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CRITICALITY SAFETY BENCHMARK CALCULATIONS FOR LOW-ENRICHED URANIUM METAL AND URANIUM OXIDE ROD-WATER LATTICES

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EXXON NUCLEAR COMPANY, Inc.

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1.0 INTRODUCTION

This report summarizes the results of benchmark calculations performed to verify the accuracy, and provide an estimate of the calculational bias, of computer code models used to calculate effective multiplication factors for low enriched uranium metal (U) and uranium-dioxide (UO_2) rod-water lattices. Data from the Yankee critical experiments[1] as well as from experiments performed at Oak Ridge National Laboratory[2] (ORNL) and the Pacific Northwest Laboratories (PNL) of Battelle[3] were used in this benchmarking effort. Descriptions of the critical and subcritical experiments and results of the criticality calculations are provided in subsequent sections of this report. The analytical methods used in these evaluations are also discussed.

2.0 SUMMARY DESCRIPTION OF BENCHMARK DATA

2.1 Yankee Critical Experiments

A number of critical experiments were performed for the "Yankee" reactor in the late 1950's. These experiments utilized stainless steel clad UO_2 fuel rods (enriched to 2.70 wt.% ^{235}U) in light water.[1] Table I lists fuel assembly parameters used for one set of experiments where the critical number of rods in a cylindrical geometry was determined for various

lattice (rod-to-rod) pitches. Table II summarizes the results of these critical experiments and gives critical cylinder radii for the respective lattice pitches.

2.2 ORNL Critical Experiments

The results of a number of critical experiments conducted at ORNL employing unclad uranium metal rods[2] were obtained from E. B. Johnson and G. E. Whitesides of ORNL. These experiments were performed for uniform lattices of 4.95 wt.% ^{235}U enriched rods, surrounded on all sides by an essentially infinite water reflector. In conducting the actual experiments, the water height above the rods was varied to control the reactivity of the array. Experiments were performed for rod-water lattices with and without the inclusion of such reflector and poison materials as depleted uranium, BORAL and stainless steel. Table III lists fuel rod, neutron absorber plate, and reflector data which describe relevant physical characteristics of the experimental equipment. Figures 1 through 5 depict graphically the arrangement of five selected experiments for which criticality calculations were performed. The experimental results of these five experiments are summarized in Table IV.

2.3 PNL Critical Experiments

In 1976 experiments were initiated at the Pacific Northwest Laboratories of Battelle to provide criticality data on systems simulating LWR fuel assembly shipping packages and storage pools.[3] The initial experiments were conducted for aluminum clad UO_2 rods in light water (enriched to 2.35

wt.% ^{235}U) arranged in lattices as depicted in Figure 6. The effect of various fixed neutron absorbers (e.g., BORAL and stainless steel) on critical array dimensions was investigated. Table V lists fuel rod and poison plate parameters describing the material and dimensional make-up of the experimental core. Table VI summarizes the results of six experimental runs, noting critical separations, dimensions, etc.

3.0 CALCULATIONAL METHODS

Methods used for criticality calculations are selected which permit accurate geometrical and neutronic modeling of the systems such that the effective multiplication factor (k_{eff}) can be computed with an acceptable degree of confidence. There are a number of Monte Carlo, transport and diffusion theory computer codes, and associated multigroup cross section data set preparation codes, which together are well suited to handle the estimation of k_{eff} for a variety of systems.

From the standpoint of applicability and flexibility, the multigroup, multiregion, three-dimensional KENO[4] Monte Carlo code is well suited to perform these calculations. The KENO code tracks individual neutrons in the system and at each neutron collision point calculates the probability of occurrence of various possible interactions (e.g., capture, fission, etc.). The assigned neutron weight is reduced after each collision by the probability of absorption. When the weight is reduced below a pre-specified level for the particular region in which the collision occurs, "Russian Roulette" is played to determine if tracking of the neutron should be

terminated or continued with an increased weigh.. Once a representative number of neutron histories have been compiled, fission rates, densities, etc. are calculated. Benchmark calculations were performed using either the KENO-II[4] code with an 18 energy group calculational model or KENO-IV[5] with a 123 energy group model. Logical computer code input for the two models is depicted in Figure 7.

3.1 Eighteen Energy Group Model

As discussed above, the KENO-II[4] Monte Carlo code was used to calculate k_{eff} values of the experimental benchmark data. Eighteen energy group cross section data input into KENO were averaged using the CCELL[6], BRT-1[7], and GAMTEC-II[8] computer codes with either ENDF/B-III or GAM-1 cross section library[9] data. Specifically, the cross sections for various material regions in the critical experiments were obtained as follows:

- FUEL REGION - The CCELL code was utilized to obtain cell-averaged multigroup ($0 \leq E \leq 10$ Mev) cross section data for the rod-water lattices. (CCELL is a pin cell calculational code developed by Exxon Nuclear. It is a combination of the HRG[10] and THERMOS[11] codes, and is designed primarily to produce broad group cell-averaged, resonance-corrected fuel region cross section data. Resonance energy cross section data are calculated using an adaptation of the Adler, Hinman, and Nordheim method[12] to an intermediate resonance approximation. The resonance integrals are allocated to the various fine energy groups with provisions made for self-shielding.) In addition CCELL was used to produce flux-weighted, epithermal multigroup cross section data ($E > 0.683$ ev) for fixed-poison material.

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• FIXED NEUTRON POISONS - The Battelle Revised Thermos (BRT-1) code was utilized to produce thermal group ($E \leq 0.683$ ev) cross section data for any fixed neutron poisons associated with the critical experiments (e.g., stainless steel, BORAL, etc.). BRT-1 performs a spatially-dependent transport calculation to provide thermal group adjusted cross section data. The neutron energy spectrum of adjacent source regions is described using a 30 x 30 scattering matrix calculated by the CCELL code.

• REFLECTORS - The GAMTEC-II code was employed to calculate multigroup cross section data for water and depleted uranium, both averaged over a neutron energy spectrum characteristic of an infinite medium. GAMTEC-II is utilized primarily for averaging cross section data in essentially homogeneous media. Epithermal group constants are averaged over a 64-group slowing down spectrum computed using the B_1 approximation to the Boltzmann equation. Thermal group constants are averaged over a Wigner-Wilkins flux spectrum[13], and resonance absorption cross sections are calculated using the narrow-resonance and narrow-resonance infinite mass approximations[12].

3.2 123 Energy Group Model

The KENO IV[5] computer code with 123 energy groups was used to calculate the effective multiplication constants for the same critical experiments. Multigroup cross section data from the XSDRN 123 energy group data library were prepared for input into KENO IV using the NITAWL and XSDRNPM codes, both of which are a part of the AMPX Modular Code System[14].

NITAWL is an acronym for Nordheim's Integral Treatment And Working Library production. The code performs resonance self-shielding calculations and combines the resonance and smooth cross section data into multigroup formats usable in other codes. Resonance calculations using the

Nordheim integral method were performed for the ^{238}U associated with each of the critical experiments. Dancoff correction factors and effective moderator cross section data necessary for the NITAWL calculations were obtained using the DASQHE[15] subroutine of the CCELL code.

The XSDRNPM code is a multiregion, multigroup, one-dimensional transport theory code used to calculate reaction rates and eigenvalues as well as produce cell-averaged fuel region cross section data. (XSDRNPM is also part of the AMPX module and is a modified version of the XSDRN[16] code.) Specifically, the code performs a forward solution of the one-dimensional Boltzmann transport equation in slab, cylindrical or spherical geometry. The solution may be performed in the multigroup discrete ordinates, diffusion, or infinite medium approximation. In addition, XSDRNPM computes multigroup constants averaged over both space and energy for use in other calculations. Hence, resonance-treated ^{238}U cross section data prepared by NITAWL were input into XSDRNPM to produce cell-averaged multigroup constants for input into KENO IV. This approach, wherein the fuel region is treated as a single homogeneous mixture (i.e., cell-averaged by XSDRNPM) not only simplifies the necessary KENO input, but also enhances the flexibility of the code in calculating reactivities of array designs which are geometrically more complex than the experimental criticals.

4.0 CALCULATIONAL RESULTS

Results of k_{eff} calculations are given in Tables VII, VIII and IX for the critical experiments summarized in Section 2. In each case the methods

of analysis used were as discussed in Section 3. Table VII summarizes the results of calculations performed for the Yankee critical experiment data. It is noted that the KENO calculated k_{eff} values agree with previously performed DTF-IV[17] transport theory calculations within the statistical uncertainty of the Monte Carlo calculations.

Table VIII tabulates calculational results for the ORNL uranium metal experimental data. For these results the eighteen group calculational model appears to do an adequate job in calculating the critical value for the first three cases which include rods in water only or rods in water reflected by depleted uranium. For the cases employing the neutron absorber (BORAL) plate, however, results are conservatively high. The 123 group calculational model gives results that remain consistent for all cases.

Calculated k_{eff} values for the experiments performed at PNL are summarized in Table IX. These experiments were performed to provide experimental criticality data on systems simulating the neutronic conditions of fuel element shipping packages and storage facilities. As indicated in the table, calculated k_{eff} values are in close agreement with the experimental data.

5.0 ASSESSMENT OF RESULTS AND CALCULATIONAL BIAS

The results of reactivity calculations for the Yankee critical experiments, using either the 18 group or the 123 group models, show a conservative bias of from +0.004 Δk to +0.013 Δk at the 95% confidence

level. This conservative bias of approximately +1.0% in $\frac{\Delta k}{k}$ is also in agreement with results of DTF IV calculations performed for the same lattices.

For the ORNL critical lattices the results of the 123 group calculations are consistently around the critical value (k_{eff} = 1.000). The average resulting k_{eff} for all cases (Cases 1B-5B) is 0.998 $\pm$ .002. For the 18 group calculations, however, the results indicate a conservative bias for systems containing a BORAL poison plate. Cases 4B and 5B indicate that the calculational results are conservatively high by not less than +0.025 Δk at the 95% confidence level. While these results are not sufficient to permit a clear definition of the calculational bias, the results strongly indicate that the BORAL cross section data averaging technique is conservative with respect to criticality safety.

The critical experiments performed by Bierman, et al., at PNL most closely resemble fuel storage and transportation systems of the three sets of critical experiment data described in this report. Hence, the results of these benchmark calculations are of particular interest. The average k_{eff} for the 18 group calculations is 1.001 $\pm$ .002 and for the 123 group calculations k_{eff} (average) is 0.998 $\pm$ .002. Both values are within one standard deviation of the critical value and results remain consistent for various fuel rod arrays and absorber plate conditions. It should also be noted that for the cases in which absorber plates were present, the attempt was made to choose several runs from many which had contrasting

critical parameters. For the BORAL cases the distance of the plates from the fuel clusters was 0.645 ± .006 cm and 4.442 ± .060 cm, respectively. These dimensions represent maximum and minimum cluster-to-plate separation distances for the data reported.

6.0 CONCLUSIONS

In validating and assessing the accuracy of calculational models via benchmark calculations, it is important that a variety of experimental data be utilized. This approach is of benefit not only in appraising the calculational bias associated with the particular method, but also in establishing the region of validity of the calculational method. From the results of calculations summarized in this report, both the 18 group and the 123 group calculational models appear to adequately reproduce the critical values. Where a significant calculational bias is indicated (i.e., the 18 energy group model calculations of the ORNL data, Cases 4B and 5B), the bias is conservative with respect to criticality safety.

This benchmarking effort was originally undertaken to determine the accuracy of the two described models which were primarily being used to calculate k_{eff} values of spent fuel shipping containers and storage pools. Hence, the calculated results using the PNL critical experiment data are especially encouraging as these results are, based on a cumulative average, within one standard deviation of the critical value for both calculational models.

Although no effort has been made to firmly establish an actual calculational bias for the two models, the theory-experiment correlations

show that the analytical methods used adequately reproduce the experimental results. Nevertheless, since changes in poison materials, fissile enrichments, and other design parameters may influence the correlation between theory and experiments, additional benchmark calculations will be made on a continuing basis to expand the region of validity of the analytical methods on an as-needed basis.

TABLE I

YANKEE CRITICAL EXPERIMENTS

(2.70 Wt.% ^{235}U Stainless Steel Clad UO_2 Rods[1])

FUEL ROD LATTICE PARAMETERS

Enrichment, wt.% ^{235}U	2.70
Uranium Form	Sintered UO_2
Pellet Diameter, cm	0.762
Pellet Density, % ρ_T	93 ± 1
Clad Material	304 SS
Clad OD, cm	0.859
Clad Thickness, cm	0.041
Active Fuel Length, cm	121.9
Rod-to-Rod Pitch, cm	1.105 - 1.689* (square)
V_m/V_f	1.40 - 4.98*
End Plugs	304 SS

*The pitch was varied from experiment to experiment.

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TABLE II

YANKEE CRITICAL EXPERIMENT RESULTS
(2.70 Wt.% ^{235}U Stainless Steel Clad UO_2 Rods[1])

Case	Square Lattice Spacing, cm		Moderator-to-Fuel Volume Ratio	$H/^{235}U$ Ratio	Critical Number of Rods	Critical Cylinder Radius, cm
1A	1.105	(0.435 in.)	1.405	150	1851	26.820
2A	1.194	(0.470 in.)	1.853	198	1301	24.295
3A	1.455	(0.573 in.)	3.357	361	826	23.599
4A	1.562	(0.615 in.)	4.078	436	790	24.770
5A	1.689	(0.665 in.)	4.984	533	813	27.173

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TABLE III

ORNL CRITICAL EXPERIMENTS

(4.95 Wt.% ^{235}U Unclad Uranium Metal Rods[2])

FUEL ROD LATTICE PARAMETERS

Enrichment, wt.% ^{235}U	4.95
Uranium Form	Metal
Uranium Density, $\%\rho_T$	99
Rod OD, cm	0.762 (unclad)
Rod Length, cm	30.0
Rod-to-Rod Pitch, cm	2.05 (square)
V_m/V_f Ratio	8.22

DEPLETED URANIUM BLOCK

Material	Uranium Metal U(0.185)
Uranium Density, g/cm^3	19.04
Length, cm	60.4
Width, cm	21.7
Height, cm	25.9 (centered)

NEUTRON ABSORBER PLATE

Material	BORAL (Brooks and Perkins)
Core Material	B_4C and Al
Wt.% B_4C in Core	38.9 (ORNL measurement)
Core Density, g/cm^3	2.63
Core Thickness, cm	0.429
Clad Material	1100 Aluminum
Clad Thickness, cm	0.104
Width, cm	47.114
Height, cm	25.876 (centered)
Total Width, cm	0.637

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TABLE IV

ORNL CRITICAL EXPERIMENT RESULTS
(4.95 Wt.% ^{235}U Unclad Uranium Metal Rods[2])

Case	Lattice Number	Number of Rods	Critical Water Height Above Lattice, cm	Reactivity at Given Water Height, ¢
		Rod-Water Lattice Only		
1B	22	203	7.1	+12.1
2B	23	195	15.24	0.0
		Rod-Water Lattice + U(0.185) Block		
3B	104 (Run)	245	9.5	+4.3
		Rod-Water Lattice + U(0.185) Block + BORAL Sheet		
4B	105 (Run)	324	15.24	0.0
5B	-	359	11.94	+0.6

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TABLE V

PNL CRITICAL EXPERIMENTS

(2.35 Wt.% ^{235}U Aluminum Clad UO_2 Rods[3])

FUEL ROD LATTICE PARAMETERS

Enrichment, wt.% ^{235}U	2.35 ± .05
Uranium Form	UO_2
Uranium Loading, gm/rod UO_2	825
^{235}U Axial Loading, gm/cm	0.187
Fuel Diameter, cm	1.118
UO_2 Density, % ρ_T	84
Clad Material	6061 Aluminum
Clad OD, cm	1.27
Clad Thickness, cm	0.076
Active Fuel Length, cm	91.44
Rod-to-Rod Pitch, cm	2.032 (square)
V_m/V_f	2.92
End Plugs	Aluminum

NEUTRON ABSORBER PLATES

	Composition	
	304-L Steel	BORAL
Density, g/cm^3	7.93	2.49
Element, wt.%		
Aℓ		62.39 ± 2.80
B		28.70 ± 0.25
C		7.97 ± 0.41
Fe	68.24 ± 0.34	0.33 ± 0.04
Cr	18.56 ± 0.10	
Mn	1.58 ± 0.05	
Ni	11.09 ± 0.06	
Plate Width, cm	35.6	35.6
Plate Height, cm	91.5	91.5
Plate Thickness, cm	3.02 ± 0.13 4.85 ± 0.15	7.13 ± 0.11 (includes 0.102 cm Aluminum on either side of core)

TABLE VI

PNL CRITICAL EXPERIMENT RESULTS
(2.35 Wt.% ^{235}U Aluminum Clad UO_2 Rods[3])

Case	Experiment Number	Fuel Clusters: No. in Array	Fuel Clusters: Lattice Size, Fuel Rods	Absorber Plates: Thickness (t_p), mm	Absorber Plates: Distance to Fuel Cluster (G), mm	Critical Separation Between Fuel Clusters (Xc), mm
			Rod-Water Lattice Only			
1C	002	1	20 x 18.08 ± 0.02	-	-	∞
2C	014	3	20 x 16	-	-	84.1 ± 0.5
			Rod-Water Lattice + 304L Steel			
3C	028	3	20 x 16	4.85 ± 0.15	6.45 ± 0.06	68.8 ± 0.2
4C	035	3	20 x 17	3.02 ± 0.13	40.42 ± 0.70	114.7 ± 0.3
			Rod-Water Lattice + BORAL			
5C	020	3	20 x 17	7.13 ± 0.11	6.45 ± 0.06	63.4 ± 0.2
6C	016	3	20 x 17	7.13 + 0.11	44.42 ± 0.60	90.3 ± 0.5

TABLE VII

CALCULATED K_{EFF} VALUES FOR YANKEE ROD-WATER CRITICAL LATTICES

(2.70 Wt.% ^{235}U Stainless Steel Clad UO_2 Rods[1])

Case	Square Lattice Spacing, in.	Moderator-to-Fuel Volume Ratio	Exp'tl. Critical Cylinder Radius, cm	CCELL-DTF-IV Calculated Reactivity (k_{eff})	CCELL-KENO II (18-group) Calculated Reactivity ($k_{eff} \pm \sigma$)	NITAWL-XSDRNPM-KENO IV (123-group) Calculated Reactivity ($k_{eff} \pm \sigma$)
1A	0.435	1.405	26.820	1.016	1.006 ± .006	1.007 ± .005
2A	0.470	1.853	24.294	1.015	1.014 ± .005	1.013 ± .005
3A	0.573	3.357	23.600	1.011	1.003 ± .005	1.008 ± .004
4A	0.615	4.078	24.771	1.009	1.010 ± .005	1.002 ± .004
5A	0.665	4.984	27.172	1.005	1.005 ± .005	1.013 ± .004
				Average:	1.008 ± .002	1.009 ± .002

TABLE VIII

CALCULATED K_{EFF} VALUES FOR ORNL CRITICAL LATTCES

(4.95 Wt.% ^{235}U Unclad Uranium Metal Rods[2])

Case	Lattice Number	Number of Rods	Critical Water Height Above Lattice, cm	CCELL-KENO II (18-group) Calculated Reactivity ($k_{eff} \pm \sigma$)	NITAWL-XSDRNPM-KENO IV (123-group) Calculated Reactivity ($k_{eff} \pm \sigma$)
			Rod-Water Lattice Only		
1B	22	203	7.1	0.988 ± .006	0.997 ± .005
2B	23	195	15.24	0.998 ± .006	0.999 ± .006
			Rod-Water Lattice + U(0.185) Block		
3B	104 (Run)	245	9.5	1.001 ± .006	0.993 ± .006
			Rod-Water Lattice + U(0.185) Block + BORAL Sheet		
4B	105 (Run)	324	15.24	1.038 ± .005	1.000 ± .005
5B	-	359	11.94	1.037 ± .006	0.999 ± .005
			Average:	1.012 ± .003	0.998 ± .002

TABLE IX

CALCULATED K_{EFF} VALUES FOR PNL CRITICAL LATTICES

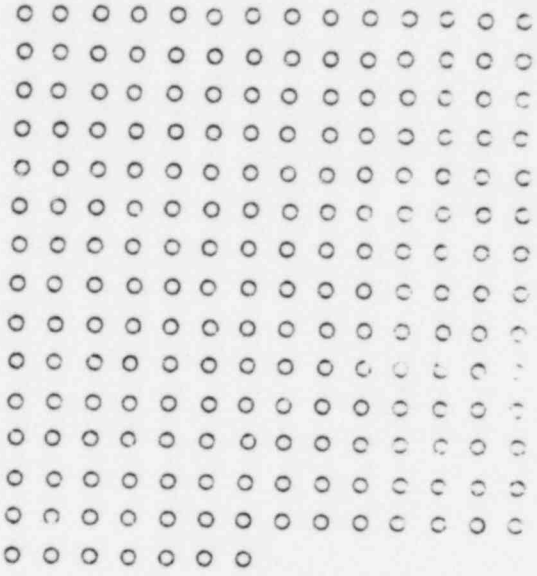
(2.35 Wt.% ^{235}U Aluminum Clad UO_2 Rods[3])

Case	Experiment Number	Number of Fuel Clusters in Array	Critical Separation Between Fuel Clusters, cm	CCELL-KENO II (18-group) Calculated Reactivity ($k_{eff} \pm \sigma$)	NITAWL-XSDRNPM-KENO IV (123-group) Calculated Reactivity ($k_{eff} \pm \sigma$)
			Rod-Water Lattice Only		
1C	002	1	∞	1.008 ± .005	1.004 ± .005
2C	014	3	8.41	1.007 ± .005	0.991 ± .005
			Rod-Water Lattice + 304L Steel		
3C	028	3	6.88	0.994 ± .004	0.997 ± .004
4C	035	3	11.47	0.997 ± .005	1.000 ± .005
			Rod-Water Lattice + BORAL		
5C	020	3	6.34*	0.995 ± .005	0.999 ± .005
6C	016	3	9.03	1.007 ± .005	0.999 ± .004
			Average:	1.001 ± .002	0.998 ± .002

*6.33 cm assumed in reactivity calculation.

Water

Water



Water

TOP VIEW

Reflector: 7.1 cm water above fuel
15.24 cm water in all other directions

FIGURE 1
ORNL Critical Assembly Arrangement
Case 1B - LATTICE #22 (203 Rods)

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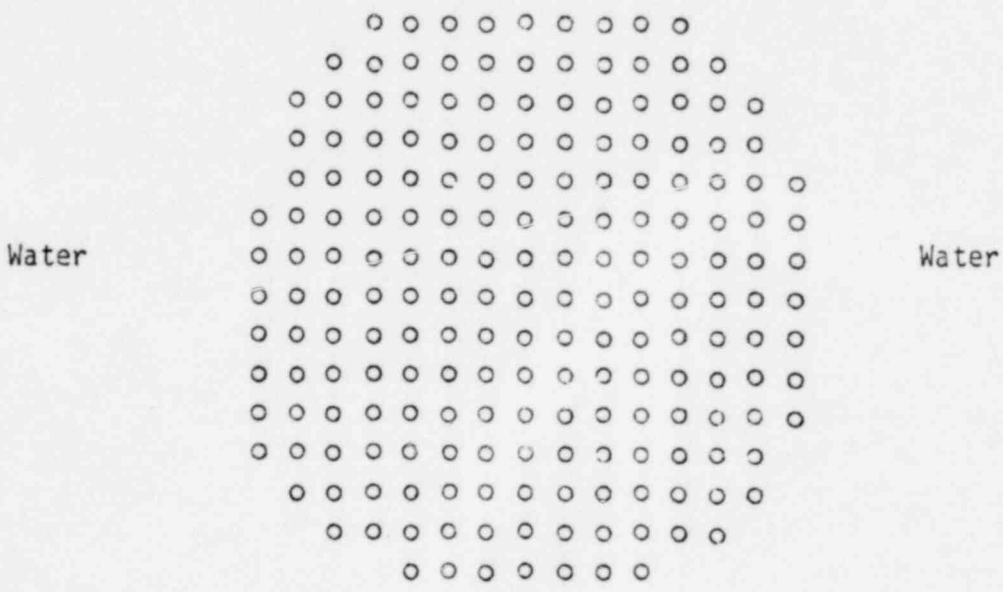
Water



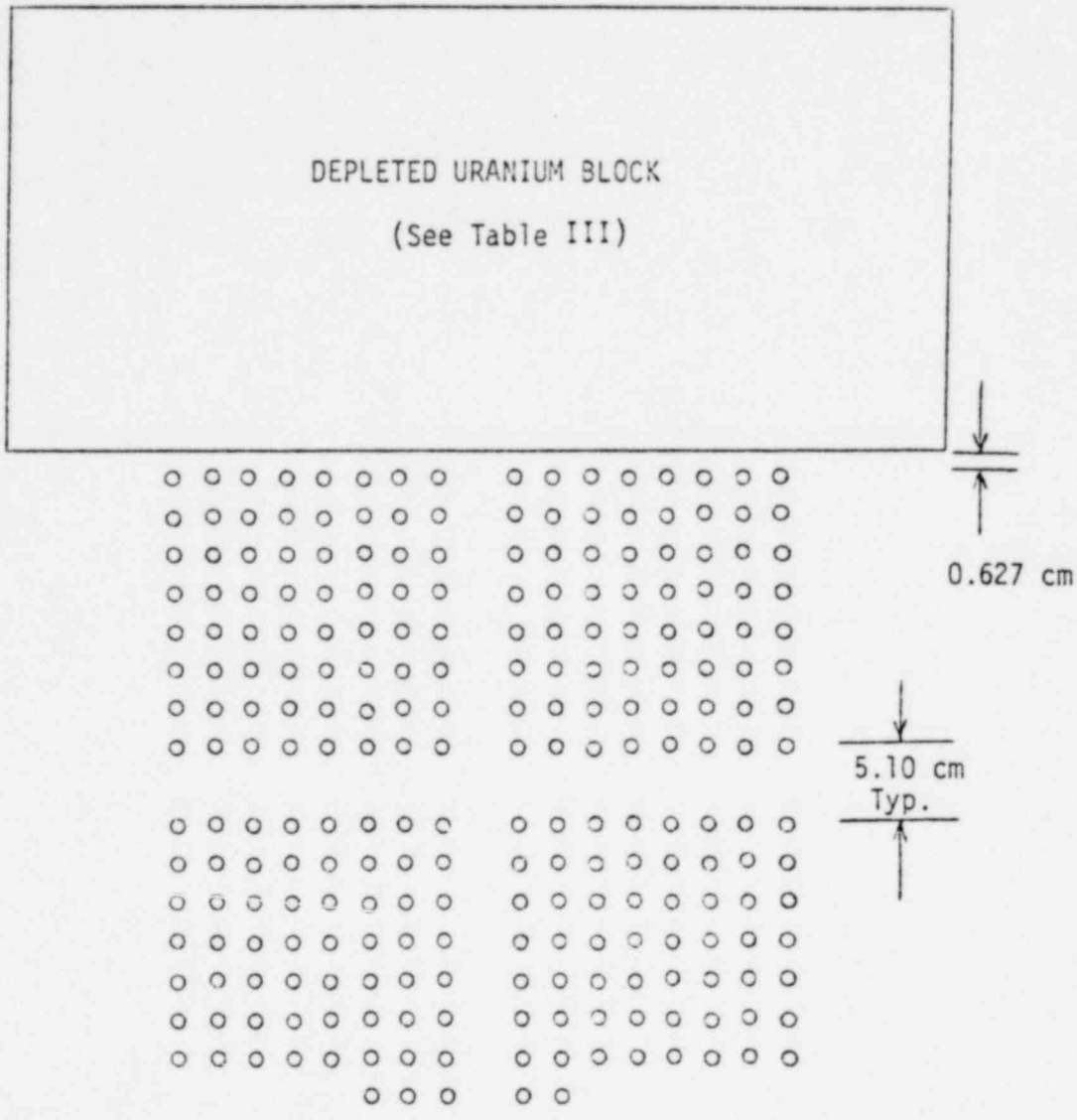
TOP VIEW

Reflector: 15.24 cm water in all directions

FIGURE 2

ORNL Critical Assembly Arrangement

Case 2B - LATTICE #23 (195 Rods)



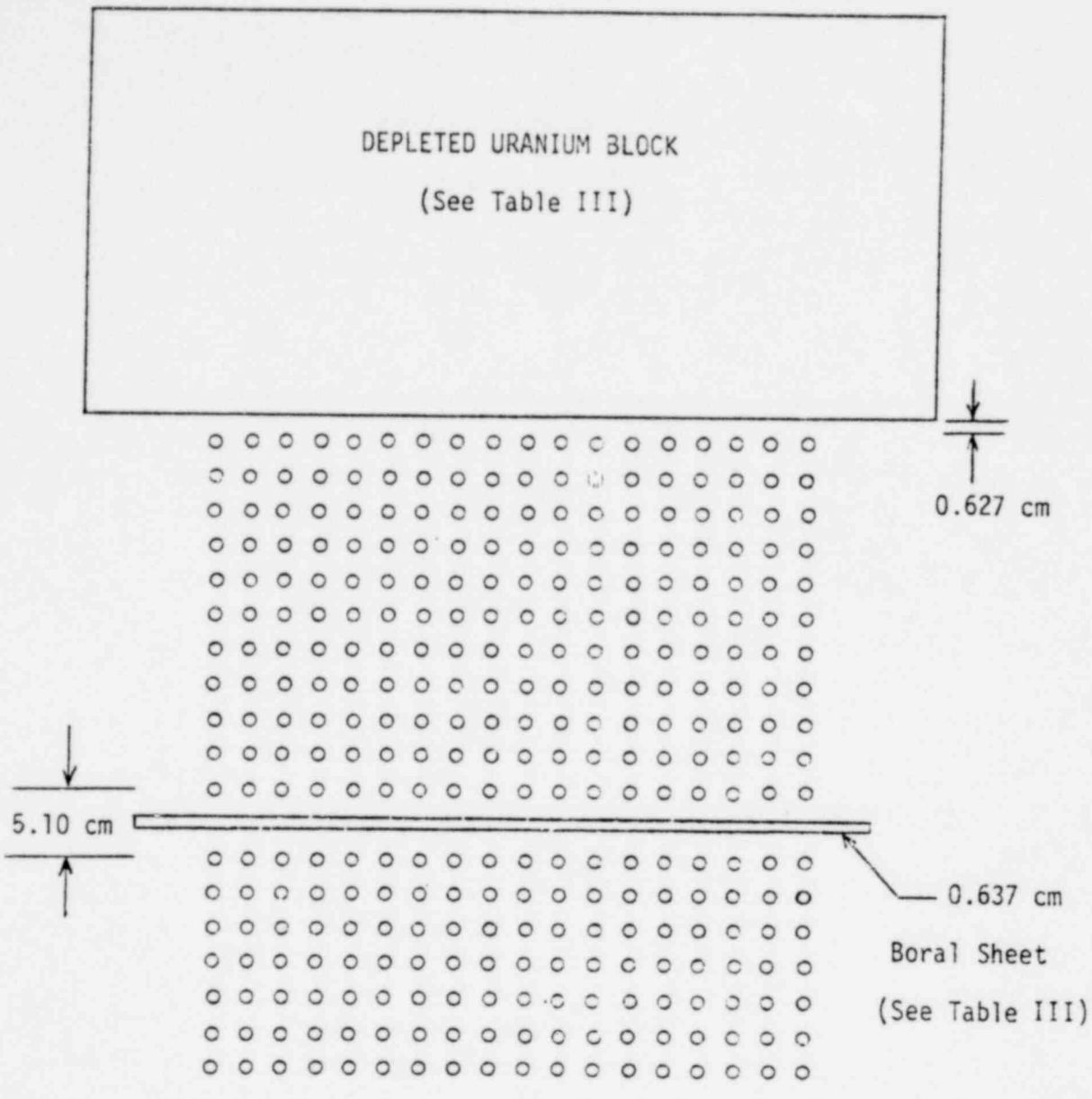
TOP VIEW

Reflector: 9.5 cm water above fuel
15.24 cm water in all other directions

FIGURE 3

ORNL Critical Assembly Arrangement

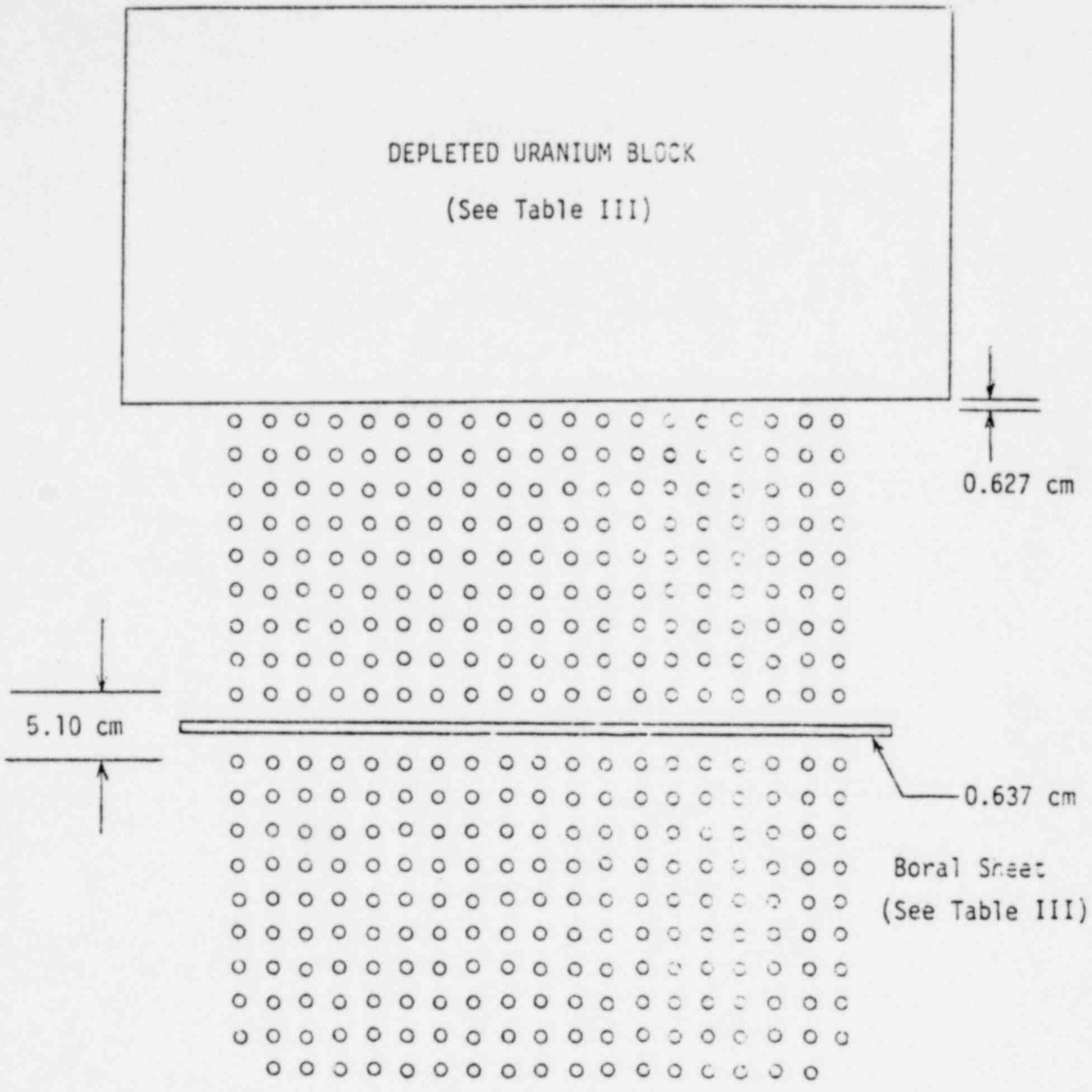
Case 3B-RUN #104 (245 Rods)



TOP VIEW

Reflector: 15.24 cm water in all directions

FIGURE 4
ORNL Critical Assembly Arrangement
Case 4B - RUN #105 (324 Rods)



TOP VIEW

Reflector: 11.94 cm water above fuel
15.24 cm water in all other directions

FIGURE 5
ORNL Critical Assembly Arrangement
Case 5B (359 Rods)

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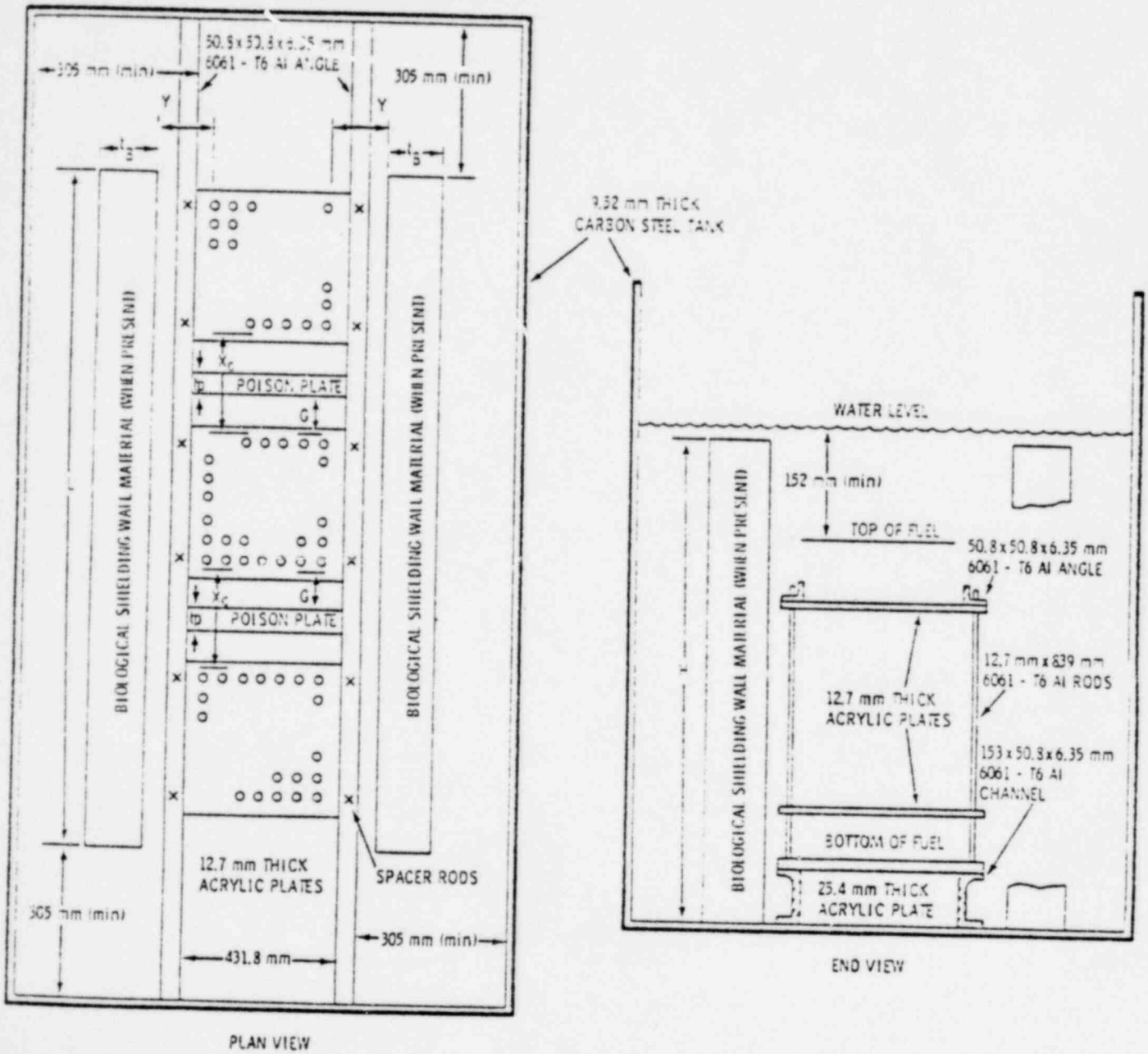
FIGURE 6

PNL CRITICAL EXPERIMENTS

GRAPHICAL ARRANGEMENT OF SIMULATED SHIPPING PACKAGE CRITICAL EXPERIMENTS



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POOR ORIGINAL

CALCULATIONAL METHODS

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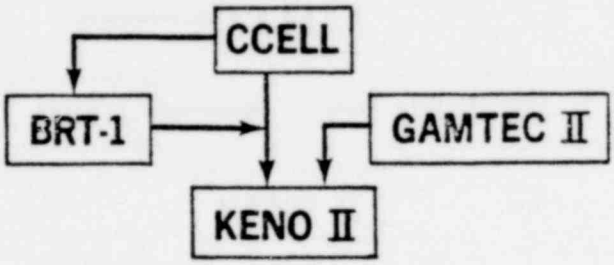
KENO II (18 Gp.) MODEL



KENO IV (123 Gp.) MODEL

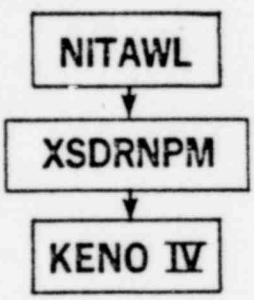


FIGURE 7

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COMPUTER CODE CALCULATONAL MODELS

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