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**Monte Carlo Analyses of Simple U233 O₂-ThO₂
and U235 O₂-ThO₂ Lattices with ENDF/B-IV Data
(AWBA Development Program)**

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MONTE CARLO ANALYSES OF
SIMPLE U233O₂-ThO₂ AND U235O₂-ThO₂
LATTICES WITH ENDF/B-IV DATA
(AWBA DEVELOPMENT PROGRAM)

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BETTIS ATOMIC POWER LABORATORY

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FOREWORD

The Shippingport Atomic Power Station located in Shippingport, Pennsylvania was the first large-scale, central-station nuclear power plant in the United States and the first plant of such size in the world operated solely to produce electric power. This program was started in 1953 to confirm the practical application of nuclear power for large-scale electric power generation. It has provided much of the technology being used for design and operation of the commercial, central-station nuclear power plants now in use.

Subsequent to development and successful operation of the Pressurized Water Reactor in the Atomic Energy Commission (now Department of Energy, DOE) owned reactor plant at the Shippingport Atomic Power Station, the Atomic Energy Commission in 1965 undertook a research and development program to design and build a Light Water Breeder Reactor core for operation in the Shippingport Station.

The objective of the Light Water Breeder Reactor (LWBR) program has been to develop a technology that would significantly improve the utilization of the nation's nuclear fuel resources employing the well-established water reactor technology. To achieve this objective, work has been directed toward analysis, design, component tests, and fabrication of a water-cooled, thorium oxide-uranium oxide fuel cycle breeder reactor for installation and operation at the Shippingport Station. The LWBR core started operation in the Shippingport Station in the Fall of 1977 and is expected to be operated for about 4 to 5 years. At the end of this period, the core will be removed and the spent fuel shipped to the Naval Reactors Expended Core Facility for a detailed examination to verify core performance including an evaluation of breeding characteristics.

In 1976, with fabrication of the Shippingport LWBR core nearing completion, the Energy Research and Development Administration, now DOE, established the Advanced Water Breeder Applications (AWBA) program to develop and disseminate technical information which would assist U.S. industry in evaluating the LWBR concept for commercial-scale applications. The program is exploring some of the problems that would be faced by industry in adapting technology confirmed in the LWBR program. Information being developed includes concepts for commercial-scale prebreeder cores which would produce uranium-233 for light water breeder cores based on the technology developed to fabricate and operate the Shippingport LWBR core, and other information and technology to aid in evaluating commercial-scale application of the LWBR concept.

All three development programs (Pressurized Water Reactor, Light Water Breeder Reactor, and Advanced Water Breeder Applications) are under the technical direction of the Division of Naval Reactors of DOE. They have the goal of developing practical improvements in the utilization of nuclear fuel resources for generation of electrical energy using water-cooled nuclear reactors.

Technical information developed under the Shippingport, LWBR, and AWBA programs has been and will continue to be published in technical memoranda, one of which is this present report.

ABSTRACT

A number of water-moderated Th-U235 and Th-U233 lattice integral experiments were analyzed in a consistent manner, with ENDF/B-IV data and detailed Monte Carlo methods. These experiments provide a consistent test of the nuclear data. The ENDF/B-IV data are found to perform reasonably well. Adequate agreement is found with integral measurements of thorium capture. Calculated K_{eff} values show a generally coherent pattern which is consistent with K_{eff} results obtained for homogeneous aqueous critical assemblies. Harder prompt fission spectra for U233 and U235 can correct the principal discrepancy observed with ENDF/B-IV, a bias trend in K_{eff} attributed to an underprediction of leakage.

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I. Introduction

To qualify nuclear data sets for use in AWBA and LWBR analyses, a survey was made of existing water-moderated Th-U233 and Th-U235 critical (and exponential) experiments.

Lattice experiments deemed potentially useful for data testing are shown in Table I-1. Very few such experiments are available with U233 fuel. Aside from the critical experiments in direct support of LWBR (the SB and BMU series and the Detailed Cell), there are only the BNL U233O₂-ThO₂ exponentials and the very hard spectrum ETA-II critical (which used the BNL fuel rods).

There are several U235-fueled ThO₂ criticals available. Among these are experiments run in the late 1950's at BAW and at ANL: the H₂O-moderated TUPE and CETR lattices, the H₂O-D₂O SSCR experiments, and the D₂O-moderated THUD lattices. One series of experiments, with 19-element cluster rods, was run at Chalk River in the center of a ZED-2 lattice of CANDU-type rods.

In exploratory studies, those experiments judged to be most promising were analyzed with Monte Carlo methods and ENDF/B-IV data. Included were five TUPE lattices, three configurations of a THUD lattice, eight H₂O-moderated BNL exponentials, eight D₂O-moderated BNL exponentials, one BMU lattice, and one LWBR Detailed Cell configuration. Two major questions were addressed: (1) To what extent do these integral experiments provide a consistent and adequately detailed test of the differential data? (2) How well do ENDF/B-IV data predict the results of these experiments?

Table I-1

Summary of Th-U233 and Th-U235 Exponential and
Critical Experiments of Potential Use for Data Testing

Experiment	TUPE Criticals	CETR Criticals
Laboratory	BAW	BAW
References	1 (1960)	2 (1960)
Fuel	U2350 ₂ -ThO ₂ rods, aluminum clad, .660 cm diam. x 152 cm Th/U235 = 15/1 and 25/1	U2350 ₂ -ThO ₂ rods, steel clad .660 cm diam. x 122 cm Th/U235 = 15/1 and 25/1
Moderator	H ₂ O, partial height	H ₂ O
Temperature	Ambient	Ambient
Lattices	Uniform square array of rods, cylindrical boundary. Five lattices with mod./fuel volume ratio from 1.4 to 5.8.	Uniform square array of rods, cylindrical boundary. Seven lattices with mod./fuel volume ratio from 1.3 to 9.5.
Parameters Measured	Critical size, material B ² , radial and axial flux shapes, reflector savings, thermal flux depression, cadmium ratio of Th232 capture and U235 fission.	Critical size, material B ² , radial and axial flux shapes, reflector savings, thermal flux depression, cadmium ratio of Th232 capture and U235 fission, differential H ₂ O worth, differential boron poison worth.
Comments	Good for criticality. Analysis of U235 and Th232 cadmium ratios requires detailed study of experimental effects.	Good for criticality. Analysis of cadmium ratios requires detailed study of experimental effects. Fuel same as Ref. 1 with different clad.

Table I-1 (Cont'd)

Experiment	SSCR Criticals	THUD Criticals	ZED-2 19-element-rod Lattices
Laboratory	BAW	ANL	CRNL
References	3 (1961)	4 (1961)	5, 6 (1968)
Fuel	U235O ₂ -ThO ₂ rods, .660 cm diam. x 152 cm, aluminum clad, Th/U235 atom ratio 15/1	U235O ₂ -ThO ₂ rods, .660 cm diam. x 152 cm, aluminum clad, Th/U235 atom ratio 15/1 and 25/1	19-element clusters of ThO ₂ containing 1.5 w/o UO ₂ (93 atom % U235)
Moderator	D ₂ O-H ₂ O (60.4 mole % D ₂ O)	D ₂ O (99.4%-97.0% purity), partial moderator height	D ₂ O (coolant: air, D ₂ O, H ₂ O, HB40)
Temperature	Ambient	Ambient	Ambient
Lattices	Uniform square array of rods, cylindrical boundary, mod./fuel volume ratio 1.4.	Uniform triangular array of rods, cylindrical boundary. 45 lattices on four pitches, from 1.9 cm to 5.7 cm.	Triangular array. Seven cluster-rods (center and first hex) in lattice of 19-element UO ₂ CANDU-type rods. Pitches of 22 cm and 28 cm (B ² also at pitches of 24 cm and 32 cm).
Parameters Measured	Critical size, reflector savings, radial and axial flux shapes, material B ² , thermal flux depression, cadmium ratios of Th232 capture and U235 fission.	Critical size, reflector savings, differential D ₂ O worth, cadmium ratio of Th232 capture, thermal flux depression, fast fission factor.	Material B ² ; neutron fine structure; relative U233, U235 and Pu239 fission ratios; δ 02, CR*.
Comments	Good for criticality. Analysis of cadmium ratios requires detailed study of experimental effects. Fuel rods same as Ref. 1.	D ₂ O purity determination in question. Good for criti- cality. Analysis of Th232 cadmium ratio and fast fis- sion factor requires detailed study of experimental effects. Fuel rods same as Ref. 1.	--

Table I-1 (Cont'd)

Experiment	BNL Exponentials	ETA-I Critical	ETA-II Critical
Laboratory	BNL	Bettis	Bettis
References	7, 8 (1966, 1970)	9, 10 (1974)	9 (1974)
Fuel	U2330 ₂ -ThO ₂ rods, 1.09 cm diam x 107 cm, Zircaloy-2 clad, Th/U233 atom ratio 32.5/1	U2350 ₂ -ThO ₂ rods, .660 cm diam. x 152 cm. aluminum clad, Th/U235 atom ratio 15/1	U2330 ₂ -ThO ₂ rods, 1.09 cm diam x 107 cm, Zircaloy-2 clad, Th/U233 atom ratio 32.5/1
Moderator	H ₂ O and D ₂ O	D ₂ O (99% purity) fully reflected	D ₂ O (98.4% purity)
Temperature	Ambient	Ambient	Ambient
Lattices	Uniform triangular array of rods, cylindrical boundary. 21 H ₂ O-moderated lattices with mod./fuel volume ratio from 1.0 to 9.3 and varying concentrations of H ₃ BO ₃ . Eight D ₂ O-moderated lattices with mod./fuel volume ratio from 3 to 120.	Inner: 2304 rods in square array of 3x3 rod clusters; cylindrical boundary 61 cm diam. Mod./fuel vol. ratio = 2.02. Driver: H ₂ O moderated lattice of TRX slightly-enriched UO ₂ rods.	Inner: 864 rods in square array of 2x2 rod clusters; cylindrical boundary, ~ 56 cm diam., mod./fuel vol. ratio = 1.70. Driver: H ₂ O moderated lattice of TRX slightly-enriched UO ₂ rods.
Parameters Measured	Material B ² , reflector savings, thermal flux depression, ρ^{02} , ρ^{02} .	δ^{02} , CR*, ρ^{02} , δ^{25} ; Th232 capture Doppler	δ^{02} , CR*, ρ^{02} , ρ^{23}
Comments	--	Central parameters in asymptotic spectrum; K_{eff} depends significantly on the driver and requires full core analysis since coupling to the driver not measured. Very hard spectrum ($\rho^{02} = 10.5$). Fuel rods same as BAW 15/1 (Ref. 1).	Central parameters in asymptotic spectrum; K_{eff} depends significantly on the driver and requires full core analysis since coupling to the driver not measured. Very hard spectrum ($\rho^{02} = 8.89$). Fuel rods same as BNL (Ref. 7).

Table I-1 (Cont'd)

Experiment	LWBR SB Criticals	LWBR BMU Criticals	LWBR Detailed Cell										
Laboratory	Bettis	Bettis	Bettis										
References	11 (1967)	12 (1975)	13 (1974)										
Fuel	Zircaloy-2 clad, 38 cm-long rods. Seed: 0.54 cm diam, 26 w/o U_{2330_2} - ZrO_2 and 26 w/o U_{2350_2} - ZrO_2 . Blanket: 1.25 cm diam, ThO_2 and 1 w/o U_{2330_2} - ThO_2 .	Axially zoned U_{2330_2} - ThO_2 and ThO_2 in Zircaloy-4 clad. Seed: 0.52 cm diam rods of four types. Blanket: 1.4 cm diam rods of four types.	Twelve types of U_{2330_2} - ThO_2 and ThO_2 seed and blanket rods ² in Zircaloy-4.										
Moderator	H ₂ O	H ₂ O	H ₂ O										
Temperature	Ambient (two of the wet-blanket assemblies were run also at 480°F.)	Ambient (except BMU-1C at 410°F)	Ambient (except Core IIIb at 477°F)										
Lattices	Small seed-blanket assemblies. Five wet-blanket lattices were square arrays with rectangular boundaries. Three dry-blanket lattices were triangular arrays with hexagonal boundaries	Multiply-zoned seed-blanket assemblies. Three BMU-1 lattices were triangular arrays with hexagonal boundary (single module). Five BMU-2 lattices were 1-, 3-, and 4-module assemblies.	Triangular array with hexagonal 270-cm-high multiply-zoned seed and blanket. Seven configurations with movable seed at different heights.										
	<table><tr><td></td><td>Mod./Fuel Volume Ratio</td></tr><tr><td>U233 Seed</td><td>27, 78</td></tr><tr><td>U235 Seed</td><td>26, 76</td></tr><tr><td>Dry Blanket</td><td>0.21</td></tr><tr><td>Wet Blanket</td><td>1.97</td></tr></table>				Mod./Fuel Volume Ratio	U233 Seed	27, 78	U235 Seed	26, 76	Dry Blanket	0.21	Wet Blanket	1.97
	Mod./Fuel Volume Ratio												
U233 Seed	27, 78												
U235 Seed	26, 76												
Dry Blanket	0.21												
Wet Blanket	1.97												

Table I-1 (Cont'd)

Experiment	LWBR SB Criticals	LWBR BMU Criticals	LWBR Detailed Cell
Parameters Measured	Critical size. Radial and axial flux shapes (U235 fiss, U233 fiss, Th cap, DY) ρ^{02} , δ^{25} , δ^{23} , thermal disadvantage factors, fast advantage factors in selected locations.	Critical size; radial and axial flux shapes; region power fractions; ρ^{02} and δ^{23} in selected locations; central worths of structural materials; Cf252 neutron importance.	Critical size; region power fractions; axial and radial flux shapes; δ^{23} , ρ^{02} , δ^{02} , at selected locations.
Comments	Good for criticality. Interpretation of parameters requires detailed study of experimental effects. Lack of asymptotic region and small size complicate analysis.	Good for criticality. Interpretation of integral parameters difficult due to geometrical complexity.	Good for criticality. Interpretation of integral parameters difficult due to geometrical complexity.

Various results of these lattice studies have appeared in each of two previous summary reports:

- (1) A review of Th-U233 and Th-U235 benchmark studies, including also results for homogeneous criticals and several other integral measurements, mostly with ENDF/B-IV data (Ref. 14).
- (2) A paper presented at the May 1978 BNL Symposium on Nuclear Data Problems for Thermal Reactors (Ref. 15). This presented results for a number of alternative data sets including several preliminary Th232 evaluations under consideration for inclusion in ENDF/B-V.

The primary purpose of the present report is to describe the analysis methods and results in somewhat more detail than appears in Refs. 14 and 15. Emphasis here is on analyses with ENDF/B-IV data, plus basic cross section sensitivities, and comparisons with the LWBR thorium data set. Detailed results for various alternative preliminary ENDF/B-V thorium data sets (Ref. 15), and comparison of Bettis results with those obtained at other laboratories (Ref. 14, 15) will not be repeated here.

Table I-2 summarizes the specific items dealt with in these studies and described in the remainder of this report.

Table I-2Summary of Benchmark Studies

1. TUPE critical experiments (U235-Th-H₂O)
Five lattices with $1.4 < M/F < 5.8$
 - a) K_{eff} by full-core Monte Carlo (RCP01)
 - b) K_{eff} by cell RCP01 with leakage corrections from P7MG and from MUFT7 with the measured B_M^2 .
 - c) Sensitivity of K_{eff} to basic cross section variations.
2. THUD critical experiments (U235-Th-D₂O)
One lattice (745 fuel rods, $M/F = 9.83$) run at three different D₂O purities and corresponding moderator heights.
 - a) K_{eff} by full-core Monte Carlo (RCP01)
 - b) K_{eff} by cell RCP01 with leakage corrections from P7MG (for sensitivity studies)
 - c) Sensitivity of K_{eff} to basic cross section variations.
3. BNL exponential lattices (U233-Th-H₂O)
Eight lattices with $1.0 < M/F < 9.3$
 - a) K_{eff} by full-core (2D) Monte Carlo (RCP01) with axial leakage correction by P7MG based on measured B_z^2 . (In addition to the clean lattices, two configurations with boron-poisoned moderators were analyzed at $M/F = 1.0$ and two at $M/F = 1.7$.)
 - b) K_{eff} by cell RCP01 with leakage corrections from P7MG and from MUFT7 with the measured B_m^2 .
 - c) ρ^{02} (the epithermal/thermal ratio of Th232 captures).
 - d) Sensitivity of K_{eff} to basic cross section variations (for three lattices).
4. BNL exponential lattices (U233-Th-D₂O)
Eight lattices with $3.0 < M/F < 120$
 - a) K_{eff} by full-core (2D) Monte Carlo (RCP01) with axial leakage corrections by P7MG based on measured B_z^2 (for four lattices).

- b) K_{eff} by cell RCP01 with leakage corrections from P7MG (four lattices) and from MUFT7 with the measured B_z^2 (all eight lattices).
- c) ρ^{02}
- 5. ETA-I critical experiment (U235-Th-D₂O)
 - a) Integral parameters by cell RCP01 with leakage corrections from P7MG.
 - b) Sensitivity of calculated integral parameters to a few cross section variations.
- 6. ETA-II critical experiment (U233-Th-D₂O)
 - a) Integral parameters by cell RCP01 with leakage corrections from P7MG.
- 7. LWBR criticals (U233-Th-H₂O)
BMU-1B and one Detailed Cell configuration.
 - a) K_{eff} by full core Monte Carlo (RCP01).

II. Calculational Methods

ENDF/B cross sections were multigroup processed with ETOMX and ETOTX, which are Bettis versions of ETOG (Ref. 16) and ETOT (Ref. 17). P3 thermal scattering kernels for hydrogen bound in H₂O were processed with FLAN2, the Bettis version of FLANGEII (Ref. 18), from ENDF/B S(α, β) files based on the Haywood kernel.

The MUFT 54-group structure was used from 0.625 eV-10 MeV with multigroup cross sections averaged over a detailed spectrum for a fission source in H₂O. Thermal data were described at 25 energies. Inelastic scattering was described by a multigroup transfer matrix which included multiplication due to the n,2n reaction. Elastic scattering was described in P3 angular approximation by multigroup.

Monte Carlo calculations were done with the RCP01 program (Ref. 19), with job libraries generated by RCPL1 (Ref. 20). In addition to the multigroup data, for each resonance absorber RCP01 employed Doppler broadened resonance profiles at approximately 25,000 energies over the ENDF/B-prescribed resonance range. S-wave resonances were treated explicitly except that only one set of unresolved parameters was allowed over the unresolved range. RCP01 used a Σ_A/Σ_T estimator and neutron weights epithermally. Thermally, a binomial estimator was used in the fuel and a terminating Σ_A/Σ_T estimator in the clad and moderator.

In the full-core RCP01 eigenvalue calculations, the entire lattice was represented in all essential detail. The representation was three dimensional except for the BNL exponential lattices which were treated as infinitely long axially.

In the RCP01/P7MG method, an infinite lattice calculation was done by RCP01, which treated the cell geometry explicitly in two dimensions. It was run as an eigenvalue problem which accounted for the very slight fission source shape in the cell. Leakage corrections were obtained with P7MG (Ref. 21), which performed a radial, one-dimensional, 54-multigroup calculation in cylinder geometry for a homogenized lattice. The calculations were P3 epi-thermally and double-P1 thermally. There was one

thermal group, with constants condensed from a 25-group calculation for each homogenized core region. Thermal cell-flux-weighting factors were derived from the RCP01 cell calculation as were flux-weighting factors for a single fast group (10 MeV-821 Kev). Alternatively leakage corrections were obtained from the measured material buckling by MUFT7, a point B1 multigroup calculation otherwise similar to P7MG. In all cases, leakage correction factors for the RCP01-calculated fast and thermal reaction rates were obtained as the ratio of reaction rate in the leaking, homogenized lattice to that in the homogenized lattice with zero buckling. Reaction rates were normalized to one neutron born of all fission.

Both P7MG and MUFT7 employed a resonance treatment (developed by E. Schmidt and L. Eisenhart) based on integral transport theory, with two-dimensional explicit geometry (including clad and void) for the rod-lattice cell. This model, which supersedes the "L-factor" method, used the same detailed cross section profile as RCP01. Within the energy range .625 eV-5530 eV (to which this method is limited at present) resonance capture rates were found to agree well with RCP01.

III. TUPE Critical Experiments

There were five H₂O-moderated simple lattices constructed from U₂₃₅O₂-ThO₂ rods with Th/U₂₃₅ atom ratios of 15/1 and 25/1. The rods were arranged on a square pitch, held in place by two "egg-crate" grids, one placed on a 10 cm-thick aluminum base plate, the other supported at the top of the core by an aluminum structure.

Table III-1 summarizes characteristics of the lattices. They are designated by the Th/U atom ratio of the fuel and a letter denoting lattice pitch.

Table III-1Characteristics of TUPE Lattices

<u>Lattice</u>	<u>Pitch (inches)</u>	<u>Moderator/Fuel Volume Ratio</u>	<u>Number of Rods</u>	<u>Moderator Critical Height (cm)</u>
15A	0.3850	1.379	1108	127.21
15B	0.4027	1.642	880	133.44
15D	0.4810	2.945	514	135.05
25√2B	0.5694	5.794	1146	135.27
25D	0.4810	3.636	1176	140.50

Table III-2 shows fuel rod dimensions and atomic number densities used in the calculations. For the 15/1 fuel, these data are the same as used in the analysis of the ETA-I experiment (Ref. 9), based on information obtained from BAW 1274 (Ref. 22). For the 25/1 fuel, the main calculations used the rod data derived from Table II of ANL 6378 (Ref. 4). However, a different fuel composition is implied by data in Table 2 of BAW 1191 (Ref. 1). The effect of these composition differences is significant, as will be discussed.

Table III-2

Basic Average Compositions and Dimensions,
and Derived Atomic Number Densities (TUPE Lattices)

<u>Basic Data</u>	<u>15/1 fuel</u>	<u>25/1 fuel</u>	
	<u>BAW 1274</u>	<u>BAW 1191 Table 2</u>	<u>ANL 6378 Table II</u>
Clad O.D.	.308 ± .001 in.	.309 in.	.788 cm
Clad I.D.	(t = .014 ± .001 in.)	.241 in.	.610 cm
Fuel O.D.	.260 ± .002 in.	.234 in.	.587 cm
Fuel Length	60.0 ± .1 in.	60 in.	152.64 cm
<u>Mass/Rod (gm)</u>			<u>Fuel Wt. %</u>
Fuel	434.6 ± .2	356.8	Th 84.13
ThO ₂	405.0 ± .2	341.8	U 3.71
U	25.80 ± .02		U235 93.18
			U234 .96
U235	24.04 ± .02	12.04	U236 .46
			U238 5.40
Fuel Density ($\frac{\text{gm}}{\text{cm}^3}$)	8.33 ± .14	8.45	8.655
N _{Th} /N _{U235}	15.00 ± .05	25.33	24.65
<u>Derived Data (Used in Calculations)</u>			
Fuel r (cm)	.3302	.2972	.2935
Clad r _{in} (cm)	.3556	.3061	.3050
Clad r _{out} (cm)	.3912	.3924	.3940
Fuel length (cm)	152.40	152.40	152.64
<u>Atomic No. Dens. (cm⁻³) × 10⁻²⁴</u>			
Fuel: Th	17705-1	1846-1	1890-1
U235	11810-2	7306-1	7666-3
U234	11961-4		7932-5
U236	60561-5		3768-5
U238	67183-4		4386-4
O	38151-1	3849-1	3958-1
Clad: Al	6025-1		
Mod: H	6676-1		
O	3338-1		

The lattices were described explicitly in three dimensions with the RCP01 Monte Carlo program. Core loading diagrams (Figures 1,3 and 4 from BAW 1191) were used in setting up the RCP01 representations, which are shown in Figures III-1 through III-3. Figure III-4 shows schematically the axial profile model for a typical lattice.

The 76 cm-radius, 1.27 cm-thick steel tank was included, surrounded by a black absorber. The small amount of water between the lower aluminum grid and fuel rods was homogenized with the grid; beyond the lattice the empty grid and water were also homogenized. For the top grid, the air gap between rod and grid was treated as aluminum; beyond the lattice, the empty grid was homogenized with air.

Since safety rods were fully withdrawn for the measurements, they were omitted entirely from the RCP01 model. The corner support posts and other peripheral grid support structure were also omitted.

Table III-3 and Figure III-5 show eigenvalues obtained in the full-core RCP01 calculations. These used rod composition data from BAW 1274 (Ref. 22) for the 15/1 fuel. For the 25/1 fuel, the results refer to fuel rod data from Table 2 of BAW 1191 which implies a thorium/uranium atom ratio of 25.33. These eigenvalues are inferred from the original full core calculations which used the somewhat different rod composition data from Table II of ANL 6378. The composition ambiguity stems from different chemical analyses which obtained values for the Th/U atom ratio of 25.33 and 24.65, as shown in Tables XLII and XLV of ANL 6378. Although the former value seems to be preferred and has been used by B&W (Ref. 1 and private communication from Warren Wittkopf), there remains a significant uncertainty in this regard. In further discussions, K_{eff} results quoted here will refer to TH/U = 25.33.

TUPE 15A

TUPE 15B

RCPO1 Quarter-Core Representations of TUPE
Lattices 15A and 15B
FIGURE III-1

TUPE 15D

TUPE 25D

RCP01 Quarter-Core Representations of TUPE Lattices
15D and 25D
FIGURE III-2

TUPE $25\sqrt{2}B$ RCP01 Quarter-Core Representation of TUPE Lattice $25\sqrt{2}B$

FIGURE III-3

DIMENSIONS
IN CM

RCPOI Axial Representation of TUPE Lattices (Schematic)

FIGURE III-4

Table III-3
 Calculated K_{eff} for TUPE Lattices
 (Full Core RCP01)

Lattice	($\frac{\text{Moderator}}{\text{Fuel}}$)	Number of Rods	Moderator Height (cm)	Calculated Net Leakage	Calculated $K_{eff} \pm \sigma^*$
	Volume Ratio				
15A	1.379	1108	127.21	0.313	$1.0002 \pm .0014$
15B	1.642	880	133.44	0.325	$.9947 \pm .0013$
15D	2.945	514	135.05	0.317	$1.0056 \pm .0014$
25D	3.636	1176	140.50	0.206	$1.0075 \pm .0013$
25 $\sqrt{2}$ B	5.794	1146	135.27	0.165	$1.0060 \pm .0013$

Detailed radial and axial activation shapes were measured with a number of detectors, and values of B_R^2 and B_Z^2 were inferred from them (Ref. 1). To test these bucklings, a zero-leakage cell calculation was done with RCP01. Leakage corrections were then obtained from a homogenized-lattice multigroup analysis with MUFT7, done first for zero leakage and then with the measured material B^2 . The cell RCP01 provided broad-group cell flux weighting factors for the fast flux (0.8-10 MeV) and for the thermal flux (0-.625 eV). The calculation employed the accurate, integral-transport resonance treatment in MUFT7 over the range .625 eV-5530 eV. This uses explicit rod cell geometry and detailed resonance cross sections derived from the RCP01 library. The resonance reaction rates produced by this method agreed very well with those of the cell RCP01 (< 1%) for these lattices. Leakage correction factors for two-group reaction rates were obtained from the MUFT7 ($B^2/B^2 = 0$) calculations and applied to the corresponding RCP01 cell rates. Eigenvalue results are shown in Table III-4. For the leakier, 15/1 fueled lattices these eigenvalues are significantly lower than obtained from the full-core Monte Carlo.

*Monte Carlo statistical error at one standard deviation. Eigenvalues refer to Th/U = 25.33.

Calculated K_{eff} Versus Moderator/Fuel Volume Ratio
for TUPE Lattices

FIGURE III-5

Table III-4

Comparison of K_{eff} from MUFT7 and P7MG
 With the Full-Core RCP01 Results*
 (TUPE Lattices)

Lattice Ident.	Measured Material B^2 (cm^{-2}) $\times 10^4$	$(K_{eff} \pm \sigma)^*$		$K_{eff}(\text{MUFT7})$	$K_{eff}(\text{MUFT7})$
		MUFT7	P7MG	K_{eff} (Full Core RCP01)	K_{eff} (Full Core RCP01)
15A	$85.31 \pm .26$	$.9756 \pm .0014$	$1.0044 \pm .0014$	$.9754 \pm .0020$	$1.0042 \pm .0020$
15B	$94.25 \pm .29$	$.9758 \pm .0018$	$1.0010 \pm .0018$	$.9810 \pm .0022$	$1.0063 \pm .0022$
15D	$114.20 \pm .70$	$.9883 \pm .0019$	$1.0137 \pm .0019$	$.9828 \pm .0024$	$1.0081 \pm .0024$
25D	$64.01 \pm .46$	$1.0046 \pm .0033$	$1.0117 \pm .0033$	$.9971 \pm .0035$	$1.0042 \pm .0035$
25 $\sqrt{2}$ B	$53.55 \pm .11$	$1.0060 \pm .0029$	$1.0129 \pm .0029$	$1.0000 \pm .0032$	$1.0069 \pm .0032$

As an alternative, the MUFT7 calculation for the buckled lattice was replaced by an explicit radial traverse out through the reflector, calculated with P7MG. Axial leakage was represented as a transverse buckling set equal to the measured B_z^2 . In Table III-4 eigenvalues from P7MG are compared with those from MUFT7 and from the full-core RCP01 (also see Figure III-6). The explicit radial calculation shows much better agreement with the Monte Carlo result, with K_{eff} running 0.5-1.0% high. This difference is attributed to approximations in the P7MG model, especially homogenization and simplified flux weighting.

*Both normalized to the same cell RCP01. Uncertainties stem from Monte Carlo statistics at one standard deviation. The MUFT7 calculations used measured material B^2 . Eigenvalues shown for lattices 25D and 25 $\sqrt{2}$ B refer to Th/U = 25.33.

Comparison of K_{eff} Values for TUPE Lattices Obtained
by Different Methods

FIGURE III-6

For the 15/1 fuel, the P7MG eigenvalues are in significantly better agreement with the full-core RCP01 than are the MUFT7 eigenvalues. Since MUFT7 and P7MG are basically similar, except for the explicit spatial treatment of P7MG, this suggests that the measured B_m^2 values are too large for the 15/1 fueled lattices. It is clear from the P7MG results that this is due to non-asymptotic spectra in the smaller lattices--that is, the calculated radial flux shapes agree reasonably well with measurement, but these shapes are not asymptotic. For the 25/1-fueled lattices, which have smaller bucklings, agreement between P7MG and MUFT7 is satisfactory.

The non-asymptotic nature of the small TUPE lattices can be illustrated by examining lattice 15A as an example. Figure III-7 shows a comparison of the measured epicadmium gold radial activation shape (Table 43 of Ref. 1) plotted against the few-group 3 flux shape (ϕ_3) from P7MG. (For a detailed quantitative comparison, the multigroup flux near 5 eV should be used, but few-group 3, which covers the range 0.625 eV-5530 eV, is perfectly adequate for illustration). Over the range of fitting, agreement appears to be reasonably good, with the measured points falling slightly above the calculation at the extremes. The radial buckling derived from the measurement is $B_R^2 = 80.28 \times 10^{-4} \text{ cm}^{-2}$.

Figure III-8 shows the same ϕ_3 along with corresponding calculated flux shapes for few-group 1 (10 MeV-800 KeV) and few-group 4 (.625 eV-0 eV). These shapes differ significantly, and the reflector thermal flux peak occupies a significant portion of the core volume. Even in the central region of the lattice an asymptotic situation is not attained. This can be seen from Figure III-9 which shows B_R^2 for the calculated few-group fluxes as a function of radius. In each case $B_R^2 = \frac{2\pi r J_R(r)}{D\phi}$, where $J_R(r)$ is the radial few-group current at radius r , and $D\phi$ is the few-group flux $\times D$ integrated over the core volume out to r . This gives a B_R^2 in excellent agreement with that derived from the calculated flux shape in an asymptotic situation, and in a non-asymptotic situation gives

Comparison of Measured and Calculated Radial Flux
Shapes in TUPE 15A

FIGURE III-7

an effective B_R^2 which reproduces the calculated few-group leakage at radius r . The different B_R^2 values for different few-groups are quite evident in Figure III-9. The integral over all groups (the total flux and total current) implies a B_R^2 which is nearly constant across the core and is close to the value $73.27 \times 10^{-4} \text{ cm}^{-2}$ which, in a simply-buckled MUFT7 calculation, gives the same eigenvalue as calculated for the explicit radial-dependent P7MG. The few-group flux ϕ_1 approaches this B_R^2 near core center, but ϕ_3 over the range of measurement gives a significantly higher B_R^2 . (In all these comparisons, the axial B^2 has been held fixed at the measured value of $5.03 \times 10^{-4} \text{ cm}^{-2}$).

To determine the effect of alternative atomic number densities and rod dimensions for the 25/1 fuel (see Table III-2), the original radial P7MG calculations for lattices 25D and 25√2B (which were based on Th/U = 24.65) were repeated with data from Table 2 of BAW 1191, which implies Th/U = 25.33. Eigenvalue changes are shown in Table III-5. The modified composition causes a ~ 0.8% reduction of eigenvalues for the 25/1-fueled lattices and brings them into noticeably better agreement with the 15/1-fueled lattices.

Table III-5

Effect of Fuel Composition Changes on
Calculated Eigenvalues for 25/1-Fueled TUPE Lattices*

<u>Lattice</u>	<u>K_{eff} (Th/U = 25.33)</u>
	<u>K_{eff} (Th/U = 24.65)</u>
25D	.99256
25√2B	.99110

*See Table III-2 for respective compositions.

Calculated Radial Few-Group Flux Shapes in TUPE 15A

FIGURE III-8

Calculated Effective Radial Buckling Versus Radius for Four-Group Fluxes
FIGURE III-9

Cadmium ratios of Th232 capture and U235 fission activations were measured with thorium metal foils and U235-Al foils, respectively. Statistics, from reproducibility, appear to be good for U235 ($\sim 1\%$ in δ^{25}); for thorium capture, uncertainties of ρ^{02} range from 2% (for lattice $25\sqrt{2}B$) to nearly 6% (for lattice 15B). Interpretation of these measurements would require detailed study of experimental effects--mainly cadmium cutoff energy and flux perturbation by the detector foils and cadmium sleeves. No attempt has been made to analyze these measurements, and such an effort is judged to be unpromising.

This conclusion is supported by the comparison shown in Table III-6 where calculated ρ^{02} is far below experiment. Since it seems unlikely that the calculations are in error by anywhere near this amount (in view of the good eigenvalues) much of the differences must be attributed to problems with the measurements or their interpretation. This suggests that useful information about thorium resonance capture is not likely to be gained by analysis of these measurements.

Table III-6
Comparison of Calculated and
Measured Values of ρ^{02} for TUPE Lattices

	<u>15A</u>	<u>15B</u>	<u>Cutoff Energy</u>
Experiment:	$2.70 \pm .09$	$2.09 \pm .12$	
Calculation:			
RCP01/P7MG	1.69	1.43	0.4 eV
	1.56	1.33	0.625 eV

ρ^{02} = epithermal thorium capture/thermal thorium capture.

Sensitivities to cross section variations were also studied by P7MG, with results shown in Table III-7. The smooth epithermal multigroup cross sections were increased by a uniform percentage to obtain the changed resonance integrals (I_c and I_f) indicated. Thermal $\sigma_f(E)$ and $\sigma_c(E)$ were increased 1%. As expected, these lattices are most sensitive to the thorium effective resonance integral. The next greatest sensitivity is generally to variations of the fission neutron spectrum.

Table III-7
Sensitivity of TUPE Eigenvalues to Selected Data Changes

	Δ	$(K_{eff}/K_{eff}^{base}) - 1$		
		15A	15D	25. $\sqrt{2}B$
U235 I_f	+ 5.0b	+ .00197	+ .00107	+ .00054
U235 I_c	+ 6.0b	- .00290	- .00149	- .00056
U235 Thermal $\sigma_f(E)$	+ 1.0%	+ .00245	+ .00307	+ .00445
U235 Thermal $\sigma_c(E)$	+ 1.0%	- .00100	- .00101	- .00086
Th232 I_c	+ 1.0b	- .00931	- .00479	- .00298
Th232 Thermal $\sigma_c(E)$	+ 1.0%	- .00112	- .00114	- .00165
U235 Fission Spectrum	ENDF/B-IV → Adams	- .00411	- .00435	- .00210

IV. THUD Critical Experiments

There were 45 D₂O-moderated, uniform single-rod lattices with two types of fuel (the same as in the TUPE experiments): U235O₂-ThO₂ rods with Th/U235 atom ratios of 15/1 and 25/1. Lattices were triangular arrays at four pitches, as summarized in Table IV-1. Spacing was maintained at three axial heights by sheets of perforated aluminum supported

above an aluminum base plate by corner posts. There were four cross-shaped control rods and guide channels at the corners of the square lattice structure.

Table IV-1
Summary of THUD Single-rod Uniform Lattices

<u>Fuel</u>	<u>Pitch</u>	<u>No. of Lattices</u>	<u>Range of Values</u>	
			<u>No. of Rods</u>	<u>Moderator Ht. (cm)</u>
25/1	2a ₀ *	14	665-1526	159.13-76.74
	3a ₀	8	325-461	> 157-103.70
	4a ₀	8	257-339	> 178-129.35
	6a ₀	2	932-1082	113.61-104.33
15/1	2a ₀	6	345-687	132.97-71.78
	3a ₀	4	163-429	150.81-59.73
	4a ₀	3	139-247	127.32-72.79
	6a ₀	3	134-176	137.15-103.58

D₂O purity was monitored periodically. Initially better than 99%, it decreased by 2% over the 2 1/2-year duration of the program. At the end, however, an independent analysis (at the Savannah River Laboratory) obtained a purity 1.6% below the ANL determination and this discrepancy was not explained.

To test overall consistency of interpretation, it was decided to analyze a lattice which was run at the beginning, middle and end of the program. This lattice had 745 fuel rods with Th/U235 atom ratio of 25/1 at the 2a₀ pitch (= 1.906 cm, M/F = 9.83). The final configuration was also analyzed with the lower D₂O purity obtained by SRL.

*a₀ = .953 cm (3/8 in.)

The original full-core RCP01 calculations used fuel composition data (from ANL 6378, Table II) which imply $\text{Th/U} = 24.65$. Eigenvalues were subsequently corrected to the preferred $\text{Th/U} = 25.33$ by means of P7MG as was done for the TUPE 25/1 lattices. The correction reduced K_{eff} by 0.75%.

The lattice was described explicitly in three dimensions by the RCP01 Monte Carlo program. As shown in Figure IV-1, the radial RCP01 representation made the boundary as nearly cylindrical as possible. Figure IV-2 shows schematically the axial profile. Because of the careful documentation it was possible to model the assembly with little ambiguity, including the corner posts, grid sheets, cross-shaped control rod guides and the tank itself. A black absorbing boundary was placed outside the tank. Control rods were represented as withdrawn to a height of 20 cm above the moderator.

RCP01 Third-Core Representation of THUD Lattice

FIGURE IV-1

D₂O purity was read from the curve in ANL 6378 (Fig. 33, p. 100). It was assumed that the values are "mole percent" although this is not explicitly stated. Moderator compositions used in the calculations are shown in Table IV-2. For the D₂O-H₂O mixtures, thermal scattering kernels were mixtures of kernels for H bound in H₂O and D bound in D₂O.

Table IV-2

Moderator Compositions Used in Analyses of THUD Lattices

<u>Core</u>	<u>Date of Run</u>	<u>D₂O Purity (%)</u>	<u>Atomic Number Density (cm⁻³) x 10⁻²⁴</u>		
			<u>Deuterium</u>	<u>Hydrogen</u>	<u>Oxygen</u>
91	3/58	98.5	65514-1	99766-3	33255-1
233	11/58	97.9	65111-1	13966-2	33254-1
456	12/59	97.2	64631-1	18618-2	33246-1
456 (-1.6)	12/59	95.6	63570-1	29258-2	33248-1

Table IV-3 shows eigenvalues obtained from the full-core RCP01 calculations. Within statistics, lattices 91, 233 and 456 are consistent with each other, averaging $1.0084 \pm .0013$, although there may be a slight downward trend. The analysis of lattice 456 with 1.6% reduced D₂O purity shows a $0.22 \pm 0.31\%$ reduction of eigenvalue.

In order to obtain sensitivities (to cross sections and to D₂O purity) without statistics problems, assembly 456 was analyzed with P7MG, which performed an explicit radial traverse of the homogenized lattice out through the reflector. As in the case of the TUPE lattices, reaction rates were normalized, via MUFT7 with $B^2 = 0$, to a cell RCP01 (zero leakage). Fast and thermal cell flux weighting factors were also obtained from the Monte Carlo cell calculation. An axial transverse $B^2 = .00038 \text{ cm}^{-2}$ was used, obtained from the measured critical moderator height, with reflector savings of 22 cm. Resonance reaction rates in the cell MUFT7

($B^2 = 0$) were in adequate agreement with RCP01 although agreement was not as good as for the H_2O moderated lattices.

The calculated eigenvalue was $1.0146 \pm .0021$, somewhat higher than the value $1.0061 \pm .0021$ obtained from the full-core RCP01. The P7MG result is very sensitive to buckling, however. For example, a change of B_z^2 from $.000380$ to $.000412 \text{ cm}^{-2}$, resulting from a 6.29 cm reduction of effective core height, reduced K_{eff} by 0.59%.

Table IV-3
Calculated K_{eff} for THUD Lattices
(Full Core RCP01)

<u>Lattice Ident.</u>	<u>Date of Run</u>	<u>D₂O Purity (%)</u>	<u>Moderator Height (cm)</u>	<u>Calculated Net Leakage</u>	<u>Calculated $K_{\text{eff}} \pm \sigma^*$</u>
91	3/58	98.5	132.84	.269	$1.0024 \pm .0023$
233	11/58	97.9	135.08	.268	$1.0018 \pm .0024$
456	12/59	97.2	139.09	.267	$.9987 \pm .0021$
				Average	$1.0010 \pm .0013$
456	12/59	95.6 (?)	139.09	.271	$.9965 \pm .0023$

P7MG showed a small (0.17%) decrease in eigenvalue due to the 1.6% reduction of D_2O purity, in good agreement with RCP01. Epithermal/thermal reaction ratios were reduced by 9%, however. Thus, the D_2O purity ambiguity is quite significant for such quantities as ρ^{02} (ratio of epithermal/thermal thorium captures) and δ^{25} (ratio of epithermal/thermal U235 fissions) although it has little effect on eigenvalue.

*One standard deviation. Eigenvalues refer to Th/U = 25.33.

The P7MG analysis of THUD 456 was repeated with the significantly different fuel composition implied by data in BAW 1191 (Table 2). This resulted in a 0.75% reduction of the predicted eigenvalue (as shown in Table IV-3).

Neutron leakage out of the tank was calculated to be approximately 10%. This suggests that questions of room return could be significant for these lattices.

There were a limited number of integral parameter measurements for these assemblies--specifically, Th232 capture cadmium ratios obtained with metal foils. Interpretation of these measurements, as in the case of the TUPE lattices, would require detailed study of experimental effects such as cadmium cutoff. Since, in most cases, only one irradiation was made and uncertainties are not quoted, it is judged that such an undertaking is not warranted.

Eigenvalue sensitivity to selected cross section variations was calculated by P7MG for THUD 456, with results shown in Table IV-4. In all cases, the smooth epithermal multigroup cross sections were increased by a uniform percentage to obtain the changed resonance integral indicated. Thermal $\sigma_A(E)$ was increased 1%. Sensitivities are fairly significant. For example, a 3% variation of Th232 σ_c (from 7.34 to 7.60b) is worth about 0.5% in eigenvalue, and a 1.0 b variation of the thorium effective resonance capture integral is worth 0.65%.

Table IV-4
Sensitivity of THUD 456 Eigenvalue to Selected Data Changes

	Δ	$(K_{eff}/K_{eff}^{base}) - 1$
U235 I_F	+ 5.0 b	+ .00115
U235 I_C	+ 6.0 b	- .00148
U235 Thermal $\sigma_F(E)$	+ 1.0 %	+ .00341
U235 Thermal $\sigma_C(E)$	+ 1.0 %	- .00095
Th232 I_C	+ 1.0 b	- .00653
Th232 Thermal $\sigma_C(E)$	+ 1.0 %	- .00177
U235 Fission Spectrum	ENDF/B-IV + Adams	- .00089

V. BNL Exponential Experiments

A series of exponential experiments was carried out at the Brookhaven National Laboratory (Ref. 7, 8) in the early 1960's. The assemblies were fueled with U233-ThO₂ elements arranged in uniform triangular pitch lattices in light and heavy water. For the light water lattices, experiments were also done with boron poison added to the moderator. Measurements were made of the material buckling B_m^2 , reflector savings, dysprosium disadvantage factor, ratio of episcadmium to subcadmium capture in thorium (ρ^{02}), and the ratio of Th232 fission to U233 fission (δ_{02}^{23}). Much of the basic data for the BNL experiments has been compiled by Price (Ref. 7), and the most recent survey of the data is presented in the paper by Windsor et al. (Ref. 8).

The D₂O lattices and the unpoisoned light-water lattices were analyzed by three different methods. In increasing order of sophistication, they were:

- 1) Infinite - lattice cell RCP01 Monte Carlo calculations corrected for neutron leakage by the MUFT7 program with measured values of the

material buckling. Resonance absorption in MUFT7 was handled by the heterogeneous collision probabilistic method. Computed reaction rates in the resonance range and other energy ranges for the unbuckled MUFT calculations generally were in good agreement with the corresponding Monte Carlo cell results.

- 2) Similar to Method 1 except that the MUFT7 calculation was replaced by P7MG. This was a one-dimensional (radial), homogenized transport calculation, with a small negative transverse buckling given by $B_z^2 \equiv 1/\lambda_z^2$, where λ_z was the measured relaxation length. (Resonance absorption in P7MG was treated in a manner similar to MUFT7.)
- 3) Two-dimensional, explicit representation of the full lattice with the RCP01 Monte Carlo program. The final K_{eff} values included a small correction for axial in-leakage which was determined using P7MG and the measured B_z^2 .

In addition, for two of the H_2O moderated lattices ($M/F = 0.997$ and 1.7134), configurations were analyzed in which the moderator and reflector were poisoned with boron (in the form of H_3BO_3). The concentration of H_3BO_3 used ranged up to 25 mg/cm^3 and was chosen to reduce the measured material buckling from its clean (pure H_2O) value to approximately zero in two steps. These analyses were done only with Method 3.

Tables V-1 through V-5 summarize fuel rod dimensions, atomic number densities, and lattice parameters used in the calculations. The RCP01 representation of a typical lattice ($M/F = 1.384$) is shown in Figure V-1.

The D_2O lattices were surrounded by a boron shield and a paraffin reflector. These were represented in the radial 2D RCP01 descriptions of the lattices along with the aluminum tank wall, and also in the radial P7MG traverses.

Table V-1

Fuel Rod Dimensions and Atomic Number
Densities Used in the Analysis of the BNL Lattices

Rod Dimensions (cm)

fuel r	.5461
clad r _{in}	.5461
clad r _{out}	.63373

Atomic Number Densities
(cm⁻³) x 10⁻²⁴

Fuel: Th232	198115-1
U233	61021-3
U235	27-6
U234 + U238	1564-4
B (natural)	22-5
O	408832-1
Clad: Zircaloy-2	451493-1

TABLE V-2

Moderator Atomic Number Densities Used For the
H₂O-Moderated BNL Lattices

(Moderator Fuel)	H ₃ BO ₃ Conc. (mg/cm ³)	Atomic Number Density (cm ⁻³) x 10 ⁻²⁴		
		Volume		
		Ratio		
		H	O	B (natural)
A11	0	667334-1	333667-1	0
0.997	13.3	66782-1	33586-1	130-3
	25.0	66790-1	33761-1	244-3
1.7134	4.74	66799-1	33469-1	462-4
	18.9	66778-1	33665-1	184-3

NOTE: For borated solutions, the atomic number densities are based on solution densities in The International Critical Tables. For the pure-H₂O cases (which were analyzed before the borated solutions) atomic number densities are slightly lower than those implied by the borated solution data.

Table V-3

Moderator Atomic Number Densities Used for the
D₂O-Moderated BNL Lattices

(Moderator Fuel)	Volume Ratio	Atomic Number Density (cm ⁻³) x 10 ⁻²⁴		
		D		
		Ratio		
		D	H	O
3.005	65994-1	46521-3	33229-1	
11.716	65941-1	49150-3	33216-1	
16.051	65994-1	46521-3	33229-1	
29.113	66033-1	44541-3	33239-1	
37.028	65931-1	49822-3	33215-1	
55.226	66020-1	43863-3	33229-1	
81.212	65762-1	69783-3	33230-1	
120.491	65931-1	49822-3	33215-1	

Table V-4

Parameters Used in Analysis of
H₂O-Moderated BNL Lattices

(Moderator) Fuel Volume Ratio	Pitch (cm)	H ₃ BO ₃ Conc. (mg/cm ³)	Number of Rods	Buckling (10 ⁻⁴ cm ⁻²)	
				B _z ²	B _m ²
0.997	1.5923	0	511	- 6.45	75.88
		13.3	889	-21.3	--
		25.0	889	-45.2	--
1.384	1.7188	0	253	-35.71	86.06
1.7134	1.8194	0	343	- 5.03	89.34
		4.74	625	- 6.10	--
		18.9	889	-52.6	--
2.1943	1.9573	0	301	- 4.98	90.35
3.0043	2.1697	0	271	- 4.664	85.54
4.2722	2.4656	0	265	- 6.60	69.80
6.8449	2.9769	0	433	- 5.60	32.20
9.2747	3.3899	0	349	-37.77	-1.22

NOTE: The axial bucklings are obtained from the measured relaxation lengths of Ref. 7 as $B_z^2 = -1/\ell^2$

Table V-5

Parameters Used in Analysis of
D₂O-Moderated BNL Lattices

(Moderator) Fuel Volume Ratio	Pitch (cm)	Number of Rods	Buckling (10^{-4} cm^{-2})	
			B_z^2	B_m^2
3.005	2.170	871	--	20.54
11.716	3.758	349	- 4.386	29.85
16.051	4.338	253	--	28.64
29.113	5.738	151	- 9.815	25.00
37.828	6.507	121	--	22.32
55.226	7.821	85	-16.30	19.13
81.212	9.456	55	--	14.67
120.491	11.481	37	-24.01	11.29

RCP01 One-Third Core Representation of BNL H₂O-
Moderated Lattice No. 2 (M/F = 1.384)

FIGURE V-1

K_{eff} results for the unpoisoned H_2O -moderated lattices are shown in Table V-6 and Figure V-2. For Method 1 (Table V-6, Column 2), eigenvalues exhibit an upward trend with moderator/fuel volume ratio (M/F) for values of M/F below 3.0. The results for lattices with M/F > 3.0 show greater consistency, with the exception of the M/F = 9.27 lattice which has a negative material buckling. The Method 2 (RCP01 Cell + P7MG) results appear to be nominally 0.5% higher than the corresponding Method 1 values of K_{eff} and appear to form a more consistent set. They also exhibit a slight rising trend in K_{eff} for M/F values below 3.0. With perhaps the exception of M/F = 1.38, the 2D Monte Carlo calculations (Method 3) yield the most consistent set of K_{eff} values (Figure V-2).

It appears that the greater overall consistency of interpretation that is achieved with the 2D Monte Carlo results compared with those based on Methods 1 and 2 may be due to the elimination of approximations involved in the homogenization of the lattices. Since the tight lattices have the smallest fueled radii, it is supposed that errors in effective resonance cross sections that occur near the core-reflector interface can significantly affect calculated results. Note that for the larger lattices (M/F > 3.0) the rising trend in K_{eff} vs M/F does not persist for Methods 1 and 2.

Table V-6

Comparison of Several Methods for Computing K_{eff} for
the BNL U233-Th232-H₂O Exponential Experiments

(Moderator) Fuel	Calculated K_{eff} *		
	Cell RCP01+MUFT7 (Method 1)	Cell RCP01+P7MG** (Method 2)	2D Full Core RCP01+P7MG (Method 3)
Volume Ratio			
0.997	0.9835 ± 0.0021	0.9993	0.9986 ± 0.0020
1.384	0.9926 ± 0.0018	0.9984	0.9907 ± 0.0022
1.7134	0.9944 ± 0.0018	1.0038	1.0077 ± 0.0028
2.1943	1.0025 ± 0.0021	1.0104	1.0040 ± 0.0019
3.0043	1.0068 ± 0.0022	1.0106	1.0028 ± 0.0024
4.2722	1.0066 ± 0.0023	1.0074	1.0055 ± 0.0025
6.8449	1.0091 ± 0.0026	1.0049	1.0015 ± 0.0025
9.2747	0.9976 ± 0.0029	1.0026	0.9969 ± 0.0023

Table V-7 shows calculated values of K_{eff} for two of the boron poisoned light water lattices. These results were obtained by Method 3, which is considered to be the most accurate. For M/F = 0.997, eigenvalues are remarkably consistent over the range of poison concentrations, with an average value of 0.9987. For M/F = 1.71 the average K_{eff} is also very close to unity (1.0008), but K_{eff} ranges from 1.0077 for the high leakage case (pure H₂O) to 0.9957 for the essentially zero net leakage lattice.

*Monte Carlo statistical errors are one standard deviation.

**Statistical errors (not shown) are the same as for Method 1.

Comparison of Three Methods to Calculate K_{eff} for the
BNL U233-Th-H₂O Lattices

FIGURE V-2

Table V-7
 Calculated Values of K_{eff} for the
 BNL U233-Th232-H₂O/H₃BO₃
Exponential Experiments

$\left(\frac{\text{Moderator}}{\text{Fuel}} \right)$ Volume Ratio	H ₃ BO ₃ Conc. (mg/cm ³)	Number of Rods	B_z^2 (10 ⁻⁴ cm ⁻²)	Calculated K_{eff} ($\pm \sigma$)
0.997	0.0	511	- 6.5	0.9986 $\pm$ 0.0020
	13.3	889	-21.3	0.9983 $\pm$ 0.0019
	25.0	889	-45.2	0.9992 $\pm$ 0.0018
1.7134	0.0	343	- 5.0	1.0077 $\pm$ 0.0028
	4.74	625	- 6.1	0.9996 $\pm$ 0.0018
	18.9	889	-52.6	0.9951 $\pm$ 0.0020

The D₂O-moderated lattices were also analyzed, in a manner similar to that for the light water lattices. Results are shown in Table V-8 and Figure V-3. With Method 1 (RCP01 Cell + MUFT7), the calculated values of K_{eff} form a nearly consistent set, but criticality is nominally underpredicted by 1.5%. Results based on Method 2 (Cell RCP01 + P7MG) and Method 3 (2D full-core RCP01 + P7MG) also underpredict criticality by 1-2%. For M/F $\leq$ 55.2, the full-core Monte Carlo results depict a slight downward trend in K_{eff} vs the M/F volume ratio.

Table V-8

Comparison of Several Methods for Computing K_{eff} for the
BNL U233-Th232-D₂O Exponential Experiments

(Moderator) Fuel	Calculated K_{eff}^*		
	Cell RCP01+MUFT/ (Method 1)	Cell RCP01+P7MG** (Method 2)	2D Full Core RCP01+P7MG (Method 3)
Volume Ratio			
3.005	0.9857 ± 0.0032	--	--
11.716	0.9806 ± 0.0020	0.9911	0.9906 ± 0.0029
16.051	0.9821 ± 0.0020	--	--
29.113	0.9822 ± 0.0019	0.9868	0.9846 ± 0.0028
37.828	0.9890 ± 0.0020	--	--
55.226	0.9792 ± 0.0020	0.9905	0.9795 ± 0.0025
81.212	0.9913 ± 0.0027	--	--
120.491	0.9892 ± 0.0033	--	--

Another key comparison of results can be made for the predicted episcadmium-to-subcadmium ratios of Th232 capture (ρ^{02}). Calculated values of ρ^{02} are compared with the measurements for the light water lattices in Table V-9. The calculations of ρ^{02} consistently underpredict the measured values by (7-10)% ± 4%.

*Monte Carlo statistical errors are one standard deviation.

**Statistical errors (not shown) are the same as for Method 1.

Calculated K_{eff} (Method 1) vs. M/F Volume Ratio for the 3NL U233-ThO₂-D₂O Lattices

FIGURE V-3

The predicted values for ρ^{02} for the D_2O lattices are compared with experiment in Table V-10. As in the case of the light water lattices, ρ^{02} tends to be underpredicted, but only slightly, with an average bias of $-3\% \pm 4\%$. There appear to be possible problems with the interpretation of the ρ^{02} values at $M/F = 81.31$ and 120.5 (both very small lattices, with only 55 and 37 rods respectively).

Table V-9

Comparison of Calculated and Measured Values of ρ^{02}
for the Unpoisoned BNL U233-Th232-H₂O Lattices

<u>(Moderator Fuel Volume Ratio</u>)	<u>Measured ρ^{02}</u>	<u>Calculated ρ^{02}</u>	<u>$\rho^{02} (Calc)/\rho^{02} (Meas)$</u>
0.997	1.380 ± 0.042	1.271	$.921 \pm .030$
1.384	0.928 ± 0.038	0.865	$.932 \pm .041$
1.713	0.754 ± 0.024	0.698	$.926 \pm .032$
2.194	0.607 ± 0.026	0.543	$.895 \pm .043$
3.004	0.435 ± 0.013	0.396	$.910 \pm .030$
4.2722	--	--	--
6.8449	0.218 ± 0.008	0.201	$.922 \pm .037$
9.2747	0.170 ± 0.007	0.158	$.929 \pm .041$
		Av.	<u>.92</u>

Table V-10

Comparison of Calculated and Measured Values of ρ^{02}
for the BNL U233-TH232-D₂O Lattices

(Moderator Fuel Volume Ratio)	Measured ρ^{02}	Calculated ρ^{02}	ρ^{02} (calc.) / ρ^{02} (meas.)
3.005	4.71 ± 0.18^a	4.377	0.929 ± 0.038^b
11.716	0.794 ± 0.028^a	0.759	0.956 ± 0.035
16.051	0.565 ± 0.017^a	0.555	0.982 ± 0.030
29.113	0.297 ± 0.011	0.297	1.000 ± 0.037
37.828	0.234 ± 0.008	0.230	0.983 ± 0.034
55.226	0.166 ± 0.006	0.164	0.987 ± 0.036
81.312	0.104 ± 0.005	0.111	1.066 ± 0.048
120.491	0.089 ± 0.005	0.079	0.888 ± 0.056
Average			.97

^aWeighted average of ρ^{02} determined by the cadmium ratio and thermal activation methods. All other values are based on the cadmium ratio method.

^bErrors are of experimental origin only.

Eigenvalue sensitivity to selected cross section variations was calculated for three H₂O-moderated lattices with results shown in Table V-11.

Table V-11
Sensitivity of Eigenvalues to Selected Data Changes
(BNL Th-U233-H₂O Lattices)

	Δ	$(K_{eff}/K_{eff}^{base} - 1)$		
		M/F=1.0	3.0	6.8
U233 I_F	+ 13.0b	+ .0044	+ .0020	+ .0074
U233 I_C	+ 6.0b	- .0024	- .0009	- .0060
U233 Thermal $\sigma_F(E)$	+ 1.0%	+ .0027	+ .0038	+ .0014
U233 Thermal $\sigma_C(E)$	+ 1.0%	- .0001	- .0004	- .0002
Th232 I_C	+ 1.0b	- .0150	- .0060	- .0029
Th232 Thermal $\sigma_C(E)$	+ 1.0%	- .0013	- .0021	- .0019
U233 Fission Spectrum	ENDF/B-IV + Std Model	- .0034	- .0041	- .0013

The effect of the LWBR thorium data set (Ref. 23, 24) was evaluated for the BNL light water lattices. The changes of K_{eff} and ρ^{02} (based on the 2D Monte Carlo calculations, corrected for axial in-leakage) are shown in Table V-12. The LWBR thorium produces ~4% higher ρ^{02} values as a result of increased resonance capture and slightly decreased thermal capture relative to ENDF/B-IV.

Table V-12

Effect of Using the LWBR Th232 Data Set on
 K_{eff} and ρ^{02} for the BNL Light Water Lattices

(Moderator) Fuel	(LWBR Th232/ENDF/B-IV Th232)		Std. Spectrum ENDF/B-IV
	ρ^{02}	K_{eff}	K_{eff}
.997	1.036	1.0086	.9967
1.384	--	1.0041	.9948
1.713	1.043	1.0057	.9945
2.1943	1.037	1.0050	.9948
3.0043	1.071	1.0050	.9960
4.2722	--	1.0031	.9962
6.8449	1.040	1.0022	.9987
9.2747	--	1.0005	1.0004

Eigenvalues with LWBR thorium are higher than with ENDF/B-IV thorium. A comparison of reaction rates for the tighter lattices reveals that the increase in LWBR thorium resonance capture more than compensates for the reduction in the thermal capture cross section. However, the higher scattering cross section of the LWBR thorium reduces core leakage and contributes to raising K_{eff} . For the looser lattices, the reduced thermal capture nearly compensates for the increased resonance capture. Since these core leakage fractions are smaller, the increased LWBR thorium scattering cross section only acts to raise K_{eff} by a slight amount above that using the ENDF/B-IV thorium.

Also shown in Table V-12 are eigenvalue changes produced by use of the Standard model fission spectrum for U233 (see p. 71).

VI. ETA-I and ETA-II Critical Experiments

The ETA-I and ETA-II critical experiments were D₂O-moderated tight lattices designed to test thorium and U233 cross sections in very hard neutron flux spectra (Ref. 9). For ETA-I, the 26" diameter test lattice contained 2304 U235O₂-ThO₂ fuel rods, with Th/U235 atom ratio of 15/1. (These were the same rods used previously in the TUPE and THUD experiments.) For ETA-II, there were 864 U233O₂-ThO₂ rods which had been used previously in the BNL exponential lattices. In both experiments it was necessary to use an H₂O-moderated driver lattice of TRX UO₂ fuel rods in order to achieve criticality. At core center, where integral parameters were measured, the flux spectrum was nearly asymptotic, despite the strong spectrum shift between the test and driver lattices. The following integral parameters were measured by activation techniques:

δ^{23} (δ^{25})	The ratio of fissions above 0.625 eV to fissions below 0.625 eV for U233 (U235)
ρ^{02}	The ratio of captures above 0.625 eV to captures below 0.625 eV for Th232
CR*	The ratio of Th232 captures to U233 (or U235) fissions
δ^{02}	The ratio of Th232 fissions to U233 (or U235) fissions

Interpretation of the parameters requires an explicit radial analysis of the full core to obtain leakage corrections. Since spatial activation shapes were not measured, the calculated K_{eff} depends significantly on the calculated leakage to the driver and hence on the driver itself. Other integral parameters are relatively insensitive to the driver, however. Due to the tightness of the inner lattice, interaction between thorium and uranium is strongly emphasized as compared to a more thermalized lattice.

Integral parameters at core center were calculated for a cell by RCP01, with leakage corrections from P7MG, which performed a homogenized multigroup P_x radial traverse. These calculations--except for the nuclear data, which were from ENDF/B-IV--followed very closely the original

analyses of these experiments as described in Ref. 9, which should be consulted for further details of the calculational model.

Table VI-1 shows a comparison of calculated and measured integral parameters for the ETA-I lattice. Agreement is reasonably good for Th232 capture (ρ^{02} and CR*) but δ^{25} is calculated $(6.9 \pm 1.3)\%$ high, and δ^{02} is $(15.1 \pm 5.5)\%$ low.

Table VI-1
Comparison of Measured and Calculated
Integral Parameters for ETA-I (U235-Th-D₂O)

<u>Integral Parameter</u>	<u>Experiment</u>	<u>Calculation</u>	<u>$(\frac{\text{Calc}}{\text{Exp.}} - 1) \times 100\%$</u>
ρ^{02}	$10.54 \pm .15$	$10.9 \pm .06$	$+ 3.4 \pm 1.5$
δ^{25}	$1.74 \pm .02$	$1.86 \pm .01$	$+ 6.9 \pm 1.3$
δ^{02}	$.0166 \pm .0009^*$	$.0141 \pm .0001$	$- 15.1 \pm 5.5$
CR*	$.867 \pm .009$	$.857 \pm .003$	$- 1.2 \pm 1.1$

Aside from some exploratory studies of alternative preliminary ENDF/B-V thorium data sets (see Ref. 15), the only data variations examined for these experiments were in ETA-I, as shown in Table VI-2. They were as follows:

1. Change from ENDF/B-IV thorium (Material 1296) to the LWBR thorium data set (Ref. 23), which is based on the Steen evaluation of thorium capture cross sections (Ref. 24).

*Measured and calculated for the central rod of the nine-rod cell. Other parameter results are for the entire cell.

+Uncertainties on calculated results are from Monte Carlo statistics.

2. Reduce the ENDF/B-IV U235 fission resonance integral by 10b (from 268b above 0.625 eV).
3. Change the ENDF/B-IV U235 fission spectrum (a Maxwellian with $\bar{E} = 1.985$ Mev) to the Adams spectrum (a Watt shape with $\bar{E} = 2.027$ Mev) and also to the Steen Standard model (with $\bar{E} = 2.073$ Mev).

Table VI-2

Effect of Data Variations on
Calculated Integral Parameters in ETA-I

Integral Parameter	% Change of Integral Parameter			
	→ LWBR Th232	U235 $\Delta I_F = -10b$	U235 Fission Spectrum	
			→ Adams	→ Std. Model
ρ^{02}	+ 2.8	- 1.0	+ 0.1	+ 0.3
δ^{25}	0	- 3.4	+ 0.1	+ 0.2
δ^{02}	+ 12.1	+ 0.5	+ 2.2	+ 5.0
CR*	+ 1.6	+ 1.2	0	+ 0.1

The LWBR thorium data set raises calculated ρ^{02} by 2.8%. This results from a $\sim 2\%$ increase of resonance capture and a $\sim 0.8\%$ reduction of thermal capture. (The LWBR thermal $\sigma_A = 7.34b$, 0.8% below the ENDF/B-IV value of 7.4b.) The 12% increase of δ^{02} can be directly attributed to the higher fission cross section of the LWBR thorium.

The 10b reduction of the U235 fission resonance integral lowers calculated δ^{25} by 3.4% and ρ^{02} by 1%, both changes which improve agreement with experiment somewhat.

The only significant effect of the fission spectrum change is on δ^{02} (via the thorium fissions): the Adams spectrum raises δ^{02} by 2.2%; the harder Standard model spectrum raises it by 5%.

Table VI-3 shows a comparison of calculated and measured integral parameters for the ETA-II lattice. In contrast to ETA-I, overall agreement is very good. The calculated ρ^{02} is slightly below experiment. Agreement for δ^{23} is excellent, and δ^{02} is low by $(9 \pm 8)\%$.

Table VI-3

Comparison of Measured and Calculated
Integral Parameters for ETA-II (U233-Th-D₂O)

<u>Integral Parameter</u>	<u>Experiment</u>	<u>Calculation</u>	<u>$(\frac{\text{Calc}}{\text{Exp.}} - 1) \times 100\%$</u>
ρ^{02}	$8.89 \pm .15$	$8.71 \pm .05$	$- 2.0 \pm 1.8$
δ^{23}	$2.96 \pm .08$	$2.90 \pm .02$	$- 2.0 \pm 2.8$
δ^{02}	$.0181 \pm .0014$	$.0165 \pm .0002$	$- 8.8 \pm 7.8$
CR*	$1.047 \pm .02$	$1.034 \pm .004$	$- 1.2 \pm 2.0$

VII. LWBR Critical Experiments

One configuration of the Detailed Cell (Ref. 13) and one BMU lattice (Ref. 12) were analyzed with RCP01 and ENDF/B-IV data. These assemblies were represented explicitly in three dimensions, including all fuel rods and lattice structural components. There was some homogenization of peripheral structure.

The BMU-1B core consisted of a symmetric hexagonal seed with 810 28-inch-long fuel rods. These were of approximately 0.25-inch diameter on a 0.32-inch triangular pitch. The upper 14 inches of each rod was 5 w/o U233O₂-ThO₂, the remainder was 9 w/o. The seed rods rested on an

equal number of 14-inch-long ThO_2 rods. The center seven lattice positions were occupied by a Zircaloy pipe. The seed was enclosed in a double-walled hexagonal Zircaloy can, and the 1/8-inch water gap between the walls provided channels for six hafnium control blades. The surrounding blanket contained 811 42-inch-long ThO_2 rods and 360 2 w/o U233O_2 - ThO_2 rods which were of approximately 0.625-inch diameter, on a 0.70-inch triangular pitch. Figure VII-1 shows the RCP01 representation of the core loading, and Figure VII-2 shows a schematic view of the axial description.

The Detailed Cell was a single seed-and-blanket core, approximately 105 inches high, with a movable central seed region. The seed was a symmetric hexagon containing 15 rows of 0.305-inch diameter fuel rods on a 0.368-inch triangular pitch. An inner blanket region surrounded the seed, separated from it by a double-walled hexagonal Zircaloy can. The 1/8-inch water gap between the walls provided channels for six hafnium control blades. The inner blanket was a nonsymmetric hexagon comprising ordinary and power-flattening regions. The outer blanket comprised a driver region with 2 w/o U233O_2 - ThO_2 rods and a reflector region of ThO_2 rods. Figure VII-3 shows the top view of the core, and Figure VII-4 shows the complex axial zoning in the seed and inner blanket regions. In the configuration analyzed, the seed was 2 inches below the axial reference position shown in Figure VII-4.

Eigenvalues obtained with RCP01 and ENDF/B-IV data are shown in Table VII-1. Analysis of the measured parameters is rendered difficult by the complexity of these cores, and no attempt has been made to calculate them.

RCP01 Planar Representation of the LWBR BMU-1B
Lattice

FIGURE VII-1

DIMENSIONS IN CM

RCPO1 Axial Representation of the LWBR BMU-1B Lattice
(Schematic)

FIGURE VII-2

Planar View of the LWBR Detailed Cell Lattice

FIGURE VII-3

NOTE: w/o DENOTES WEIGHT PERCENT OF URANIUM / TOTAL FUEL. SEED IS SHOWN IN AXIAL - ZERO POSITION.

Axial Arrangement of the LWBR Detailed Cell Showing Fuel Zoning

FIGURE VII-4

Table VII-1
Eigenvalues of LWR Criticals Calculated With RCP01

<u>Assembly</u>	<u>Calculated $K_{eff} \pm \sigma$</u>		
	<u>ENDF/B-IV Data</u>		
	<u>All ENDF/B-IV Data</u>	<u>Except LWR Thorium</u>	<u>LWR Data Set (Ref. 23)</u>
Detailed Cell (-2 inches)	.9949 $\pm$.0012	--	1.0015 $\pm$.0018
BMU-1B	.9963 $\pm$.0014	1.0080 $\pm$.0015	1.0069 $\pm$.0019

Table VII-2
Comparison of Major Reaction Rates for
BMU-1B Obtained with ENDF/B-IV and
LWR Thorium Data Sets*

<u>Fast</u>	<u>ENDF/B-IV Th232</u>	<u>LWR Th232</u>
Th fiss.	.0081 (.26%)	.0088
cap.	.1991 (.20%)	.2047
U233 fiss.	.1692 (.20%)	.1706
Q (0.625 eV)	.5725 (.17%)	.5652
<u>Thermal</u>		
Th cap.	.2220 (.26%)	.2168
U233 fiss.	.2213 (.23%)	.2239

*Rest of data were ENDF/B-IV in both cases. Uncertainties for LWR Th232 are the same as shown for ENDF/B-IV. They represent Monte Carlo statistics at one standard deviation.

VIII. Evaluation of Results

In this section, the results are examined as a whole in an attempt to answer the major questions addressed initially:

- (1) To what extent do these integral experiments provide a consistent and adequately detailed test of the differential data?
- (2) How well do ENDF/B-IV data predict the results of these experiments?

The major questions of consistency are as follows:

A) Th232 Capture

- 1) How consistent are the following measured integral parameters:
 - a) effective resonance integrals for ThO₂ rods
 - b) ρ^{02} in BNL H₂O-moderated lattices
 - c) ρ^{02} in BNL D₂O-moderated lattices
 - d) ρ^{02} in ETA-I
 - e) ρ^{02} in ETA-II
- 2) How well are these predicted by ENDF/B-IV?
- 3) How do the ENDF/B-IV and LWBR thorium data sets compare?

B) Eigenvalues

- 1) U235-Th: How consistent are eigenvalues of TUPE and THUD lattices with homogeneous U235-H₂O criticals?
- 2) U233-Th: How consistent are eigenvalues of BNL H₂O-moderated lattices with homogeneous U233-H₂O criticals? BNL D₂O moderated lattices?
- 3) Are ρ^{02} results for BNL H₂O-moderated lattices consistent with K_{eff} ?
- 4) How do the ENDF/B-IV and LWBR thorium data sets compare?

A. Overall Comparison of Thorium Capture

Basic characteristics of the ENDF/B-IV and LWBR thorium data sets are shown in Tables VIII-1 and 2 and Figures VIII-1 and 2. The LWBR set has a 0.8% lower thermal σ_A and a slightly lower dilute resonance integral than ENDF/B-IV. However, it produces 3% more shielded resonance capture. The ENDF/B-IV calculated effec-

tive resonance integral is 6.3% (and the LWBR 3.3%) below the Hellstrand recommended experimental values which are uncertain to $\pm 4.5\%$ (Table VIII-2 and Figure VIII-1). Note however that consistent use of the LWBR $\sigma_A = 7.34b$ will lower the experimental effective resonance integrals by 0.8% (since they are normalized via σ_A taken to be 7.4b), putting LWBR only 2.5% below the measured resonance integral. The LWBR elastic scattering cross section is significantly higher than ENDF/B-IV as shown in Figure VIII-2.

Table VIII-1

Comparison of Resonance Integrals and
Thermal Capture Cross Sections for Thorium Data Sets

	<u>I(> 0.625 eV)</u>	<u>$\sigma_c(.0253 \text{ eV})$</u>
ENDF/B-IV	85.2b	7.40b
LWBR	84.8b	7.34b

Table VIII-2

Comparison of Measured and Calculated
Effective Resonance Integrals for ThO₂ Rods

$\sqrt{\left(\frac{S}{M}\right)_{\text{ThO}_2}}$ (cm ² /g-in) ^{1/2}	Measured I (b)	Calculated I (b)		
	Hellstrand Recom. (Ref. 25)	ENDF/B-IV Th232		
		(Ref. 26)	This Work	LWBR Th232 (Ref. 24)
.3709	11.99		11.49 ± .23	
.4639	13.37	12.47		12.95
.6117	15.75	14.74		15.25
.7278	17.64	16.52		17.05
.8092			17.64 ± .32	
.8652	19.87	18.74		19.19
.9977	22.14		20.87 ± .28	

Hellstrand recommended (Ref. 25): $I = 5.85 + 16.2 \sqrt{\frac{S}{M}} (\pm 4.5\%) \quad b$

LWBR Th232 (Ref. 24): $I = 5.74 + 15.54 \sqrt{\frac{S}{M}} \quad b$

Comparison of Measured and Calculated Effective Resonance Capture Integrals for ThO₂ Rods

FIGURE VIII-1

Comparison of High Energy Elastic Scattering Cross Sections for ENDF/B-IV and LWBR Thorium Data Sets

FIGURE VIII-2

In Figure VIII-3 experiment/calculation ratios are displayed for the limited number of integral Th232 capture measurements which are available. Allowing for the uncertainties shown (which are experimental only), consistency is quite good, although the ETA-I lattice seems somewhat low.

In comparison with ENDF/B-IV, calculated results based on the LWBR thorium evaluation are in slightly better overall agreement with experiment. This is due to its greater resonance capture, and 0.8% smaller thermal capture cross section. Collectively, these comparisons suggest that thorium resonance capture should be slightly above--or at least not much below--ENDF/B-IV.

B. Eigenvalues

In the study of homogeneous U233-H₂O and U235-H₂O criticals with ENDF/B-IV data (Ref. 14, 15, 27), a significant dependence of K_{eff} on hydrogen/uranium ratio was observed. It was concluded that this was due primarily to an underprediction of fast leakage which stemmed in turn from the fact that the ENDF/B-IV prompt fission spectra for U233 and U235 were too soft.

Four recent differential experiments show that the prompt neutron spectrum for low-energy U235 fission is significantly harder than that of ENDF/B-IV, a Maxwellian with $\bar{E} = 1.985$ MeV. A description of the experiments and an analysis of them by J. M. Adams appeared in the Proceedings of the Specialists Meeting on Inelastic Scattering and Fission Neutron Spectra, which was held at Harwell in April 1975. Although it did not provide an exact fit to the data, the Watt model fit quite well and was clearly better than a Maxwellian. The Adams best-fit Watt spectrum had a prompt mean energy of 2.016 MeV.

Comparison of Measured and Calculated Thorium Capture Parameters

FIGURE VIII-3

Recently Steen has performed a least squares adjustment of data for U233 and U235 systems and obtained best-fit fission spectra for both nuclides (Ref. 28). For U235, a good fit was obtained with a Watt shape ($\bar{E}_p = 2.027 \pm .004$ MeV). This result is based on four differential experiments, three of which were used by Adams. A more complex prompt spectrum model (two fully accelerated fragments plus a stationary source) produced an equally good fit to the differential data and a substantially higher mean energy of $2.073 \pm .005$ MeV. This is denoted the Standard model. For U233, based on the differential experiment of L. Green et al. (Ref. 29), a good fit was obtained for a Standard model with $\bar{E}_p = 2.082$ MeV. The Watt and Maxwellian models failed to provide adequate representation of these data.

Figure VIII-4 shows the ENDF/B-IV-calculated K_{eff} versus leakage for homogeneous U235-H₂O criticals and the U235-Th lattices. Although there is some scatter (TUPE 15B is particularly low) the lattices generally fit in very well with the rising trend of K_{eff} shown by the homogeneous criticals.

The effect of the hardened fission spectrum on K_{eff} of U235 systems is shown in Figure VIII-5. Here, where the situation is complicated by a sensitivity to U235 resonance absorption (Ref. 27), both the Watt and Standard models can, with suitable choice of U235 resonance fission and capture integrals, eliminate the trend of K_{eff} with leakage. Figure VIII-5 shows the effect of a particular choice: a 10b reduction of the U235 resonance fission integral plus use of an equilibrium spectrum based on a Watt prompt spectrum with $\bar{E}_p = 2.027$ MeV. This combination removes most of the eigenvalue variation with leakage.

Calculated K_{eff} vs. Leakage Fraction for Homogeneous U235-H₂O Criticals and U235-Th Lattices (ENDF/B-IV)

FIGURE VIII-4

Calculated K_{eff} vs. Leakage Fraction for Homogeneous
U235 H₂O Criticals and U235 Th Lattices (Modified Data)

FIGURE VIII-5

Although their eigenvalues show a fair amount of spread, the U235-Th lattices respond (with sensitivities of Tables III-7 and IV-4) in a manner similar to the homogeneous criticals. To see whether the lattice eigenvalues in Figure VIII-5 exhibit a trend with Th232 resonance capture, they are replotted in Figure VIII-6 versus calculated Th232 resonance capture (above 0.625 eV), along with the zero-leakage limit of K_{eff} for the homogeneous U235-H₂O criticals. There is no evidence of a trend--in fact, overall consistency is quite good except that TUPE 15B is low. Although the 25/1-fueled lattices are slightly high, they would be considerably higher with the alternative fuel composition (Th/U=24.65, see p. 14), which tends to support the Th/U=25.33 values used.

A somewhat more consistent picture is obtained for the U233-H₂O criticals. (These in fact show remarkably little scatter.) Figure VIII-7 shows the ENDF/B-IV calculated K_{eff} versus total neutron leakage fraction for the homogeneous U233-H₂O criticals, the BNL H₂O-moderated exponentials and the two LWBR criticals. The BNL exponentials and the LWBR cores fit nicely into the pattern that was established for the homogeneous criticals. As shown in Figure VIII-8, when the Standard model U233 fission spectrum is employed much of the rising trend in K_{eff} vs leakage is eliminated.

The BNL D₂O-moderated exponentials are not consistent with this picture since K_{eff} is already underpredicted by 1.5% with ENDF/B-IV. It is expected that a harder U233 fission neutron spectrum would worsen this underprediction. However, it should be recognized--a point emphasized by the Brookhaven experimenters--that all the D₂O-moderated lattices were so small as to present significant questions of interpretation. For this reason,

Calculated K_{eff} vs. Th232 Capture Fraction (E > 0.625 eV)
for U235 Th Lattices (Modified Data)

FIGURE VIII-6

preference is given to the H_2O -moderated BNL lattices in attempts to establish a consistent picture. Although there remains the possibility that the lower eigenvalues of the D_2O -moderated exponentials are significant--indicating for example too much fast leakage in D_2O --the good agreement of the THUD U235-Th- D_2O lattices with the U233- H_2O systems seems to argue against this.

Table VIII-3 shows the eigenvalues of the BNL H_2O -moderated lattices (Method 3) corrected by use of the Standard model spectrum, and these are plotted versus calculated fast Th232 capture rate in Figure VIII-9. Eigenvalues are quite consistent with the zero leakage limit of the homogeneous U233- H_2O criticals (as was apparent in Figure VIII-8) and there is little sign of a trend with Th232 fast capture fraction.

Calculated K_{eff} vs. Leakage Fraction for Homogeneous U233-H₂O Criticals and U233-Th Lattices (ENDF/B-IV)

FIGURE VIII-7

Calculated K_{eff} vs. Leakage for Homogeneous U_{233} - H_2O
Criticals and U_{233} -Th Lattices (Modified Data)

FIGURE VIII-8

Table VIII-3

Eigenvalues of BNL H₂O-Moderated
Lattices With Various Thorium Data Sets

Lattice	$\frac{\% \Delta K_{eff}}{\% \Delta \rho^{02}}$	Calculated K_{eff}^*			
		ENDF/B-IV Th232	Modified ENDF/B-IV Th232	LWBR Th232	ENDF/B-IV Th232 (σ_s from LWBR Th232)
			($\Delta \rho^{02} = + 8\%$)		
1	- .1421	.9953	.9839	1.0039	.9997
2	--	--	--	--	--
3	- .0977	1.0021	.9943	1.0078	1.0055
4	- .0817	.9987	.9922	1.0037	--
5	- .0642	.9988	.9937	1.0036	1.0011
6	--	1.0016	--	1.0047	--
7	- .0333	1.0002	.9975	1.0024	1.0009
8	- .0259	.9973	.9952	.9978	--

- *Notes: 1) Data other than for thorium are from ENDF/B-IV in every case.
 2) All eigenvalues are adjusted by use of the Standard spectrum.
 3) Lattices are listed in order of increasing moderator/fuel ratio.

Calculated K_{eff} vs. Th232 Capture Fraction ($E > 0.625 \text{ eV}$)
for U233-Th Lattices (Modified Data)

FIGURE VIII-9

The display of Figure VIII-9 offers a convenient way of examining the consistency of measured ρ^{02} and K_{eff} for the BNL H₂O-moderated lattices. The ENDF/B-IV calculated values of ρ^{02} are 8% below measured values on the average (see Table V-9). Although there remain some questions about cut-off energy (0.51 eV in the calculation) and thorium thermal σ_A (~ 1% uncertain), it would seem that these cannot account for much of the 8% difference. From the calculational end, the difference is most likely due to an under-prediction of Th232 resonance capture.

An 8% increase of calculated Th232 resonance capture (to match the measured ρ^{02}) lowers calculated K_{eff} significantly* (as shown by the dashed line in Figure VIII-9) and produces a strong downward trend of K_{eff} with Th232 capture fraction.

Before any inferences about Th232 resonance capture can be drawn from the plots in Figure VIII-9, however, it is necessary to take into account the sensitivity of K_{eff} to thorium scattering cross section. This is illustrated by the LWBR thorium data set, which produces 3% more resonance capture than ENDF/B-IV-- ρ^{02} is ~ 4% below experiment-- and significantly higher K_{eff} . The increased K_{eff} is due only partly to the 0.8% lower thermal σ_A of the LWBR thorium (worth 0.1-0.2% in K_{eff}). The major factor is the larger scattering cross section of the LWBR thorium (see Figure VIII-2), which reduces leakage. (The effect of the scattering cross section difference was calculated by P7MG and is also shown in Table VIII-3.) Thus, the use of these calculated K_{eff} values to make judgments about Th232 resonance capture depends on having a reasonably accurate knowledge of its scattering cross section.

*Values of $\Delta K_{eff}/\% \Delta \rho^{02}$ and resulting modified eigenvalues, as shown in Table VIII-1, were obtained from the Th232 resonance integral sensitivity calculations.

In any case, the consistency of eigenvalue results (between the BNL H₂O-moderated lattices and the homogeneous U233-H₂O criticals) is lessened for the LWBR thorium, but this is due mostly to the effects of the higher thorium scattering cross section which was adopted in that evaluation and which acts to reduce leakage and raise K_{eff} . The LWBR thorium raises K_{eff} for the BMU-1B core by 1.2%. This is also attributed to reduced leakage with the LWBR set since the overall thorium capture rate was virtually unchanged compared to that for ENDF/B-IV (see Table VIII-2).

IX. Summary

This report has described the analysis of those Th-U233 and Th-U235 critical and exponential experiments considered to be most promising as thermal reactor data-testing benchmarks. Included were five TUPE (Th-U235-H₂O) lattices, three configurations of a THUD (Th-U235-D₂O) lattice, eight H₂O-moderated BNL exponentials (Th-U233), eight D₂O-moderated BNL exponentials, one BMU lattice (Th-U233-H₂O) and one LWBR Detailed Cell configuration (Th-U233-H₂O). Accurate Monte Carlo methods and ENDF/B-IV data were used in all cases. Two major questions were addressed:

1. To what extent do these experiments provide a consistent and adequately detailed test of the differential data?
2. How well do ENDF/B-IV data predict the integral results?

The existing integral experiments provide good beginning-of-life criticality information for these systems. However, except for a few thorium capture measurements (which are fairly consistent) integral parameter results are limited in number and scope.

For H₂O-moderated thorium-uranium lattices, eigenvalues are consistent with the trends observed for homogeneous U233-H₂O and U235-H₂O criticals. This suggests that leakage is underpredicted with ENDF/B-IV for these lattices, as is observed for the homogeneous criticals, and that thorium capture is reasonably well predicted. For the BNL D₂O-moderated exponentials, on the other hand, calculated eigenvalues are low by 1.5%.

In the area of integral parameters, the number of useful measurements is limited. Although the ENDF/B-IV thorium evaluation does not reflect recent experimental data, predicted thorium resonance capture in lattices is only slightly below the nominal best integral result. However, the spread of integral values is large--from ~8% above calculation to ~3% below. It may be noteworthy that in the D₂O-moderated systems calculated thorium capture is slightly higher (relative to experiment) than in the H₂O-moderated systems.

These analyses support hardening of the ENDF/B-IV prompt fission neutron spectrum of U233. The best spectrum representation is obtained with the Standard model, which uses two fully-accelerated fission fragments and a stationary source. This model yields a prompt mean energy of $\bar{E}_p = 2.082$ MeV, and effectively removes the trend in calculated K_{eff} versus leakage.

The ENDF/B-IV U235 prompt fission spectrum is also too soft. Both the Standard and Watt spectrum models can eliminate the trend of K_{eff} versus leakage depending on choice of resonance alpha.

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