did not come from the dissociation of UO_2F_2 molecules but from the solution synthesis process. Table 22 contains the Δk_{eff} value results of this analysis; the uncertainty was treated as a bounding limit.

[a] Jordan, W. C., et al., "Estimated Critical Conditions for UO_2F_2-H_2O Systems in Fully Water Reflected Spherical Geometry," ORNL/TM-12292, December 1992.
[b] Barber, E. J., et al., "Investigation of Breached Depleted UF6 Cylinders", POEF-2086, ORNL/TM-11988, September 1991.

Table 22. Δk_{eff} Results with all Fe in FeF_3 Compound.

Experiment	Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	-0.00073	±	0.00007	2√3	-0.00021	±	0.00002
109	-0.00065	±	0.00007	2√3	-0.00019	±	0.00002
110	-0.00077	±	0.00007	2√3	-0.00022	±	0.00002
111	-0.00070	±	0.00007	2√3	-0.00020	±	0.00002
112	-0.00060	±	0.00007	2√3	-0.00017	±	0.00002

2.2 Uncertainty in Other Material Properties

Neither the logbook nor Reference 1 gave any information regarding the composition of the Lucite® box and spacers, water reflector, or the surroundings.

2.2.1 Lucite® Purity

Lucite® was used for the spacer blocks, the thickness varying inserts, and the box. Lucite® is a polymer of methyl methacrylate (MMA). Generally the monomer is 99.5% pure or better. By today's standards the Lucite is greater than 99.9% pure. Impurities in the Lucite® generally come from the initiator and internal release agent used during the polymerization process. At times other impurities are purposely added to the Lucite® for experimental purposes although there would most likely have not been any special additions in the Lucite® used for these experiments.[a,b] Rocky Flats has performed experiments using Lucite® (or similar materials) that contain boron.[c] All benchmarks from Rocky Flats using Lucite were reviewed and no boron was included in the Lucite®. Although the Lucite® most likely did not contain boron in the experiment and was assumed to be pure in the benchmark specifications the effect of 1 ppm (at.%) was calculated The results are given in Table 23.

Table 23. Δk_{eff} Results with 1 ppm Boron Included in the Lucite®.

Experiment	Δk_{eff}	±	$\sigma_{\Delta k}$
105	-0.00039	±	0.00007
109	-0.00040	±	0.00007
110	-0.00035	±	0.00007
111	-0.00019	±	0.00007
112	-0.00037	±	0.00007

[a] Personal Email Communication with John Daniels of Lucite International on May 20, 2009 and June 2, 2010.
[b] Personal Phone Communication with Dr. Robb Hermes of LANL of May 26, 2009 and Personal Email Communication on June 20, 2010.
[c] Personal Communication with Calvin M. Hopper of Oak Ridge National Laboratory on May 5, 2010.

2.2.2 Lucite® Density

The composition of Lucite® was calculated using an average density of 1.19 g/cm^3 and the empirical chemical formula of the material ($C_5O_2H_8$). Density ranges from 1.18 to 1.2 g/cm^3 and thus a bounding uncertainty of ±0.01 g/cm^3 was used with values uniformly distributed.[a] Table 24 contains the results of the Δk_{eff} values obtained for the uncertainty in the Lucite® density.

Table 24. Δk_{eff} Results Due to Uncertainties in Lucite® Density.

Experiment	Density (g/cm3)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	1.19	+ 0.01	0.00024	±	0.00007	√3	0.00014	±	0.00004
	1.19	- 0.01	-0.00037	±	0.00007	√3	-0.00021	±	0.00004
109	1.19	+ 0.01	0.00034	±	0.00007	√3	0.00020	±	0.00004
	1.19	- 0.01	-0.00031	±	0.00007	√3	-0.00018	±	0.00004
110	1.19	+ 0.01	0.00040	±	0.00007	√3	0.00023	±	0.00004
	1.19	- 0.01	-0.00023	±	0.00007	√3	-0.00013	±	0.00004
111	1.19	+ 0.01	0.00034	±	0.00007	√3	0.00020	±	0.00004
	1.19	- 0.01	-0.00017	±	0.00007	√3	-0.00010	±	0.00004
112	1.19	+ 0.01	0.00032	±	0.00007	√3	0.00018	±	0.00004
	1.19	- 0.01	-0.00022	±	0.00007	√3	-0.00013	±	0.00004

2.2.3 Water Reflector

No information was given regarding the purity of the water reflector, thus pure water was assumed. The density of water is a function of the system temperature, thus uncertainty in the water reflector properties is tied to the uncertainty in temperature. The effect of temperature on the system can be seen in Table 17 of Section 2.1.3.

2.2.4 Surroundings

Effects of the surroundings on k_{eff} are discussed in Section 3.1.1.1.

2.3 Uncertainty in Measurements

2.3.1 Solution Height

The height of the uranium oxyfluoride solution was measured using a selsyn reader. For all experiments it is assumed with a high degree of confidence that the reported fuel height is the actual fuel height not the selsyn reading unless otherwise stated. No uncertainty in the solution height was reported in the logbook or Reference 1. Evaluated in HEU-SOL-THERM-050 is a uranium oxyfluoride experiment performed by some of the same experimenters at about the same time as these experiments. That evaluation uses a

[a] Personal Email Communication with John Daniels of Lucite International on May 20, 2009.

bounded solution height uncertainty of ±0.5 cm.[a] For the purpose of this evaluation the same uncertainty value was used but was not assumed to be bounding. The Δk_{eff} values are given in Table 25.

Table 25. Δk_{eff} Results Due to Uncertainties in Solution Height.

Experiment	Solution Height (cm)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	71.5772	+ 2.000	0.00142	±	0.00007	4	0.00035	±	0.00007
	71.5772	- 2.000	-0.00162	±	0.00007	4	-0.00040	±	0.00007
109	115.2652	+ 2.000	0.00035	±	0.00007	4	0.00009	±	0.00007
	115.2652	- 2.000	-0.00056	±	0.00007	4	-0.00014	±	0.00007
110	88.5444	+ 2.000	0.00085	±	0.00007	4	0.00021	±	0.00001
	88.5444	- 2.000	-0.00084	±	0.00007	4	-0.00021	±	0.00001
111	93.2942	+ 2.000	0.00076	±	0.00007	4	0.00019	±	0.00007
	93.2942	- 2.000	-0.00066	±	0.00007	4	-0.00016	±	0.00007
112	130.2512	+ 2.000	0.00023	±	0.00007	4	0.00006	±	0.00001
	130.2512	- 2.000	-0.00031	±	0.00007	4	-0.00008	±	0.00001

2.3.2 Reflector

No information was given regarding uncertainty in reflector height so 1σ values were chosen based on the least significant digit reported by the experimenter. However, in order to calculate Δk_{eff} values larger than the uncertainty of the Monte Carlo methods, the reflector height had to be scaled by unreasonably large amounts. Thus the effect of uncertainty in reflector height measurements is considered negligible.

The experimenters were attempting to simulate an infinite reflector, but the thickness is not known. A reflector thickness of 30 cm was used to simulate infinite reflection. Appendix E contains calculation results that demonstrate that a reflector thickness of 30 cm is effectively infinite and the uncertainty in the reflector thickness is considered negligible.

2.3.3 Slab Thickness

The thickness of the UO_2F_2 slab was "altered by inserting plastic sheets of various thicknesses adjacent to one inside surface" (Reference 1). This could lead one to think that multiple sheets were used to reduce slab thickness to the desired value. However, the logbook often refers to a single Lucite® plate insert from which it can be inferred that a single Lucite® insert was made for each unique slab thickness.

Reference 1 and the logbook both refer to a change in slab thickness due to hydrostatic forces. Spacers are used to mitigate this problem although Experiment 109 still reports a change in slab thickness.[b] In Reference 1 the results from Experiment 109 are reported being for a slab thickness of 1.995-inches, but the logbook reports a thickness of 2.00-inches. At the end of the experiment it was reported that a 2 inch gauge block could only be moved to the center of the slab with difficulty and could not be inserted to the

[a] HEU-SOL-THERM-050.
[b] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 258.

bottom of the slab. Based on this observation and the discrepancy in slab thickness it is assumed that the reported slab thickness was adjusted by the experiments to account for box deformation due in part to hydrostatic forces. This same reasoning can also be applied to Experiment 112 which also has a slab thickness of 1.995-in. in Reference 1, but 2.00-inches in the logbook. This evaluation used 1.995-inches as slab thickness for Experiment 109 and 112. It is assumed this value of "slab thickness was measured with gauge blocks" (Reference 1). For all other cases the slab thickness reported in the logbook is used. The uncertainties in slab thickness reported in Reference 1 (see Table 11) are used as 1σ-uncertainties. The Δk_{eff} values for this uncertainty are given in Table 26.

Table 26. Δk_{eff} Results Due To Uncertainties in Slab Thickness.

Experiment	Slab Thickness (cm)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	5.39750	+ 0.0254	-0.00155	±	0.00007	1	-0.00155	±	0.00007
	5.39750	- 0.0254	0.00129	±	0.00007	1	0.00129	±	0.00007
109	5.06730	+ 0.0127	-0.00077	±	0.00007	1	-0.00077	±	0.00007
	5.06730	- 0.0127	0.00080	±	0.00006	1	0.00080	±	0.00006
110	5.23875	+ 0.0254	-0.00159	±	0.00007	1	-0.00159	±	0.00007
	5.23875	- 0.0254	0.00150	±	0.00007	1	0.00150	±	0.00007
111	5.23875	+ 0.0254	-0.00161	±	0.00007	1	-0.00161	±	0.00007
	5.23875	- 0.0254	0.00157	±	0.00007	1	0.00157	±	0.00007
112	5.06730	+ 0.0127	-0.00081	±	0.00007	1	-0.00081	±	0.00007
	5.06730	- 0.0127	0.00077	±	0.00007	1	0.00077	±	0.00007

2.3.4 Box Length

Uncertainty in the cutting of the Lucite® could lead to an incorrect box length. A possible cutting error of 0.1-inches of the box is used as an evenly distributed bounded uncertainty.[a] Ten times the uncertainty in box length was used in order to find Δk_{eff} values larger than the Monte Carlo uncertainty. The scaling factor used was $10\sqrt{3}$ to account for the scaling of the uncertainty and the fact that the uncertainty is considered bounding with a uniform distribution. The adjusted Δk_{eff} values are given in Table 27.

[a] Cutting sensitivity obtained from personal communication with Renee Fitch of Countryside Woodturners on June 2, 2009.

Table 27. Δk_{eff} Results Due to Uncertainties in Box Length.

Experiment	Box Length (Inner Dimension) (cm)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	147.32	+ 2.54	0.00014	±	0.00007	10√3	0.00001	±	0.000004
	147.32	- 2.54	-0.00035	±	0.00007	10√3	-0.00002	±	0.000004
109	147.32	+ 2.54	0.00033	±	0.00007	10√3	0.00002	±	0.000004
	147.32	- 2.54	-0.00016	±	0.00007	10√3	-0.00001	±	0.000004
110	147.32	+ 2.54	0.00030	±	0.00007	10√3	0.00002	±	0.000004
	147.32	- 2.54	-0.00025	±	0.00007	10√3	-0.00001	±	0.000004
111	147.32	+ 2.54	0.00033	±	0.00007	10√3	0.00002	±	0.000004
	147.32	- 2.54	-0.00019	±	0.00007	10√3	-0.00001	±	0.000004
112	147.32	+ 2.54	0.00023	±	0.00007	10√3	0.00001	±	0.000004
	147.32	- 2.54	-0.00028	±	0.00007	10√3	-0.00002	±	0.000004

2.3.6 Lucite® Thickness

In Reference 1 the uncertainty in the slab thickness was 0.01 inches for most cases. This uncertainty was used as the uncertainty is the Lucite® thickness as an evenly distributed bounding uncertainty. This uncertainty was scaled by a factor of ten (verified to be within the linear range). The adjusted Δk_{eff} values are in Table 28.

Table 28. Δk_{eff} Results Due to Uncertainties in Lucite® Thickness.

Experiment	Thickness (cm)		Δk_{eff}	±	$\sigma_{\Delta k}$	Scaling Factor	Δk_{eff} (1σ)	±	$\sigma_{\Delta k}$
105	1.905	+0.254	0.00244	±	0.00007	10√3	0.00014	±	0.000002
	1.905	-0.254	-0.00270	±	0.00007	10√3	-0.00016	±	0.000002
109	1.905	+0.254	0.00257	±	0.00007	10√3	0.00015	±	0.000002
	1.905	-0.254	-0.00252	±	0.00007	10√3	-0.00015	±	0.000002
110	1.905	+0.254	0.00257	±	0.00007	10√3	0.00015	±	0.000002
	1.905	-0.254	-0.00260	±	0.00007	10√3	-0.00015	±	0.000002
111	1.905	+0.254	0.00250	±	0.00007	10√3	0.00014	±	0.000002
	1.905	-0.254	-0.00247	±	0.00007	10√3	-0.00014	±	0.000002
112	1.905	+0.254	0.00244	±	0.00007	10√3	0.00014	±	0.000002
	1.905	-0.254	-0.00261	±	0.00007	10√3	-0.00015	±	0.000002

2.3.7 Spacer Placement

The logbook states that spacers were used to overcome the hydrostatic pressure placed on the box. These spacers were "12[-inches] on centers in each direction [with the] highest row at 48[-inches] up [plus] 2 spacers at the top of [the] tank."[a] As can be seen in Section 3.1.2.7 if these spacers are homogenized into the solution the effect on k_{eff} is small and therefore the uncertainty in the placement of the spacers is negligible. However, to be sure, an uncertainty analysis was performed. The results are given in Appendix D.

2.4 Summary and Conclusions

The amount of uranium in the system is strongly dependent upon both the uranium weight fraction and the specific gravity measurements. In order to avoid double-counting of the uncertainty in the uranium content the uranium weight fraction and the specific gravity uncertainties were correlated using the following equation.

$$\sigma_k^2 = \sigma_{gU/gT}^2 \left[\frac{\Delta\left(k_{gU/gT}\right)}{\Delta(gU/gT)}\right]^2 + \sigma_{Sp.G}^2 \left[\frac{\Delta\left(k_{Sp.G}\right)}{\Delta(Sp.G)}\right]^2 + 2 \cdot r_{x_U,Sp.G} \cdot \sigma_{gU/gT} \cdot \sigma_{Sp.G} \left[\frac{\Delta\left(k_{gU/gT}\right)}{\Delta(gU/gT)}\right]\left[\frac{\Delta\left(k_{Sp.G}\right)}{\Delta(Sp.G)}\right]$$

Where the correlation coefficient, $r_{x_U,Sp.G}$, is approximately 0.3 for all experiments. Further explanation of the correlation coefficients and the derivation of the above equation can be found in Appendix G.

Total uncertainties were found by taking the square root of the sum of the squares of each individual components of uncertainty and the results are summarized in Table 29. All total uncertainties were between 0.19 and 0.27 % $\Delta k/k_{eff}$. Based on these uncertainties, five of the ten possible cases are deemed acceptable as benchmark evaluations. All uncertainties below 0.0001 are deemed negligible and left off of Table 29. Any uncertainty values higher than 0.00080 are highlighted.

[a] Oak Ridge National laboratory, Critical Experiment Logbook, 81R, page 255.

Table 29. Summary of Uncertainties.

Experiment	105	109	110	111	112
Case → / Parameter ↓	1	2	3	4	5
U_{total} Weight Fraction[(a)]	*0.00125*	*0.00117*	*0.00117*	*0.00107*	*0.00090*
Specific Gravity[(a)]	*0.00229*	*0.00215*	*0.00212*	*0.00215*	*0.00211*
U_{total} Weight Fraction and Specific Gravity	0.00199	0.00186	0.00184	0.00158	0.00158
Temperature	0.00018	0.00016	0.00017	0.00016	0.00016
Enrichment	0.00018	0.00016	0.00018	0.00016	0.00015
^{234}U wt.%	0.00037	0.00037	0.00038	0.00035	0.00036
^{236}U wt.%	NG[(b)]	NG	NG	NG	NG
Impurities	0.00032	0.00031	0.00030	0.00028	0.00034
Compounds in Solution	0.00021	0.00019	0.00022	0.00020	0.00017
Lucite® Purity	0.00039	0.00040	0.00035	0.00019	0.00037
Lucite® Density	0.00021	0.00020	0.00023	0.00020	0.00018
Solution Height	0.00040	0.00014	0.00021	0.00019	NG
Reflector Height	NG	NG	NG	NG	NG
Slab Thickness	0.00155	0.00080	0.00159	0.00161	0.00081
Box Length	NG	NG	NG	NG	NG
Lucite® Thickness	0.00016	0.00015	0.00015	0.00014	0.00015
Spacer Placement	NG	NG	NG	NG	NG
Overall	0.00266	0.00216	0.00255	0.00235	0.00191

(a) Values are not used in calculation of overall uncertainty because they accounted for with the correlated uncertainty.
(b) Negligible uncertainties, below 0.0001, are denoted with an NG and not included in the overall uncertainty calculation.

3.0 BENCHMARK SPECIFICATIONS

3.1 Description of Model

For this evaluation both detailed and simplified models are provided. Biases were determined using MCNP5 and the ENDF/B-VI.8 cross section library.

3.1.1 Detailed Model

The detailed model of this experiment is a Lucite® box with a plate, also made of Lucite®, inserted along one side of the box to vary the thickness of the UO_2F_2 slab. There are 1-inch square blocks within the slab to keep a constant slab thickness. The fuel is aqueous UO_2F_2 and the box is surrounded by an effectively infinite water reflector. Fuel and reflector height and slab thickness are varied for each experiment.

3.1.1.1 Surroundings

A support structure to hold up the box, reinforced stiffening members on the outside of the Lucite® box, and a reflector tank were not included in the detailed model and a bias (considered to be negligible) could not be quantified because no reference to and/or detail about the structure was provided. However, room return would have no effect because of the effectively infinite water reflection except from above the opening in the top of the box. To test room return effects, concrete[a] was placed directly on top of the Lucite® box. The effect on k_{eff} was negligible therefore excluding the surrounding room from the detailed model contributes no additional bias.

3.1.1.2 Spacer Placement

The logbook defines the vertical position of the spacer blocks (see Section 1.2.6). The horizontal position is not defined. For the detailed model five columns of spacers are assumed to be centered in the box. The effect of moving these spacers is insignificant. Results of this analysis for Configurations 1 and 5 are provided in Appendix D.

3.1.2 Simplified Model

The following simplifications were made from the detailed model:

- Air is replaced with void,
- The Lucite® insert is merged with the box,
- Spacers above the solution were ignored,
- Spacers within the solution were homogenized,
- Reflector width was reduced to 30 cm on all sides and on the bottom,
- The Lucite® box protruding above the reflector height was ignored,
- Impurities in the solution were removed, and
- Lucite® spacers were homogenized into the solution.

For the purpose of this study a bias is defined as the difference in the k value for the simplified model and the detailed model. The statistical uncertainty in the bias values determined with MCNP5 is 0.00007.

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[a] Concrete composition used from PU-SOL-THERM-008.

3.1.2.1 Removing Air

When air above the solution and water reflector is replaced with void the effect on k_{eff} is negligible. Results are in Table 30.

3.1.2.2 Exclusions of Impurities in Fuel Solution

The logbook gives definite impurity concentrations as well as maximum impurity concentrations (see Table 13). In Section 2.1.7 the effect of uncertainty in the concentrations of the impurities has on k_{eff} is evaluated. Table 30 has the bias on k_{eff} if all impurities are excluded from the solution.

3.1.2.3 Lucite® Insert Merged with the Lucite® Box

Modeling the Lucite® thickness-varying insert as part of the box instead of as a separate cell has negligible effects on k_{eff}. The Δk value of this simplification can be found in Table 30.

3.1.2.4 Lucite® Spacers Above Solution Ignored

The effects on k_{eff} from removing Lucite® spacers from the model that are above the solution level were so small that the bias for removing these spacers is not included in Table 30.

3.1.2.6 Exclusion of Box above Reflector height

For the simplified model the Lucite® box was modeled as being as tall as the reflector height rather than the full 180.34 cm. This created a minor bias which can be found in Table 30.

3.1.2.7 Homogenization of Lucite® Spacers within the Solution

Table 30 contains the Δk value for the homogenization of the Lucite® spacers. It should be noted that each case has different number of spacers homogenized into the solution based on the number of spacers that were located below the solution height.

3.1.2.8 Total Simplification Bias

Once the individual effects of the above simplifications were found, a model with all the simplifications was created. See Table 29 for a correlation between case numbers and experiment numbers, from this point forward each experiment will be referred to by case number. The bias of this model is the total simplification bias.

Table 30. Effects of Simplifications in Detailed Model.

Case	No Air Δk	No Impurities Δk	Insert Merged with Box Δk	Cut Box at Reflector Height Δk	Homo-genized Spacers Δk		Total Simplification Bias[b] $\Delta k \pm \sigma_{calc}$		
1	-0.00009	0.00013	-0.00005	-0.00011	-- [a]		0.00024	±	0.00007
2	0.00006	0.00037	-0.00002	0.00011	0.00070		0.00100	±	0.00007
3	0.00005	0.00028	-0.00003	0.00011	0.00062		0.00114	±	0.00007
4	-0.00010	0.00028	-0.00009	-0.00016	0.00049		0.00081	±	0.00007
5	0.00003	0.00037	0.00014	0.00011	0.00051		0.00101	±	0.00007

(a) Case 1 has no Lucite® spacers.
(b) Bias in k_{eff} when all simplifications are performed at the same time.

3.1.3 Other Simplifications

The effect of replacing the Lucite® box with water as well as homogenizing the Lucite® box into the 30-cm-wide water reflector was also considered but not included in the simplified model because they are on the order of ~2%. The biases of these simplifications are summarized in Table 31.

Table 31. Effects of Other Simplifications.

Case	Water Replaces Lucite® Box Δk	Homogenized Lucite® Box in Reflector Δk
1	-0.02016	-0.01787
2	-0.02213	-0.01960
3	-0.02112	-0.01875
4	-0.02135	-0.01897
5	-0.02234	-0.01991

3.2 Dimensions

Figures 2 and 3 are sketches of the detailed and simplified models, respectively, for Case 1. Case 1 does not have Lucite® spacers like Cases 2-5.

Figures 4 and 5 are the detailed and simple models for Cases 2-5.

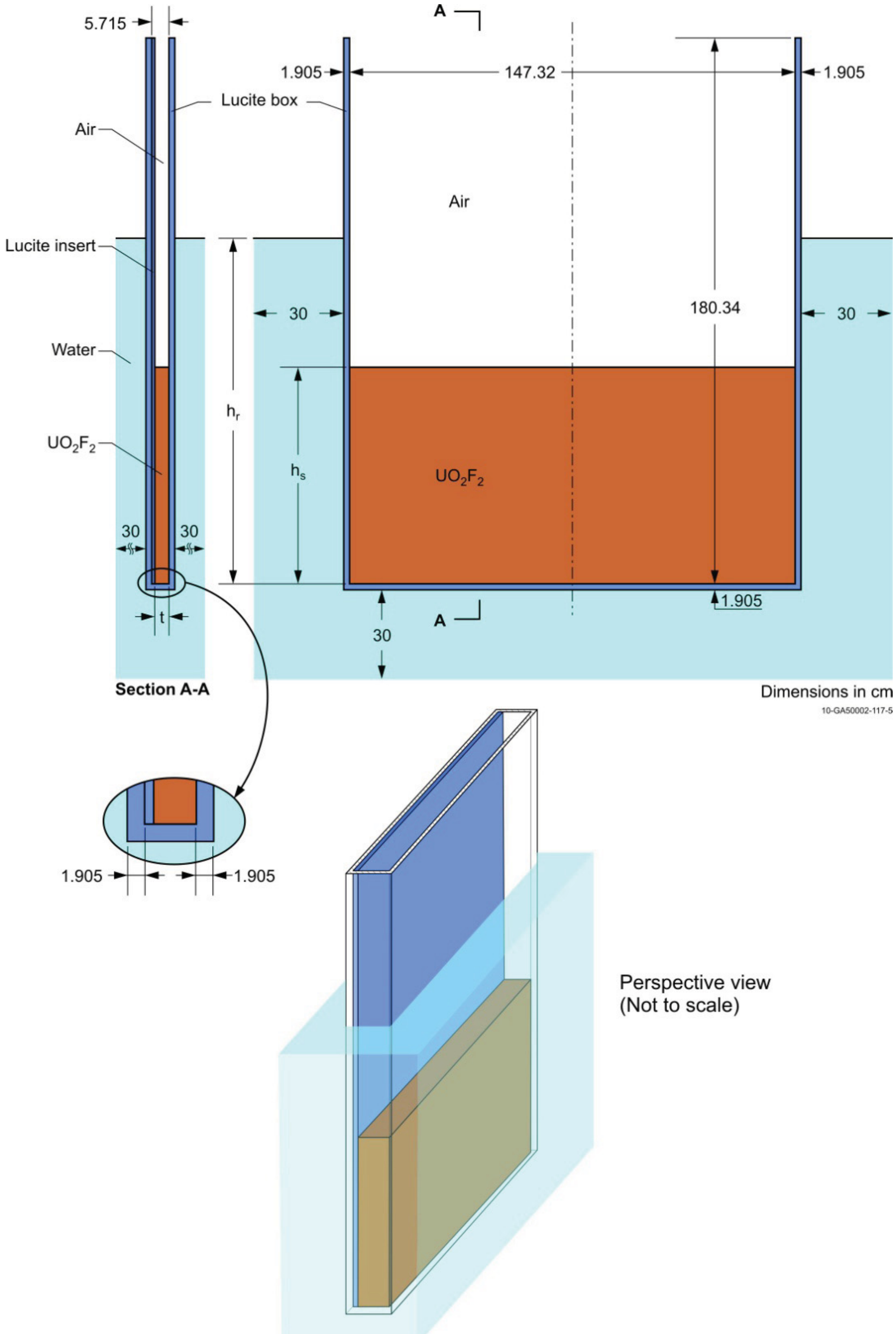


Figure 2. Detailed Model of Case 1 of UO_2F_2 Slab Experiments.[a]

[a] All figures courtesy of Christine White, Idaho National Laboratory.

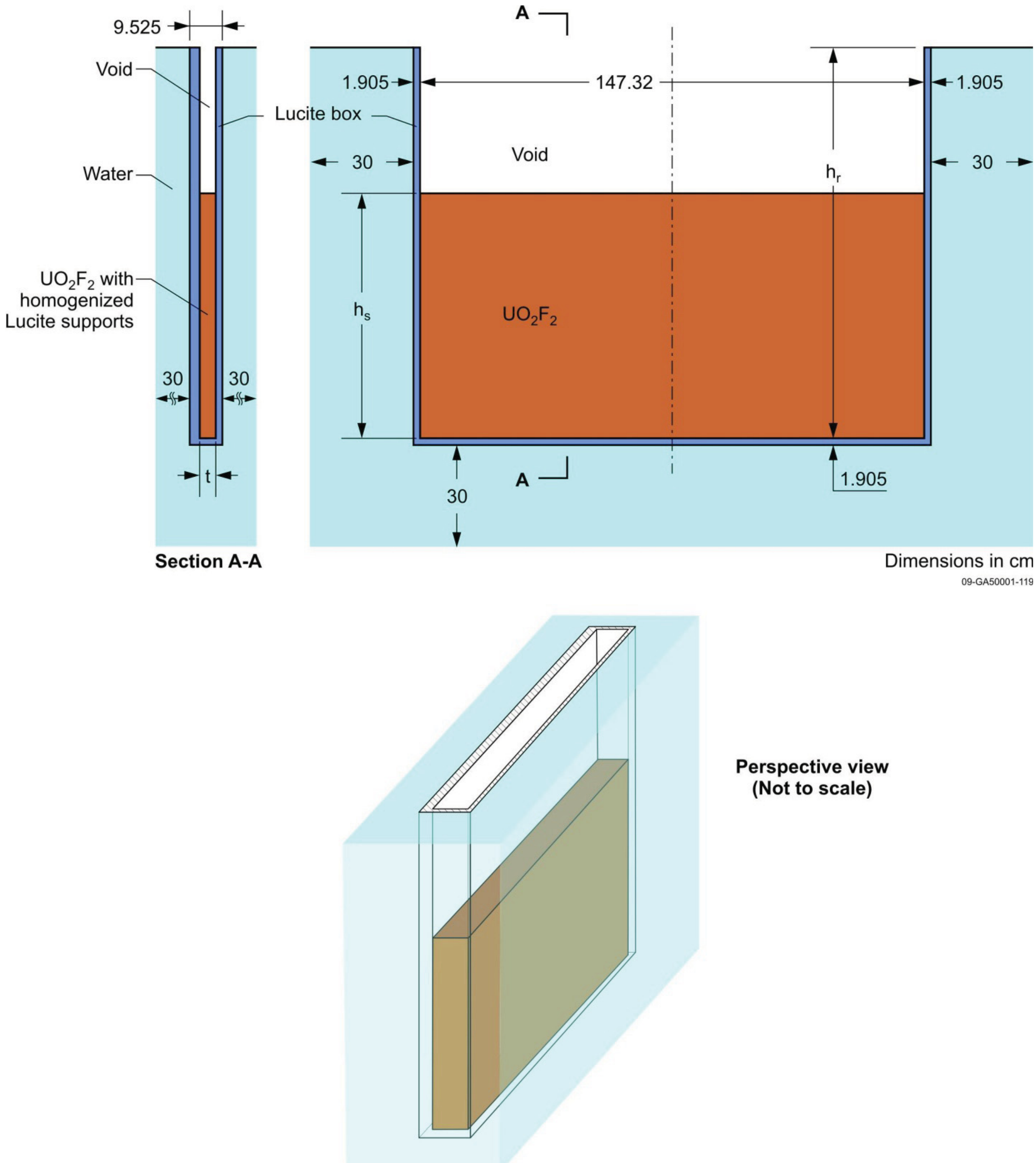


Figure 3. Simple Benchmark Model for Case 1 of the UO_2F_2 Slab Experiments.

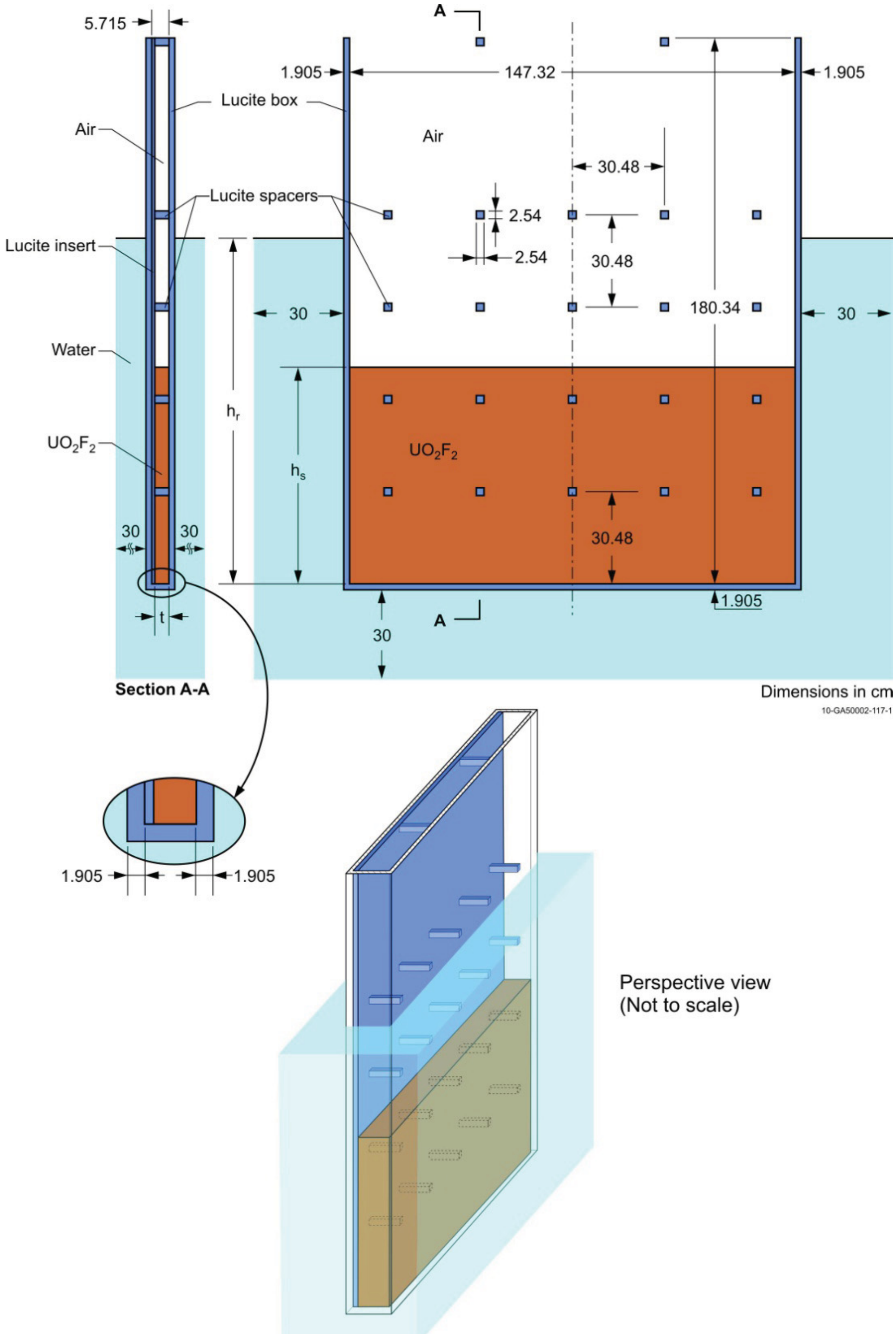
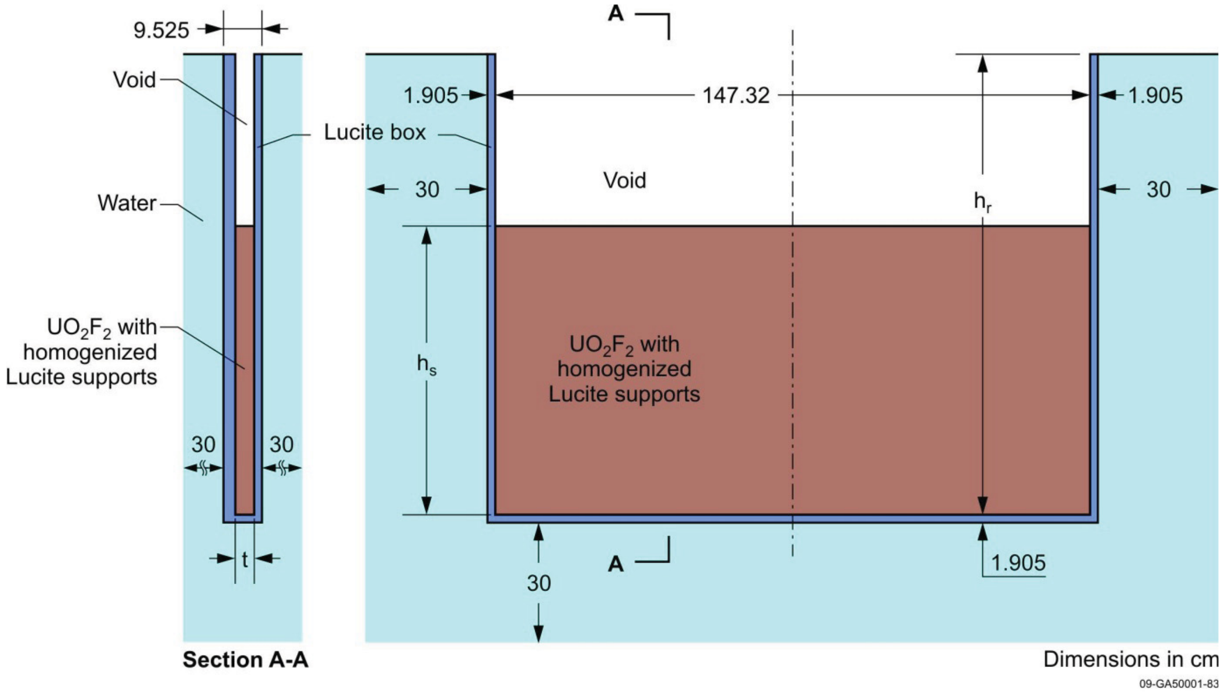


Figure 4. Detailed Benchmark Model of Cases 2 – 5 of the UO_2F_2 Slab Experiments.



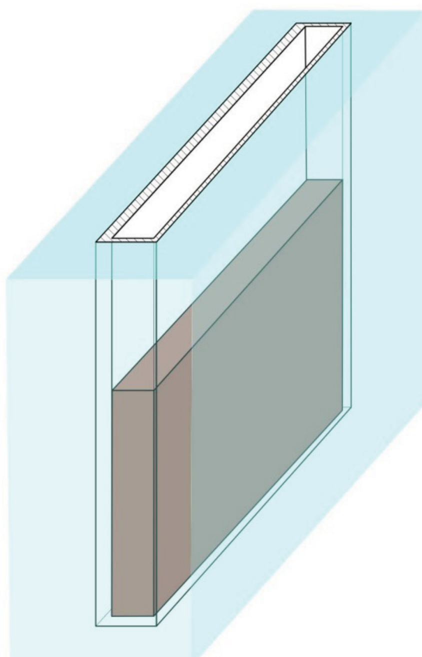


Figure 5. Simple Benchmark Model of Cases 2 – 5 of the UO_2F_2 Slab Experiments.

Table 32 contains the parameters that vary between experiments: slab thickness, solution height, and water reflector height for the simple and detailed models. Table 33 contains all other dimensions for the system.

Table 32. Detailed Model Dimensions.

Case	Slab Thickness (t, cm)	Solution Height (h_s, cm)	Reflector Height (h_r, cm)
1	5.39750	71.5772	116.6
2	5.06730	115.2652	149.4
3	5.23875	88.5444	127.0
4	5.23875	93.2942	135.5
5	5.06730	130.2512	162.3

Table 33. Summary of Dimensions.

	Detailed Model		Simple Model	
Nominal Inner Box Dimensions	height	180.34 cm	height	Equal to reflector height.
	width	147.32 cm	width	147.32 cm
	thickness	5.715 cm	thickness	5.715 cm
Lucite® Thickness	1.905 cm		1.905 cm	
Slab Thickness	Varies for each experiment using a Lucite® insert on one side of the box -see Table 32		Varies for each experiment using a Lucite® insert on one side of the box -see Table 32	
Spacer Insert Dimensions (Cases 2-5)	height	2.54 cm	Spacers have been homogenized into solution.	
	width	2.54 cm		
	length	varies with slab thickness		
Solution and Reflector Height	see Table 32		see Table 32	
Spacer Placement (Cases 2-5)	30.48 cm on centers with top row 121.92 cm high. Centered in the 147.32 cm dimension. Two additional spacers located at the top of the Lucite® box.		Spacers have been homogenized into solution.	

3.3 Material Data

3.3.1 Solution for Detailed Model

Solution properties in Tables 12 and 13, a ^{235}U enrichment of 93.2%, a ^{234}U enrichment of 1.14% (see Section 2.1.4), and nuclear constants provided in ICSBEP Document Content and Format Guide were used to calculate the following atom densities. Sample atom density calculations can be found in Appendix C. Solution atom densities for the detailed benchmark model are provided in Table 34.

Table 34. Solution Atom Densities for Detailed Model.

Isotope	Isotopic Compositions/ Totals	Atom Densities (atom/b-cm)	
		Cases 1-3	Cases 4-5
H/^{235}U ratio (calculated)		44.5	51.2
U	total	1.4587E-03	1.2871E-03
U-234	--	1.6711E-05	1.4746E-05
U-235	--	1.3604E-03	1.2004E-03
U-238	--	8.1573E-05	7.1977E-05
O	--	3.3188E-02	3.3274E-02
F	--	2.9174E-03	2.5742E-03
H	--	6.0542E-02	6.1399E-02
Be	--	1.6523E-08	1.5779E-08
Ni	total	2.9602E-06	2.8267E-06
Ni-58	68.08%	2.0153E-06	1.9244E-06
Ni-60	26.22%	7.7615E-07	7.4116E-07
Ni-61	1.14%	3.3746E-08	3.2225E-08
Ni-62	3.63%	1.0745E-07	1.0261E-07
Ni-64	0.93%	2.7529E-08	2.6288E-08
Sn	total	4.1813E-08	3.9929E-08
Sn-112	0.97%	4.0560E-10	3.8731E-10
Sn-114	0.65%	2.7179E-10	2.5954E-10
Sn-115	0.34%	1.4217E-10	1.3576E-10
Sn-116	14.54%	6.0798E-09	5.8057E-09
Sn-117	7.68%	3.2113E-09	3.0666E-09
Sn-118	24.22%	1.0127E-08	9.6708E-09
Sn-119	8.59%	3.5918E-09	3.4299E-09
Sn-120	32.59%	1.3627E-08	1.3013E-08
Sn-122	4.63%	1.9360E-09	1.8487E-09
Sn-124	5.79%	2.4210E-09	2.3119E-09
Si	total	1.7673E-07	1.6877E-07
Si-28	92.23%	1.6300E-07	1.5566E-07
Si-29	4.67%	8.2536E-09	7.8816E-09
Si-30	3.10%	5.4789E-09	5.2319E-09

Table 34 (cont'd). Solution Atom Densities for Detailed Model.

Isotope	Isotopic Compositions/ Totals	Atom Densities (atom/b-cm) Cases 1-3	Cases 4-5
Li	total	1.4303E-07	1.3658E-07
Li-6	7.50%	1.0727E-08	1.0243E-08
Li-7	92.50%	1.3230E-07	1.2634E-07
P	--	5.4563E-07	5.2103E-07
Na	--	2.1591E-07	2.0618E-07
Mn	--	4.1562E-07	3.9688E-07
Mg	total	3.2676E-06	3.1204E-06
Mg-24	78.99%	2.5811E-06	2.4648E-06
Mg-25	10.00%	3.2676E-07	3.1203E-07
Mg-26	11.01%	3.5977E-07	3.4355E-07
K	total	6.3478E-07	6.0617E-07
K-39	93.26%	5.9198E-07	5.6530E-07
K-40	0.01%	7.4269E-11	7.0921E-11
K-41	6.73%	4.2722E-08	4.0796E-08
Fe	total	2.6665E-05	2.5463E-05
Fe-54	5.85%	1.5599E-06	1.4895E-06
Fe-56	91.75%	2.4465E-05	2.3362E-05
Fe-57	2.12%	5.6529E-07	5.3980E-07
Fe-58	0.28%	7.4660E-08	7.1295E-08
Cu	total	4.3743E-07	4.1771E-07
Cu-63	69.17%	3.0257E-07	2.8893E-07
Cu-65	30.83%	1.3486E-07	1.2878E-07
Cr	total	3.0549E-06	2.9172E-06
Cr-50	4.35%	1.3289E-07	1.2690E-07
Cr-52	83.79%	2.5597E-06	2.4443E-06
Cr-53	9.50%	2.9021E-07	2.7713E-07
Cr-54	2.36%	7.2095E-08	6.8845E-08
Ca	total	6.1926E-07	5.9135E-07
Ca-40	96.94%	6.0032E-07	5.7326E-07
Ca-42	0.65%	4.0066E-09	3.8260E-09
Ca-43	0.14%	8.3600E-10	7.9832E-10
Ca-44	2.09%	1.2918E-08	1.2335E-08
Ca-46	0.00%	2.4770E-11	2.3654E-11
Ca-48	0.19%	1.1580E-09	1.1058E-09

Table 34 (cont'd). Solution Atom Densities for Detailed Model.

Isotope	Isotopic Compositions/ Totals	Atom Densities (atom/b-cm) Cases 1-3	Cases 4-5
Ba	total	3.6145E-08	3.4516E-08
Ba-130	0.11%	3.8314E-11	3.6587E-11
Ba-132	0.10%	3.6507E-11	3.4861E-11
Ba-134	2.42%	8.7472E-10	8.3529E-10
Ba-135	6.59%	2.3831E-09	2.2756E-09
Ba-136	7.85%	2.8374E-09	2.7095E-09
Ba-137	11.23%	4.0591E-09	3.8762E-09
Ba-138	71.70%	2.5916E-08	2.4748E-08
B	total	4.5914E-08	4.3844E-08
B-10	19.90%	9.1369E-09	8.7250E-09
B-11	80.10%	3.6777E-08	3.5119E-08
Al	--	5.7030E-06	5.4459E-06
Ag	total	2.0423E-08	1.9502E-08
Ag-107	51.84%	1.0587E-08	1.0110E-08
Ag-109	48.16%	9.8358E-09	9.3924E-09
Total		9.8151E-02	9.8577E-02

3.3.2 Other Materials

Lucite® mass density is 1.19 g/cm^3 and the empirical chemical formula was used to obtain the atom densities in Table 35.

Oak Ridge National Laboratory is approximated to be at an elevation of about 300 meters above sea level. Air density as a function of elevation was taken from Perry's Chemical Engineering Handbook.[a] An average air density of 0.00119101 g/cm^3 and pure air (i.e. 79.0% N_2 and 21.0 % O_2) was used to find the atom densities in Table 35.

Reference 1 gives a system temperature range of 72-75 ^{o}F. Density was obtained from the CRC Handbook[b] for water at 73.5 ^{o}F. Water was assumed to be pure.

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[a] *Perry's Chemical Engineering Handbook 7th ed.*
[b] Standard water densities at various temperatures from: *The CRC Handbook of Chemistry and Physics, 89th ed. (Internet version 2009)*.

Table 35. Atom Densities for Other Materials.

Material	Element	Atom Density (atom/b-cm)
Lucite®	total	1.0737E-01
	H	5.7263E-02
	C	3.5790E-02
	O	1.4316E-02
Air	total	4.9721E-05
	N	3.9280E-05
	O	1.0441E-05
Water	total	1.0004E-01
	H	6.6690E-02
	O	3.3345E-02

Lucite®, air, and water atom densities are the same for the detailed and simple models.

3.3.3 Solution for Simple Model

For the simple model all impurities were removed from the solution and for Cases 2-5 spacers were homogenized into the solution. Solution atom densities for the simple benchmark model are provided in Table 36.

Table 36. Atom Densities of Simple Model Solution.

Case →	1	2	3	4	5
Isotope ↓	Atom Density (atoms/b-cm)				
^{235}U	1.3604E-03	1.3527E-03	1.3537E-03	1.1919E-03	1.1923E-03
^{234}U	1.6711E-05	1.6616E-05	1.6629E-05	1.4642E-05	1.4646E-05
^{238}U	8.1573E-05	8.1109E-05	8.1170E-05	7.1470E-05	7.1493E-05
Oxygen	3.3188E-02	3.3080E-02	3.3095E-02	3.3140E-02	3.3146E-02
Fluorine	2.9174E-03	2.9008E-03	2.9030E-03	2.5561E-03	2.5569E-03
Hydrogen	6.0542E-02	6.0522E-02	6.0525E-02	6.1368E-02	6.1369E-02
Carbon	-- [a]	2.0311E-04	1.7627E-04	2.5094E-04	2.3965E-04

(a) Case 1 does not have any spacers and thus no carbon in the homogenized solution.

3.4 Temperature Data

The temperature of the benchmark models is 23.06 ^oC.

3.5 Benchmark Model k_{eff}

All experiments were measured at critical and no biases were applied to the benchmark k_{eff} for the detailed model (Table 37). Uncertainties in k_{eff} were calculated in Section 2.

Table 37. Benchmark Model k_{eff} and Uncertainties (1σ) for Detailed Model.

Case	k_{eff}	Uncertainty
1	1.0000	± 0.0027
2	1.0000	± 0.0022
3	1.0000	± 0.0026
4	1.0000	± 0.0023
5	1.0000	± 0.0019

The simplified model had no additional uncertainty. The biased benchmark k_{eff} for the simple models are shown in Table 38.

Table 38. Benchmark Model k_{eff} and Uncertainties (1σ) for Simplified Model.

Case	k_{eff}	Uncertainty
1	1.0002	± 0.0027
2	1.0010	± 0.0022
3	1.0011	± 0.0026
4	1.0008	± 0.0023
5	1.0010	± 0.0019

4.0 RESULTS OF SAMPLE CALCULATIONS

All calculations were performed with the MCNP5 code using both continuous energy ENDF/B-VI.8 and ENDF/B-VII.0 cross section data. Typical input listings are provided in Appendix A. A thermal scattering treatment for water was used for Lucite®. The effect of various scatter treatments was investigated and the results can be found in Appendix F.

A basic execution of the detailed and simple models using KENO-VI and KENO-V.a,[a] respectively, serves as a comparison to the MCNP results. Results are shown in Table 39.

Table 39. Sample Calculation Results for Detailed Model.

Case	MCNP5 (Continuous Energy ENDF/B-VI.8)		MCNP5 (Continuous Energy ENDF/B-VII.0)		KENO-VI (238-Group ENDF/B-VII.0) (b)	
	$k_{eff} \pm 1\sigma$	% Deviation(a)	$k_{eff} \pm 1\sigma$	% Deviation(a)	$k_{eff} \pm 1\sigma$	% Deviation(a)
1	0.9943 ± 0.00005	-0.57%	0.9996 ± 0.00005	-0.04%	0.9987±0.0021	-0.13%
2	0.9912 ± 0.00005	-0.88%	0.9968 ± 0.00005	-0.32%	0.9948±0.0023	-0.52%
3	0.9936 ± 0.00005	-0.64%	0.9992 ± 0.00005	-0.08%	0.9973±0.0020	-0.27%
4	0.9932 ± 0.00005	-0.69%	0.9987 ± 0.00005	-0.13%	0.9974±0.0020	-0.26%
5	0.9913 ± 0.00005	-0.87%	0.9969 ± 0.00005	-0.31%	0.9910±0.0021	-0.90%

(a) Percent deviation is with respect to benchmark k_{eff}.
(b) KENO results provided by John Bess at INL

Calculations were also performed for the simple models. The results are listed in Table 40.

[a] "SCALE: A Modular Code System for Performing Standardized Computer Analyses," ORNL/TM-2005/39, Version 6, Oak Ridge National Laboratory (2009).

Table 40. Sample Calculation Results for Simplified Model.

Case	MCNP5 (Continuous Energy ENDF/B-VI.8)		MCNP5 (Continuous Energy ENDF/B-VII.0)		KENO-VI (238-Group ENDF/B-VII.0) [b]	
	$k_{eff} \pm 1\sigma$	% Deviation[a]	$k_{eff} \pm 1\sigma$	% Deviation[a]	$k_{eff} \pm 1\sigma$	% Deviation[a]
1	0.9944 ± 0.00005	-0.58%	0.9997 ± 0.00005	0.05%	0.9969±0.0021	0.33%
2	0.9920 ± 0.00005	-0.90%	0.9974 ± 0.00005	0.36%	0.9946±0.0020	0.64%
3	0.9945 ± 0.00005	-0.66%	0.9998 ± 0.00005	0.13%	0.9991±0.0019	0.20%
4	0.9939 ± 0.00005	-0.69%	0.9993 ± 0.00005	0.15%	0.9991±0.0022	0.17%
5	0.9921 ± 0.00005	-0.89%	0.9975 ± 0.00005	-0.35%	0.9968±0.0021	0.42%

(a) Percent deviation is with respect to benchmark k_{eff}.
(b) KENO results provided by John Bess at INL

5.0 REFERENCES

1. J. K. Fox, L. W. Gilley, and J. H. Marable, "Critical Parameters of a Proton-Moderated and Proton-Reflected Slab of ^{235}U," *Nucl. Sci. Eng.*, **3**, 694 (1958).

APPENDIX A: SAMPLE INPUT LISTINGS

A.1 MCNP

MCNP5 calculations were performed using continuous energy, ENDF/B-VI.8 and VII.0 neutron cross section data and a water thermal scattering treatment for the solution and Lucite®. Calculations were performed with 4,000 generations with 100,000 neutrons per generation. The k_{eff} estimates did not include the first 150 generations and are the result of 385,000,000 neutron histories. The statistical uncertainty in k_{eff} is 0.0005.

MCNP Input Listing for Case 1 Simple Model, Table 40.

```
Experiment 105: simple model
C    No air; insert part of box; reflector 30 cm wide;
C    box cut at reflector height; no impurities
C    Experiment 105  has no support blocks
C
C
100   2   1.0737e-01  100 -101 imp:n=1 $lucite box 71x58x2.25
103   1   9.8106E-02 -100 -113  imp:n=1 $uranium oxyfluoride solution
107   0    -100  113   imp:n=1 $void above solution
400   3   1.0004e-01 101 -114 -300  imp:n=1 $water reflector
500   0     101  114 -300  imp:n=1 $void above reflector and box
600   0     300    imp:n=0

C    Lucite box cut at reflector height
100   rpp -2.5400 2.8575 -73.66 73.66 0 116.6 $inside of box + insert
101   rpp -4.7625 4.7625 -75.565 75.565 -1.905 116.6 $outside of box
C    liquid surfaces
113    pz  71.5772      $ height of solution
114    pz  116.6        $ height of reflector
c
300    rpp -34.7625 34.7625 -105.565 105.565 -31.905 210.34

c    m1: uranium oxyfluoride solution
m1   92235.66c  1.3604E-03
     92234.66c  1.6711E-05
     92238.66c  8.1573E-05
      8016.62c  3.3188E-02
      9019.62c  2.9174E-03
      1001.62c  6.0542E-02  $ 9.8106E-02
mt1  lwtr.60t
c    m2: lucite
m2    1001.62c 5.7263e-02
      6000.66c 3.5790e-02
      8016.62c 1.4316e-02
mt2  lwtr.60t
c    m3: light water reflector
m3    8016.62c 3.3345e-02
      1001.62c 6.6690e-02
mt3  lwtr.60t
kcode 100000 1 150 4000
ksrc 0 -60.96 5.08    0 -30.48 5.08   0 0 5.08   0 30.48 5.08   0 60.96 5.08
```

```
0 -60.96 35.56   0 -30.48 35.56  0 0 35.56  0 30.48 35.56  0 60.96 35.56
0 -60.96 66.04   0 -30.48 66.04  0 0 66.04  0 30.48 66.04  0 60.96 66.04
```

MCNP Input Listing for Case 1 Detailed Model, Table 40.

```
Experiment 105
C    Experiment 105  has no support blocks
C
C
100   2   1.0737e-01  100 -101 imp:n=1 $lucite box 71x58x2.25
101   2   1.0737E-01  -100 -150 imp:n=1 $thickness varying insert
103   1   9.8151E-02 -100 -113 150 imp:n=1 $uranium oxyfluoride solution
107   4   4.9721e-05 -100  113 150  imp:n=1 $space above solution
400   3   1.0004e-01 101 -114 -300  imp:n=1 $water reflector
500   4   4.9721e-05  101  114 -300  imp:n=1 $space above reflector and box
600   0      300    imp:n=0

C    Lucite box
100   rpp -2.8575 2.8575 -73.66 73.66 0 180.34 $inside of box
101   rpp -4.7625 4.7625 -75.565 75.565 -1.905 180.34 $outside of box
C    liquid surfaces
113    pz  71.5772      $ height of solution
114    pz  116.6        $ height of reflector
C    insert to control slab thickness
150    px -2.5400
c
300    so  600

c    m1: uranium oxyfluoride solution
m1   92235.66c 1.3604E-03
     92234.66c 1.6711E-05
     92238.66c 8.1573E-05
      8016.62c 3.3188E-02
      9019.62c 2.9174E-03
      1001.62c 6.0542E-02
      4009.62c 1.6523e-08
     28058.62c 2.0153E-06
     28060.62c 7.7615E-07
     28061.62c 3.3746E-08
     28062.62c 1.0745E-07
     28064.62c 2.7529E-08
     50000.42c 4.1814e-08
     14000.60c 1.7674E-08
      3007.66c 1.4303E-07
     15031.66c 5.4563E-07
     11023.62c 2.1591E-07
     25055.62c 4.1562E-07
     12000.62c 3.2676E-06
     19000.62c 6.3478E-07
     26054.62c 1.5599E-06
     26056.62c 2.4465E-05
     26057.62c 5.6529E-07
     26058.62c 7.4660E-08
     29063.62c 3.0257E-07
     29065.62c 1.3486E-07
     24050.62c 1.3289E-07
     24052.62c 2.5597E-06
     24053.62c 2.9021E-07
```

```
     24054.62c 7.2095E-08
     20000.62c 6.1926E-07
     56138.66c 3.6146E-08
      5010.66c 4.5914E-08
     13027.62c 5.7030E-06
     47107.60c 1.0587E-08
     47109.66c 9.8358e-09
mt1  lwtr.60t
c    m2: lucite
m2    1001.62c 5.7263e-02
      6000.66c 3.5790e-02
      8016.62c 1.4316e-02
mt2  lwtr.60t
c    m3: light water reflector
m3    8016.62c 3.3345e-02
      1001.62c 6.6690e-02
mt3  lwtr.60t
C    m4: air
m4    8016.62c 1.0441e-05
      7014.62c 3.9280e-05
kcode 100000 1 150 4000
ksrc 0 -60.96 5.08    0 -30.48 5.08   0 0 5.08   0 30.48 5.08   0 60.96 5.08
     0 -60.96 35.56   0 -30.48 35.56  0 0 35.56  0 30.48 35.56  0 60.96 35.56
     0 -60.96 66.04   0 -30.48 66.04  0 0 66.04  0 30.48 66.04  0 60.96 66.04
C     0 -60.96 38   0 -30.48 38  0 0 38  0 30.48 38  0 60.96 38
C     0 -60.96 50   0 -30.48 50  0 0 50  0 30.48 50  0 60.96 50
C     0 -60.96 62   0 -30.48 62  0 0 62  0 30.48 26  0 60.96 62
```

MCNP Input Listing for Case 5 Simple Model, Table 40.

```
Experiment 112:  simple model
C    No air; insert part of box; no out of solution supports; reflector 30 cm
C    wide; box cut at reflector height; no impurities; homogenized supports
C    in solution
C
C
100  2   1.0737e-01  100 -101 imp:n=1 $lucite box 71x58x2.25
150  1   9.8590E-02 -100 -113 imp:n=1 $solution
160  0      -100 113 imp:n=1 $space above solution
400  3   1.0004e-01 101 -114 -300  imp:n=1 $water reflector
500  0       101  114 -300  imp:n=1 $space above reflector
600  0       300    imp:n=0

C    Lucite box
100   rpp -2.2098 2.8575 -73.66 73.66 0 164.35 $inside of box
101   rpp -4.7625 4.7625 -75.565 75.565 -1.905 164.35 $outside of box
C    liquid surfaces
113    pz  130.2512      $ height of solution
114    pz  162.3     $ height of reflector
c
300    rpp -34.7625 34.7625 -105.565 105.565 -31.905 210.34

c    m1: uranium oxyfluoride solution
m1   92235.66c   1.1923E-03
     92234.66c  1.4646E-05
     92238.66c  7.1493E-05
      8016.62c  3.3146E-02
      9019.62c  2.5569E-03
      1001.62c  6.1369E-02
      6000.66c  2.3965E-04
mt1  lwtr.60t
c    m2: lucite
m2    1001.62c 5.7263e-02
      6000.66c 3.5790e-02
      8016.62c 1.4316e-02
mt2  lwtr.60t
c    m3: light water reflector
m3    8016.62c 3.3345e-02
      1001.62c 6.6690e-02
mt3  lwtr.60t
kcode 100000 1 150 4000
ksrc 0 -60.96 5.08    0 -30.48 5.08   0 0 5.08   0 30.48 5.08   0 60.96 5.08
     0 -60.96 35.56   0 -30.48 35.56  0 0 35.56  0 30.48 35.56  0 60.96 35.56
     0 -60.96 66.04   0 -30.48 66.04  0 0 66.04  0 30.48 66.04  0 60.96 66.04
print 40
```

MCNP Input Listing for Case 5 of Detailed Model, Table 40.

```
Experiment 112
C
C
100  2   1.0737e-01  100 -101 imp:n=1 $lucite box 71x58x2.25
101  2   1.0737E-01  -100 -150 imp:n=1 $thickness varying insert
102  2   1.0737E-01  -102  u=1 imp:n=1 $support blocks
103  1   9.8577E-02  102   u=1 imp:n=1 $UO2F2 around support blocks
104  0      -106 105 -108 107  lat=1 fill=1 u=2 imp:n=1
105  0      -100 -113 150 109 fill=2 imp:n=1 $support blocks and UO2F2
106  2   1.0737E-01  -102  u=3 imp:n=1 $support blocks
107  4   4.9721e-05     102  u=3 imp:n=1 $void around support blocks
108  0      -106 105 -108 107  lat=1 fill=3 u=4 imp:n=1
109  0      -100 113 150 -110 fill=4 imp:n=1 $support blocks and void
112  2   1.0737E-01 -103 -100 150 105 imp:n=1 $ upper support block
113   like 112 but trcl (0 -60.96 0) imp:n=1 $upper support block
150  1   9.8577E-02 -100 150 -113 #105 imp:n=1 $solution w/o supports
160  4   4.9721E-05  -100 110 113 150 #112 #113 imp:n=1 $space w/o supports
400  3   1.0004e-01 101 -114 -300  imp:n=1 $water reflector
500  4   4.9721E-05    101  114 -300  imp:n=1 $space above reflector
600  0       300    imp:n=0

C    Lucite box
100   rpp -2.8575 2.8575 -73.66 73.66 0 180.34 $inside of box
101   rpp -4.7625 4.7625 -75.565 75.565 -1.905 180.34 $outside of box
C    Support blocks
102   rpp -2.9 2.9 -1.27 1.27 29.21 31.75
103   rpp -2.9 2.9 29.21 31.75 177.8 180.34
C    lattice window
105   py  -15.24
106   py   15.24
107   pz   15.24
108   pz   45.72
109   pz   24.4
110   pz   127
C    liquid surfaces
113    pz  130.2512      $ height of solution
114    pz  162.3     $ height of reflector
C    insert to control thickness
150    px -2.2098
c
300    so  600

c    m1: uranium oxyfluoride solution
m1   92235.66c 1.2004E-03
     92234.66c 1.4746E-05
     92238.66c 7.1977E-05
      8016.62c 3.3274E-02
      9019.62c 2.5742E-03
      1001.62c 6.1399E-02
      4009.62c 1.5779e-08
     28058.62c 1.9244E-06
     28060.62c 7.4116E-07
     28061.62c 3.2225E-08
```

```
     28062.62c 1.0261E-07
     28064.62c 2.6288E-08
     50000.42c 3.9929e-08
     14000.60c 1.6877E-07
      3007.66c 1.3658E-07
     15031.66c 5.2103E-07
     11023.62c 2.0618E-07
     25055.62c 3.9688E-07
     12000.62c 3.1203E-06
     19000.62c 6.0616E-07
     26054.62c 1.4895E-06
     26056.62c 2.3362E-05
     26057.62c 5.3980E-07
     26058.62c 7.1295E-08
     29063.62c 2.8893E-07
     29065.62c 1.2878E-07
     24050.62c 1.2690E-07
     24052.62c 2.4443E-06
     24053.62c 2.7713E-07
     24054.62c 6.8845E-08
     20000.62c 5.9135E-07
     56138.66c 3.4516E-08
      5010.66c 4.3844E-08
     13027.62c 5.4459E-06
     47107.66c 1.0110E-08
     47109.66c 9.3924e-09
mt1  lwtr.60t
c    m2: lucite
m2    1001.62c 5.7263e-02
      6000.66c 3.5790e-02
      8016.62c 1.4316e-02
mt2  lwtr.60t
c    m3: light water reflector
m3    8016.62c 3.3345e-02
      1001.62c 6.6690e-02
mt3  lwtr.60t
C    m4: air
m4    8016.62c 1.0441e-05
      7014.62c 3.9280e-05
kcode 100000 1 150 4000
ksrc 0 -60.96 5.08    0 -30.48 5.08   0 0 5.08   0 30.48 5.08   0 60.96 5.08
     0 -60.96 35.56   0 -30.48 35.56  0 0 35.56  0 30.48 35.56  0 60.96 35.56
     0 -60.96 66.04   0 -30.48 66.04  0 0 66.04  0 30.48 66.04  0 60.96 66.04
```

A.2 KENO Input Listing

KENO Input Listing for Case 1 Simple Model, Table 40.

```
'Input generated by GeeWiz SCALE 6.0.2 Compiled on February 18, 2009
=csas5
hst034 case 1 simple
v7-238
read composition
 u-234       1 0 1.6609e-05 296.21   end
 u-235       1 0 0.0013521 296.21   end
 u-238       1 0 8.1074e-05 296.21   end
 o           1 0 0.033073 296.21   end
 f           1 0 0.0028996 296.21   end
 h           1 0 0.060522 296.21   end
 c           1 0 0.00021897 296.21   end
 h           2 0 0.057263 296.21   end
 c           2 0 0.03579 296.21   end
 o           2 0 0.014316 296.21   end
 h           3 0 0.06669 296.21   end
 o           3 0 0.033345 296.21   end
end composition
read celldata
  infhommedium 1 end
  infhommedium 2 end
  infhommedium 3 end
end celldata
read parameter
 htm=yes
end parameter
read geometry
global unit 1
com='global unit 1'
 cuboid 1 1     2.54  -2.8575    73.66   -73.66  71.5772        0
 cuboid 0 1     2.54  -2.8575    73.66   -73.66    116.6        0
 cuboid 2 1   4.7625  -4.7625   75.565  -75.565    116.6   -1.905
 cuboid 3 1  34.7625  -34.7625  105.565  -105.565    116.6  -31.905
end geometry
end data
end
```

KENO Input Listing for Case 1 Detailed Model, Table 40.

```
'Input generated by GeeWiz SCALE 6.0.2 Compiled on February 18, 2009
=csas6
hst034 case 1
v7-238
read composition
 u-234       1 0 1.6711e-05 296.21   end
 u-235       1 0 0.0013604 296.21   end
 u-238       1 0 8.1573e-05 296.21   end
 o           1 0 0.033188 296.21   end
 f           1 0 0.0029174 296.21   end
 h           1 0 0.060542 296.21   end
 be          1 0 1.6523e-08 296.21   end
 ni          1 0 2.9602e-06 296.21
                                28058 68.08
                                28060 26.22
                                28061 1.14
                                28062 3.63
                                28064 0.93   end
 sn          1 0 4.1814e-08 296.21
                                50112 0.97
                                50114 0.65
                                50115 0.34
                                50116 14.54
                                50117 7.68
                                50118 24.22
                                50119 8.59
                                50120 32.59
                                50122 4.63
                                50124 5.79   end
 si          1 0 1.7674e-07 296.21
                                14028 92.23
                                14029 4.67
                                14030 3.1   end
 li          1 0 1.4303e-07 296.21
                                3006 7.5
                                3007 92.5   end
 p           1 0 5.4563e-07 296.21   end
 na          1 0 2.1591e-07 296.21   end
 mn          1 0 4.1562e-07 296.21   end
 mg          1 0 3.2676e-06 296.21
                                12024 78.99
                                12025 10
                                12026 11.01   end
 k           1 0 6.3478e-07 296.21
                                19039 93.26
                                19040 0.01
                                19041 6.73   end
 fe          1 0 2.6664e-05 296.21
                                26054 5.85
                                26056 91.75
                                26057 2.12
                                26058 0.28   end
 cu          1 0 4.3743e-07 296.21
```

```
                                29063 69.17
                                29065 30.83   end
 cr          1 0 3.0549e-06 296.21
                                24050 4.35
                                24052 83.79
                                24053 9.5
                                24054 2.36   end
 ca          1 0 6.1926e-07 296.21
                                20040 96.94
                                20042 0.65
                                20043 0.14
                                20044 2.09
                                20048 0.18   end
 ba          1 0 3.6146e-08 296.21
                                56130 0.11
                                56132 0.1
                                56134 2.42
                                56135 6.59
                                56136 7.85
                                56137 11.23
                                56138 71.7   end
 b           1 0 4.5914e-08 296.21
                                5010 19.9
                                5011 80.1   end
 al          1 0 5.703e-06 296.21   end
 ag          1 0 2.0423e-08 296.21
                                47107 51.84
                                47109 48.16   end
 h           2 0 0.057263 296.21   end
 c           2 0 0.03579 296.21   end
 o           2 0 0.014316 296.21   end
 h           3 0 0.06669 296.21   end
 o           3 0 0.033345 296.21   end
 n           4 0 3.928e-05 296.21   end
 o           4 0 1.0441e-05 296.21   end
end composition
read celldata
  infhommedium 1 end
  infhommedium 2 end
  infhommedium 3 end
  infhommedium 4 end
end celldata
read parameter
 htm=yes
 nub=no
end parameter
read geometry
global unit 1
com='uo2f2 slab'
 cuboid 1   2.8575  -2.8575    73.66   -73.66  71.5772        0
 cuboid 2   2.8575  -2.8575    73.66   -73.66   180.34        0
 cuboid 3     2.54  -2.8575    73.66   -73.66   180.34        0
 cuboid 4   4.7625  -4.7625  75.5655  -75.5655   180.34   -1.905
 cuboid 5  34.7625  -34.7625  105.5655  -105.5655    116.6  -31.905
 cuboid 6  34.7625  -34.7625  105.5655  -105.5655   180.34  -31.905
```

```
 media 1 1 1 3
 media 4 1 3 -1
 media 2 1 2 -3
 media 2 1 -2 4
 media 3 1 -4 5
 media 4 1 6 -4 -5
 boundary 6
end geometry
read start
 nst=0
 xsm=0
 xsp=2.5
 ysm=0
 ysp=70
 zsm=0
 zsp=70
  end start
end data
end
```

KENO Input Listing for Case 5 Simple Model, Table 40.

```
'Input generated by GeeWiz SCALE 6.0.2 Compiled on February 18, 2009
=csas5
hst034 case 1 simple
v7-238
read composition
 u-234       1 0 1.4646e-05 296.21   end
 u-235       1 0 0.0011923 296.21   end
 u-238       1 0 7.1493e-05 296.21   end
 o           1 0 0.033146 296.21   end
 f           1 0 0.0025569 296.21   end
 h           1 0 0.061369 296.21   end
 c           1 0 0.00023965 296.21   end
 h           2 0 0.057263 296.21   end
 c           2 0 0.03579 296.21   end
 o           2 0 0.014316 296.21   end
 h           3 0 0.06669 296.21   end
 o           3 0 0.033345 296.21   end
end composition
read celldata
  infhommedium 1 end
  infhommedium 2 end
  infhommedium 3 end
end celldata
read parameter
 htm=yes
end parameter
read geometry
global unit 1
com='global unit 1'
 cuboid 1 1   2.2098  -2.8575    73.66   -73.66  130.2512        0
 cuboid 0 1   2.2098  -2.8575    73.66   -73.66    162.3        0
 cuboid 2 1   4.7625  -4.7625   75.565  -75.565    162.3   -1.905
 cuboid 3 1  34.7625  -34.7625  105.565  -105.565    162.3  -31.905
end geometry
end data
end
```

KENO Input Listing for Case 5 Detailed Model, Table 40.

```
'Input generated by GeeWiz SCALE 6.0.2 Compiled on February 18, 2009
=csas6
hst034 case 5
v7-238
read composition
 u-234        1 0 1.4746e-05 296.21   end
 u-235        1 0 0.0012004 296.21   end
 u-238        1 0 7.1977e-05 296.21   end
 o            1 0 0.033274 296.21   end
 f            1 0 0.0025742 296.21   end
 h            1 0 0.061399 296.21   end
 be           1 0 1.5779e-08 296.21   end
 ni           1 0 2.8267e-06 296.21
                                28058 68.08
                                28060 26.22
                                28061 1.14
                                28062 3.63
                                28064 0.93   end
 sn           1 0 3.9929e-08 296.21
                                50112 0.97
                                50114 0.65
                                50115 0.34
                                50116 14.54
                                50117 7.68
                                50118 24.22
                                50119 8.59
                                50120 32.59
                                50122 4.63
                                50124 5.79   end
 si           1 0 1.6877e-07 296.21
                                14028 92.23
                                14029 4.67
                                14030 3.1   end
 li           1 0 1.3658e-07 296.21
                                3006 7.5
                                3007 92.5   end
 p            1 0 5.2103e-07 296.21   end
 na           1 0 2.0618e-07 296.21   end
 mn           1 0 3.9688e-07 296.21   end
 mg           1 0 3.1203e-06 296.21
                                12024 78.99
                                12025 10
                                12026 11.01   end
 k            1 0 6.0616e-07 296.21
                                19039 93.26
                                19040 0.01
                                19041 6.73   end
 fe           1 0 2.5462e-05 296.21
                                26054 5.85
                                26056 91.75
                                26057 2.12
                                26058 0.28   end
 cu           1 0 4.1771e-07 296.21
```

```
                                29063 69.17
                                29065 30.83   end
 cr          1 0 2.9171e-06 296.21
                                24050 4.35
                                24052 83.79
                                24053 9.5
                                24054 2.36   end
 ca          1 0 5.9135e-07 296.21
                                20040 96.94
                                20042 0.65
                                20043 0.14
                                20044 2.09
                                20048 0.18   end
 ba          1 0 3.4516e-08 296.21
                                56130 0.11
                                56132 0.1
                                56134 2.42
                                56135 6.59
                                56136 7.85
                                56137 11.23
                                56138 71.7   end
 b           1 0 4.3844e-08 296.21
                                5010 19.9
                                5011 80.1   end
 al          1 0 5.4459e-06 296.21   end
 ag          1 0 1.9502e-08 296.21
                                47107 51.84
                                47109 48.16   end
 h           2 0 0.057263 296.21   end
 c           2 0 0.03579 296.21   end
 o           2 0 0.014316 296.21   end
 h           3 0 0.06669 296.21   end
 o           3 0 0.033345 296.21   end
 n           4 0 3.928e-05 296.21   end
 o           4 0 1.0441e-05 296.21   end
end composition
read celldata
  infhommedium 1 end
  infhommedium 2 end
  infhommedium 3 end
  infhommedium 4 end
end celldata
read parameter
 htm=yes
 nub=no
end parameter
read geometry
unit 1
com='lucite pegs'
 cuboid 1   2.8575  -2.8575     1.27    -1.27     1.27    -1.27
 media 2 1 1
 boundary 1
global unit 2
com='uo2f2 slab'
 cuboid 1   2.8575  -2.8575    73.66   -73.66  130.2512        0
```

```
 cuboid 3   2.2098  -2.8575    73.66   -73.66   180.34        0
 cuboid 4   4.7625  -4.7625  75.5655  -75.5655   180.34   -1.905
 cuboid 5  34.7625  -34.7625  105.5655  -105.5655    162.3  -31.905
 cuboid 6  34.7625  -34.7625  105.5655  -105.5655   180.34  -31.905
 cuboid 2   2.8575  -2.8575    73.66   -73.66   180.34        0
 hole 1   origin  x=0 y=-60.96 z=30.48
 hole 1   origin  x=0 y=-30.48 z=30.48
 hole 1   origin  x=0 y=0 z=30.48
 hole 1   origin  x=0 y=30.48 z=30.48
 hole 1   origin  x=0 y=60.96 z=30.48
 hole 1   origin  x=0 y=-60.96 z=60.96
 hole 1   origin  x=0 y=-30.48 z=60.96
 hole 1   origin  x=0 y=0 z=60.96
 hole 1   origin  x=0 y=30.48 z=60.96
 hole 1   origin  x=0 y=60.96 z=60.96
 hole 1   origin  x=0 y=-60.96 z=91.44
 hole 1   origin  x=0 y=-30.48 z=91.44
 hole 1   origin  x=0 y=0 z=91.44
 hole 1   origin  x=0 y=30.48 z=91.44
 hole 1   origin  x=0 y=60.96 z=91.44
 hole 1   origin  x=0 y=-60.96 z=121.92
 hole 1   origin  x=0 y=-30.48 z=121.92
 hole 1   origin  x=0 y=0 z=121.92
 hole 1   origin  x=0 y=30.48 z=121.92
 hole 1   origin  x=0 y=60.96 z=121.92
 hole 1   origin  x=0 y=-30.48 z=179.07
 hole 1   origin  x=0 y=30.48 z=179.07
 media 1 1 1 3
 media 4 1 3 -1
 media 2 1 2 -3
 media 2 1 -2 4
 media 3 1 -4 5
 media 4 1 6 -4 -5
 boundary 6
end geometry
read start
 nst=0
 xsm=0
 xsp=2.5
 ysm=0
 ysp=70
 zsm=0
 zsp=70
  end start
end data
end
```

APPENDIX B: EXPERIMENT 108 RESULTS

Analysis was done for Experiment 108 which was rejected as an acceptable criticality safety benchmark because of experimenters' lack of confidence in the data and the fact that Experiment 109 is a repeat of Experiment 108. Analyses were performed similar to those discussed for the accepted benchmark experiments.

B.1 Uncertainty Analysis Results

Table B.1. Results of Uncertainty Analysis for Exp. 108.

Experiment → / Parameter ↓	Exp. 108
Uranium Weight Fraction	*0.00119*[(a)]
Specific Gravity	*0.00212*[(a)]
U_{total} Weight Fraction and Specific Gravity	0.00190
Temperature	0.00016
Enrichment	0.00018
^{234}U wt.%	0.00037
^{236}U wt.%	NG[(b)]
Impurities	0.00035
Compounds	0.00021
Lucite® Purity	0.00032
Lucite® Density	0.00021
Solution Height	0.00015
Reflector Height	NG
Slab Thickness	0.00157
Box Length	NG
Lucite® Thickness	0.00016
Spacer Placement	NG
Overall	0.00257

(a) Values are not used in calculation of overall uncertainty because they accounted for with the correlated uncertainty.
(b) Negligible uncertainties are denoted with an NG and not included in to overall uncertainty calculation.

B.2 Results of Bias Assessment

Table B.2. Results of Bias Assessment for Exp. 108.

Experiment	No Air Δk	No Impurities Δk	Insert Merged with Box Δk	Cut Box at Reflector Height Δk	Homo-genized Spacers Δk	Simple Model Δk
108	-0.00006	0.00026	-0.00011	-0.00005	0.00053	0.00087

These results follow the same pattern as other biases set forth in Table 30 of Section 3.1.2.

B.3 Model Characteristics

B.3.1 Dimensions

The detailed and simple models of Experiment 108 are the same as Figures 4 and 5. Table B.3 contains the corresponding slab thickness and solution and reflector height for both the detailed and simple models. All other values are the same as those in Table 33.

Table B.3. Dimensions for Exp. 108.

Experiment	Slab Thickness (t, cm)	Solution Height (h_s, cm)	Reflector Height (h_r, cm)
108	5.080	99.4664	119.1

B.3.2 Materials

The composition of the detailed model solution is the same as Cases 1-3 in Table 34. The Lucite®, air, and water compositions are the same as in Table 35. Table B.4 contains the atom densities for the simple model of Experiment 108.

Table B.4. Simple Model Atom Densities for Exp. 108.

Experiment →	108
Isotope ↓	Atom Density (atom/b-cm)
U-235	1.3514E-03
U-234	1.6601E-05
U-238	8.1035E-05
Oxygen	3.3063E-02
Fluorine	2.8981E-03
Hydrogen	6.0519E-02
Carbon	2.3537E-04

The temperature of the Experiment 108 model is 23.05 ºC

B.4 Model k_{eff} and Uncertainties

Table B.5. Benchmark Model k_{eff} and Uncertainty (1σ).

Detailed Model		
Exp.	keff	Uncertainty
108	1.0000	± 0.0031
Simple Model		
Exp.	keff	Uncertainty
108	1.0009	± 0.0031

B.5 Results of Sample Calculations

Table B.6. Sample Calculation Results.

Detailed Model				
Experiment	MCNP5 (Continuous Energy ENDF/B-VI.8)		MCNP5 (Continuous Energy ENDF/B-VII.0)	
	$k_{eff} \pm 1\sigma$	% Deviation[(a)]	$k_{eff} \pm 1\sigma$	% Deviation[(a)]
108	0.9878 ± 0.00005	-1.22%	0.9936 ± 0.00004	-0.64%
Simple Model				
Experiment	MCNP5 (Continuous Energy ENDF/B-VI.8)		MCNP5 (Continuous Energy ENDF/B-VII.0)	
	$k_{eff} \pm 1\sigma$	% Deviation[(a)]	$k_{eff} \pm 1\sigma$	% Deviation[(a)]
108	0.9887 ± 0.00005	-1.22%	0.9942 ± 0.00005	-0.67%

(a) Percent deviation compared to accepted benchmark k_{eff}.

APPENDIX C: SUMMARY OF SOLUTION ATOM DENSITY CALCULATIONS

It should be noted that the following method of calculating atom density requires the knowledge of both the uranium weight fraction and the solution density. Because of the non-additive behavior of uranium oxyfluoride solutions methods such as those set forth in *Calculating Atomic Number Densities for Uranium Compounds*[a] should be followed if the uranium weight fraction and solution density are not accurately known.

To find the atom density of the fuel the molar density, *M.D.*, of the uranium oxyfluoride was calculated first:

$$M.D_{U_i} = Sp.G\ \rho_{water} x_U \gamma_i \frac{1}{MM_{U_i}} \tag{C.1}$$

$$M.D_j = A.R_j \sum_i M.D_{U_i} \tag{C.2}$$

$M.D_{U_i}$	=	Molar Density of i^{th} uranium isotope (moles/cm^3)
$Sp.G$	=	Specific Gravity of Solution
ρ_{water}	=	Standard density of water at solution temperature (g/cm^3)
x_U	=	Weight fraction of uranium in solution ($g_{Uranium}/g_{solution}$)
γ_i	=	Enrichment of i^{th} uranium isotope
MM_z	=	Molecular Weight of isotope, element, or molecule *z*.
$M.D_j$	=	Molar Density of j^{th} non-uranium element in uranium oxyfluoride molecule (moles/cm^3)
$A.R_j$	=	Atomic ratio of j^{th} non-uranium element in uranium oxyfluoride molecule (atom of *j*/atom of U)

Next the density of water in the solution was found by first converting all molar densities to mass density. Mass density of the uranium oxyfluoride and impurities (including any compounds formed) was then subtracted from the total solution density to find the density of water. This density and the impurity densities were then converted into molar densities. Finally the molar densities were converted to atom densities.

$$\rho_{UO_2F_2} = \sum_i \left(M.D_{U_i} MM_{U_i}\right) + \sum_j M.D_j MM_j \tag{C.3}$$

$$\rho_{imp} = Sp.G\ \rho_{water} \sum_i x_n \tag{C.4}$$

[a] R. W. Tayloe and T. C. Davis. *Calculating Atomic Number Densities for Uranium Compounds*. Martin Marietta Energy Systems, POEF-T-3545, Jan. 1993.

$$\rho_{H_2O} = Sp.G\ \rho_{water} - \rho_{UO_2F_2} - \rho_{imp} \tag{C.5}$$

$$M.D_{H_2O} = \rho_{H_2O}\frac{1}{MM_{H_2O}} \tag{C.6}$$

$$M.D_{n^{th}\ imp.} = x_n Sp.G\ \rho_{water}\frac{1}{MM_{n^{th}\ imp.}} \tag{C.7}$$

$$N_k = M.D_k N_A \frac{1\ cm^2}{10^{24}\ barn} \tag{C.8}$$

$\rho_{UO_2F_2}$	=	Density of uranium oxyfluoride in solution (g UO_2F_2/cm^3)
ρ_{imp}	=	Density of impurities and compounds in solution (g /cm^3)
x_n	=	Concentration of n^{th} impurity/compound (g impurity/ g solution)
ρ_{H_2O}	=	Density of water in solution (g H_2O/cm^3)
$M.D_{H_2O}$	=	Molar density of water (moles H_2O/cm^3)
$M.D_{n^{th}\ imp.}$	=	Molar density of n^{th} impurity in solution (mole/cm^3)
N_k	=	Atom density of k^{th} element/isotope (atom/b-cm)
N_A	=	Avogadro's number (atoms/mole)

The following is an example of all these calculations for Experiment 109. Only one example of the use of each equation is shown. All values calculated by the evaluator and used below are highlighted in red and truncated to three decimal places although all this was not done during the actual calculations.

Molar Density of ^{235}U:

$$M.D._{U_{235}} = 1.6525 \cdot 0.9975 \cdot 0.34559 \cdot 0.932 \cdot {}^{1}/_{235.0439} = 2.259x10^{-3}$$

Molar Density of oxygen:

$$M.D._{O} = 2 \cdot 2.422x10^{-3} = 4.844x10^{-3}$$

Density of uranium oxyfluoride:

$$\rho_{UO_2F_2} = 5.697x10^{-1} + 1.700\ x10^{-1} = 7.393x10^{-1}$$

Density of impurities: Only the first term of the summation representing the Be impurity is shown below.

$$\rho_{imp.} = 1.6525 \cdot 0.9975 \cdot 2.243x10^{-3} = 3.370x10^{-3}$$

Density of pure water:

$$\rho_{H_2O} = 1.625 \cdot 0.9975 - 7.393x10^{-1} - 3.370x10^{-3} = 9.056x10^{-1}$$

Molar Density of pure water:

$$M.D._{H_2O} = 9.056x10^{-1} \cdot \frac{1}{2 \cdot 1.0079 + 15.9994}$$

Molar Density of Be:

$$M.D._{Be} = \frac{0.15}{10^6} \cdot 1.6526 \cdot 0.9975 \cdot \frac{1}{9.0122} = 9.7438x10^{-8}$$

Atom Density of ^{235}U:

$$N_{U_{235}} = 2.259x10^{-3} \cdot 0.60221x10^{24} \cdot \frac{1\,cm}{10^{24} barn}$$

APPENDIX D: RESULTS OF UNCERTAINTY IN LUCITE® SPACER PLACEMENT

Analysis of the effect of spacer placement in the experiments.

D.1 Spacer Movements to Analyze Uncertainty in Spacer Placement

Table D.1. Spacer Movements.

Configuration	Movement of Spacers
1	left 5.5-in.
2	left and up 5.5-in.
3	up 5.5-in.
4	right and up 5.5-in.
5	right 5.5-in.
6	right and down 5.5-in.
7	down 5.5-in.
8	left and down 5.5-in.

D.2 Δk Results Due to Uncertainty in Spacer Placement

Table D.2. Uncertainty in Spacer Placements.

Configuration:	1	2	3	4	5	6	7	8
Case	Δk	Δk	Δk	Δk	Δk	Δk	Δk	Δk
2	0.00000	0.00023	0.00018	0.00013	-0.00005	0.00015	0.00016	0.00023
3	0.00005	0.00007	0.00023	0.00015	0.00004	0.00024	0.00014	0.00023
4	-0.00001	0.00017	0.00021	0.00021	0.00013	0.00016	0.00015	0.00030
5	-0.00001	0.00024	0.00001	0.00003	0.00002	0.00016	0.00004	0.00008

The effect of spacer placement is effectively negligible.

APPENDIX E: RESULTS OF REFLECTOR THICKNESS ANALYSIS

The following are summaries of Δk results for the varying of reflector thickness. Table E.1 is varying the reflector thickness of Case 1. Table E.2 is the Δk results for each case with a reflector thickness of 30 cm. All results are compared with results for a 600 cm radius spherical reflector around the system.

Table E.1. Δk Results for Varying the Reflector Thickness using Exp. 105.

Reflector Width (cm)	Δk
6	-0.02123
10	-0.00269
15	-0.00025
20	-0.00011
25	-0.00001
30	0.00000
35	-0.00004
40	-0.00013
45	-0.00006
50	-0.00002

Table E.2. Bias of Reduction of Reflector Thickness to 30 cm in Detailed Model.

Case	Δk
1	0.00000
2	-0.00002
3	0.00000
4	-0.00011
5	0.00007

APPENDIX F: EFFECTS OF THERMAL SCATTERING TREATMENT

Within the MCNP data libraries there is no thermal neutron scattering treatment, S(α,β), for Lucite® or a similar material. For the detailed and simple models, a light-water S(α,β) was used because the experimenters chose a Lucite® box to simulate part of the water reflector. The deviation from the benchmark k_{eff} for the light water and polyethylene S(α,β) as well as a free gas treatment, i.e. no S(α,β) are shown in Table F.1. Values were computed with the ENDF/B.VII.0 cross section libraries.

Table F.1. Results of Δk Due to S(α,β) Treatment.

Case	Benchmark k_{eff}	Light Water[(a)]	Polyethylene[(a)]	Free Gas[(a)]
1	1.0000	-0.0004	-0.0070	0.0438
2	1.0000	-0.0029	-0.0098	0.0450
3	1.0000	-0.0008	-0.0077	0.0451
4	1.0000	-0.0010	-0.0077	0.0438
5	1.0000	-0.0031	-0.0098	0.0437
Average % Deviation		-0.16%	-0.84%	4.43%

(a) All statistical uncertainties were 0.00005. Δk's are reference to the benchmark k_{eff}.

APPENDIX G: DERIVATION OF CORRELATION EQUATION AND COEFFICIENT

In order to find the combines variance, $\sigma_c^2(y)$, of uranium weight fraction (grams uranium per gram solution) and specific gravity the following general equation was used:

$$\sigma_c^2(y) = \sum_{i=1}^{N} \left(\frac{\partial f}{\partial x_i}\right)^2 \sigma_{x_i}^2 + 2\sum_{i=1}^{N-1} \sum_{j=i+1}^{N} \frac{\partial f}{\partial x_i}\frac{\partial f}{\partial x_j}\sigma_{x_i,x_j} \quad ^{a} \qquad \text{(G.1)}$$

Where $\sigma_c^2(y)$ is the variance of a parameter y that depends on both x_i and x_j which are correlated variables, f is the dependence of y on x_i and x_j, and σ_{x_i,x_j} is the estimated covariance of x_i and x_j. In order to find the correlated uncertainty in k_{eff} with respect to uranium weight fraction (x_U) and specific gravity ($Sp.G.$) the following equation for the variance is derived from Equation G.1.

$$\sigma_k^2 = \left(\frac{\partial k}{\partial x_U}\right)^2 \sigma_{x_U}^2 + \left(\frac{\partial k}{\partial Sp.G}\right)^2 \sigma_{Sp.G}^2 + 2\frac{\partial k}{\partial x_U}\frac{\partial k}{\partial Sp.G}\sigma_{x_U,Sp.G} \qquad \text{(G.2)}$$

Because there is not a continuous function for k the partial derivatives are approximated by finding the change in k caused by a change in each parameter independently.

$$\frac{\partial k}{\partial x_U} \approx \frac{\Delta k_{x_U}}{\Delta x_U}$$
$$\frac{\partial k}{\partial Sp.G} \approx \frac{\Delta k_{Sp.G}}{\Delta Sp.G} \qquad \text{(G.3)}$$

Where Δk_{x_U} is the change in k corresponding to a Δx_U change in uranium weight fraction and $\Delta k_{Sp.G}$ is the change in k corresponding to a $\Delta Sp.G$ change in the specific gravity.

The estimated covariance of the uranium weight fraction and specific gravity is found using the correlation coefficient, $r_{x_{x_u},x_{Sp.G}}$.

$$\sigma_{x_U,Sp.G} = r_{x_{U,Sp.G}} \cdot \sigma_{x_U}\sigma_{Sp.G} \quad ^{b} \qquad \text{(G.4)}$$

The correlation coefficient can be approximated using the following:

$$r_{x_U,Sp.G} \approx {\sigma_{Sp.G}\Delta x_U} \big/ {\sigma_{x_U}\,\Delta Sp.G} \quad ^{c} \qquad \text{(G.5)}$$

[a] "American Nation Standard for Expressing Uncertainty-U.S. Guide to the Expression of Uncertainty in Measurement" ANSI/NCSL Z540-2-1997, Section 5.2, Equation 13.
[b] "American National Standard for Expressing Uncertainty-U.S. Guide to the Expression of Uncertainty in Measurement" ANSI/NCSL Z540-2-1997, Section 5.2, Equation 14.
[c] "American National Standard for Expressing Uncertainty-U.S. Guide to the Expression of Uncertainty in Measurement" ANSI/NCSL Z540-2-1997, Annex C.3.6.

Where Δx_U is the change in the uranium weight fraction associated with a $\Delta Sp.G$ change in the specific gravity of the solution. Because these values are not available from experimental measurements an equation for uranium weight fraction's dependence on specific gravity is derived (G.8-G.14) that can be differentiated to find the change in uranium weight fraction with respect to density. Using this and the fact that $\sigma_{Sp.G}$ is equal to σ_{x_U} Equation G.5 simplifies to the following

$$r_{x_U,Sp.G} \approx \frac{\partial x_U}{\partial Sp.G} \tag{G.7}$$

The relationship between uranium weight fraction and specific gravity is derived as follows:

First the uranium weight fraction is equated to the mass density of uranium in the solution, ρ_U, and the total solution density.

$$x_U = \frac{\rho_U}{\rho_{sol}} \tag{G.8}$$

ρ_{sol} is the total solution density and is equal to:

$$\rho_{sol} = \rho_{UO_2F_2} + \rho_{water} + \rho_{imp.} \tag{G.9}$$

Where ρ_{water} is the mass density of water in the solution and $\rho_{UO_2F_2}$ is the mass density of the uranium oxyfluoride molecules in the solution and is equal to the sum of the uranium mass density, ρ_U, and the oxyfluoride mass density, $\rho_{O_2F_2}$. The $\rho_{imp.}$ is the density of the impurities in the solution and can be found using Equation C.4. The density of the solution can also be found using the specific gravity and the standard density of water at the solution temperature.

$$\rho_{sol} = Sp.G \cdot \rho_{water} \tag{G.10}$$

Equation G.9 can now be written as:

$$\rho_{sol} = \rho_U + \rho_{O_2F_2} + \rho_{water} + \mathrm{Sp.G} \cdot \rho_{water} \sum_n x_n = Sp.G \cdot \rho_{water} \tag{G.11}$$

Where $\sum_n x_n$ is the sum of the mass fractions of the impurities. Equation G.10 can be rearranged and solved for the density of water.

$$\begin{gathered} \rho_U + \rho_{O_2F_2} = Sp.G \cdot \rho_{water} - \rho_{water} - \mathrm{Sp.G} \cdot \rho_{water} \sum_n x_n \\ \rho_{water} = \rho_U + \rho_{O_2F_2} \Big/ \left(\mathrm{Sp.G} - 1 - \mathrm{Sp.G} \textstyle\sum_n x_n\right) \end{gathered} \tag{G.12}$$

Because all uranium in the solution is uranium oxyfluoride the density of the uranium and the density of the oxyfluoride are proportional by their molar masses (MM):

$$\rho_{O_2F_2} = \rho_U \frac{MM_{O_2F_2}}{MM_U} \tag{G.13}$$

Finally Equations G.8, G.10, G.12, and G.13 can be combined and simplified to obtain the following:

$$x_U = \frac{Sp.G - 1 - Sp.G \sum_n x_n}{\left(1 + \frac{MM_{O_2F_2}}{MM_U}\right) Sp.G} \tag{G.14}$$

By applying Equation G.7 to Equation G.14 the following is found for the correlation coefficient.

$$r_{x_U,Sp.G} \approx \frac{\partial x_U}{\partial Sp.G} = \frac{1}{1+\frac{MM_{O_2F_2}}{MM_U}} \left(\frac{Sp.G(1-\sum_n x_n) - Sp.G + 1 + Sp.G \sum_n x_n}{Sp.G^2}\right) \tag{G.15}$$

Now Equation G.3 and G.4 can be combined with Equation G.2 to find the following equation.

$$\sigma_k^2 = \left(\frac{\Delta k}{\Delta x_U}\right)^2 \sigma_{x_U}^2 + \left(\frac{\Delta k}{\Delta Sp.G}\right)^2 \sigma_{Sp.G}^2 + 2\frac{\Delta k}{\Delta x_U}\frac{\Delta k}{\Delta Sp.G}\sigma_{x_U}\sigma_{Sp.G} r_{x_U,Sp.G} \tag{G.16}$$

Equation G.15 yields a correlation coefficient of about 0.3 for all experiments. This correlation coefficient is then used in Equation G.16 to find the correlated Δk_{eff} in Table 29.

When Equation G.14 is used to calculate the uranium weight fraction the calculated value differs from the measured value by about 12% for all cases. To account for this difference the correlation coefficient was varied by 12%. It was found that this variation of the correlation coefficient yielded negligible changes in the correlated Δk_{eff}'s.