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**REVIEW OF THORIUM - U233 CYCLE THERMAL
REACTOR BENCHMARK STUDIES**
(AWBA Development Program)

MARCH 1980

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BETTIS ATOMIC POWER LABORATORY
WEST MIFFLIN, PENNSYLVANIA

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REVIEW OF THORIUM-U233 CYCLE THERMAL REACTOR BENCHMARK STUDIES

(AWBA DEVELOPMENT PROGRAM)

J. J. Ullo
J. Hardy, Jr.
N. M. Steen

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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 while producing electric power, improvements for 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 survey is made of existing integral experiments for U233 systems and thorium-uranium based fuel systems. The aim is to understand to what extent they give a consistent test of ENDF/B-IV nuclear data. A principal result is that ENDF/B-IV leads to an underprediction of neutron leakage. Results from testing alternate thorium data sets are presented. For one evaluation due to Leonard, the results depict a possibly growing discrepancy between measured integral parameters such as ρ^{02} and I^{232} and the differential data, which underpredicts these parameters. Sensitivities to other nuclear data components, notably the fission neutron spectrum, were determined. A new harder U233 spectrum significantly reduces a bias trend in K_{eff} vs leakage.

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REVIEW OF THORIUM-U233 CYCLE THERMAL REACTOR BENCHMARK STUDIES

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INTRODUCTION

Not unexpected due to the renewed interest in the U233-thorium fuel cycle is the desire to establish the adequacy of existing clean thorium-U233 experiments to provide a test of theoretical techniques and nuclear data. This paper summarizes the results of a survey of U233 and thorium-uranium critical experiments which may be of potential use as thermal reactor benchmarks.

The presentation has been divided into two parts. The first part describes analyses of existing thorium-uranium experiments in order to assess their reliability as benchmarks. ENDF/B-IV data were used throughout. Experiments studied included homogeneous U233-H₂O criticals (Ref. 1), simple thorium-U235 critical lattices moderated with H₂O (TUPE (Ref. 2)) and D₂O (THUD (Ref. 3)), the BNL thorium-U233 H₂O and D₂O exponential lattices (Ref. 4, 5), and critical experiments in support of LWBR including the D₂O ETA-I and ETA-II experiments (Ref. 6, 7), the H₂O BMU series (Ref. 8) and the H₂O detailed cells (Ref. 9).

In the second part, the sensitivities of the integral parameters for selected experiments to various thorium data sets are summarized and discussed. The alternate thorium sets tested included the Leonard evaluation (Ref. 10), the Derrien evaluation (Ref. 11), and the LWBR data set based on the Steen evaluation (Ref. 12). Sensitivities to several other

data changes were also determined with the representation of the fission neutron spectrum for U233 and U235 being the most significant.

I. Calculation of Uranium-Thorium Experiments With ENDF/B-IV Data

In this section, the analyses of homogeneous U233 criticals and thorium-uranium lattice critical and exponential experiments which are potentially useful for data testing are discussed. In addition, related analyses performed at other laboratories using ENDF/B-IV data are summarized for comparison.

A. Analyses of Homogeneous U233-H₂O Critical Experiments

In a study done at Oak Ridge (Ref. 13) to compare Hanson-Roach and ENDF/B-IV data sets, McNeany and Jenkins reported that ENDF/B-IV produced errors of several percent in calculated neutron multiplication factors for homogeneous U233 assemblies with low hydrogen/uranium atom ratios (H/U). It was concluded that the ENDF/B-IV data file was not satisfactory for calculating criticality of such assemblies.

More recently, a set of fourteen U233 criticals (including several of those considered in the Oak Ridge study) was analyzed at Bettis (Ref. 1), and a corresponding set of seventeen U235 criticals was analyzed for comparison. The purpose was to examine in detail the ability of ENDF/B-IV data to predict criticality of such systems over a wide range of H/U, with the intent of drawing specific conclusions about the data set. These systems span a wide range of neutron spectrum hardness (with as much as 50% epithermal fission) and of neutron leakage (from 1%-50%). The critical eigenvalue and detailed reaction rates were calculated, and eigenvalue sensitivities to certain major data changes were determined.

The criticals were analyzed with the Monte Carlo program RCP01 (Ref. 14) and with P7MG, an extension of P3MG (Ref. 15), a one-dimensional, multigroup P_0 program. RCP01 was used for the overall study of criticality versus H/U ratio. Cross section sensitivities were derived from P7MG and are presented in Part II of this paper. The agreement between RCP01 and P7MG was checked for five specific experiments and found to be very good.

1. Criticality Versus Hydrogen/Uranium Ratio

Eigenvalues for the U233 criticals (Table I) show generally good agreement with the Oak Ridge calculations. This suggests that the use of different analysis programs and nuclear data processing procedures had little effect on the calculated results. For both U233 and U235, the ENDF/B-IV-calculated eigenvalues (Ref. 1) become increasingly high relative to experiment as the H/U ratio is decreased from well thermalized systems (Figure 1).

Although there remain questions of interpretation about individual experiments, these are judged not to be significant for the overall pattern. Errors in calculated eigenvalue can stem from energy-dependent errors of η which are emphasized as the spectrum hardens, but arguments were presented in Reference 1 which tended to discount this possibility. The other source of eigenvalue error is under-prediction of neutron leakage, which is emphasized in the smaller cores. The most significant factors potentially affecting leakage are considered to be:

Table I - Results for Homogeneous U233-H₂O Critical Experiments Calculated with ENDF/B-IV Data

Experiment	H/U233 Atom Ratio	Calculated		Calculated K _{eff}	
		Total Leakage	δ^{23***}	Ref. (1)*	Ref. (13)**
L1	119	.5149	.4493	1.0116 $\pm$.0034	
L2	154	.5081	.3466	1.0226 $\pm$.0027	1.027 $\pm$.007
L3	381	.4617	.1526	1.0110 $\pm$.0035	1.026 $\pm$.006
L4	581	.4081	.1094	1.0111 $\pm$.0034	
9	1324	.1742	.0635	1.0007 $\pm$.0037	
		.1736	.0635	1.0029	
8	1369	.1743	.0633	1.0035	
7	1417	.1751	.0610	1.0035	
6	1470	.1759	.0588	1.0037	
5	1533	.1776	.0548	1.0017 $\pm$.0016	1.005 $\pm$.003
		.1769	.0563	1.0032	
17	1820	.1094	.0505	.9990	
18	1901	.0880	.0491	1.0002	
11	1986	.0683	.0463	.9974 $\pm$.0031	.994
		.0686	.0477	.9981	
19	1997	.0649	.0476	.9991	
20	2106	.0402	.0461	.9956 $\pm$.0008	
		.0398	.0461	.9967	

*Uncertainty is two standard deviations for RCP01 results.
Eigenvalues without uncertainties are from P7MG.

**Uncertainty is one standard deviation.

*** δ^{23} is the ratio of epithermal fission to thermal fission in U233.

FIGURE 1: U233-H₂O Homogeneous Criticals, Calculated Eigenvalue vs. Total Neutron Leakage Fraction

- (1) Multigroup averaging and limited P_0 treatment in RCP01.
- (2) Oxygen scattering cross section and angular pattern (MeV).
- (3) Fission spectrum of U233 and of U235.

Since the trend in calculated eigenvalue error is nearly the same for U233 and for U235 systems, it is tempting to seek a common source of difficulty (e.g., items (1) and (2) above), but this has not proved fruitful. Furthermore, calculational approximations (including data processing) were deemed to be relatively unimportant. Sensitivities to the fission spectrum mean energy and shape were significant and are further examined in Part II.

B. TUPE Lattices (Th-U235-H₂O)

The TUPE (Thorium-Uranium-Physics-Experiment) criticals were operated at Babcock and Wilcox in the late 1950's (Ref. 2). There were five H₂O-moderated simple lattices constructed from U235O₂-ThO₂ rods having Th/U235 atom ratios of 15/1 and 25/1. The lattices were square arrays of four rod spacings, with moderator/fuel volume ratios ranging from 1.38 to 5.79.

The five uniform lattices have been analyzed with ENDF/B-IV data and the RCP01 Monte Carlo program. The cores were described explicitly in three dimensions, including the lattice plates, core support structure and tank, with a black absorbing boundary placed outside the tank.

Table II and Figure 2 present eigenvalues (K_{eff}) obtained in the full-core analyses with ENDF/B-IV data. These show relatively good agreement with experiment, although there is a distinct downward trend of K_{eff} in the tighter lattices.

Table II - Calculated Criticality of TUPE Lattices
(Full Core RCP01)

<u>Lattice Ident. (Ref. 2)</u>	<u>Mod./Fuel Volume Ratio</u>	<u>Number of Rods</u>	<u>Moderator Height (cm)</u>	<u>Calculated Net Leakage</u>	<u>Calculated $K_{eff} \pm \sigma^*$</u>
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

* Monte Carlo statistical error at one standard deviation.

FIGURE 2: TUPE U235-ThO₂-H₂O Lattices, Full Core FCP01 Calculated K_{eff} vs. (M/F) Volume Ratio

Material bucklings were reported (Ref. 2), inferred from careful measurements of radial and axial activation shapes. For comparison with the full-core Monte Carlo results, eigenvalues have been calculated from a zero-leakage cell Monte Carlo, with leakage correction obtained from MUFT7, an extension of MUFT5 (Ref. 16), using the measured material buckling. Fast advantage factors and thermal disadvantage factors were obtained from the RCP01 cell region fluxes for the fast (10 MeV - 820 keV) and thermal (0 - 0.625 eV) groups. The MUFT7 calculation used a recently developed resonance absorption treatment, based on integral transport theory, with the same detailed cross section profile as used in RCP01. This produced reaction rates in good agreement with the cell RCP01 over the range 0.625 eV - 5530 eV in which it was applied. An alternative calculation was done with the P7MG program. This used the small measured axial buckling ($\sim 0.0004 \text{ cm}^2$) and did an explicit radial traverse of the homogenized core out through the reflector. The calculation was otherwise similar to MUFT7.

Results are shown in Table III and in Figure 3. Two points are noteworthy:

- (1) The P7MG leakage-corrected eigenvalues are somewhat higher than the full-core RCP01 but in reasonable agreement in view of the approximations (homogenization, few-group flux weighting) in P7MG.

Table III - Comparison of Eigenvalues for the TUPE Lattices

Lattice Ident.	Measured Material B^2 (cm ⁻²) $\times 10^4$	$K_{eff} \pm \sigma^*$		K_{eff} (MUFT7)	K_{eff} (P7MG)	K_{eff}^{**} (GE-San Jose)	K_{eff}^{***} (Combustion Engineering)
		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	1.006	--
15B	94.25 $\pm$.29	.9758 $\pm$.0018	1.0010 $\pm$.0018	.9810 $\pm$.0022	1.0063 $\pm$.0022	1.005	0.9873, 1.0023
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	--	--

* Both normalized to the same cell RCP01. Uncertainties stem from Monte Carlo statistics at one standard deviation. The MUFT7 calculations used measured material B_m^2 .

** Work reported (Ref. 17) used BWR lattice methods.

*** Work reported (Ref. 18) consisted of a point CEPAC calculation (low eigenvalue) and a 2D PDQ spatial calculation.

FIGURE 3: TUPE Lattices, Alternate Calculated K_{eff}

- (2) For the 15/1-fueled lattices, use of the measured B_m^2 values in MUFT7 produces eigenvalues significantly below those calculated with the explicit radial traverse by P7MG or by the full-core RCP01. Since MUFT7 and P7MG contain basically similar approximations, except for the explicit spatial treatment in P7MG, this suggests that the measured bucklings are too large. It is clear from the P7MG results that this is due to nonasymptotic spectra in the smaller cores (Ref. 2) - that is, the calculated radial flux shapes agree reasonably well with measurement, but these are not the correct asymptotic shapes. For the 25/1-fueled lattices, which have smaller bucklings, agreement is satisfactory.

Other analyses of lattices 15A and 15B using ENDF/B-IV data have been reported. These were done at GE San Jose (Ref. 17) and Combustion Engineering (Ref. 18). Eigenvalue results are compared in Table III. These show good agreement for the spatially dependent calculations. For the point calculations with measured B_m^2 , the CEPAC result is not as low as obtained with MUFT7.

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} , the ratio of epithermal fission to thermal fission for U235); for thorium capture, uncertainties of ρ^{02} , the ratio of epithermal capture to thermal capture for thorium, range from 2% (for core 25 $\sqrt{2}B$) to nearly 6% (for core 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 unfruitful.

This conclusion is supported by the calculated ρ^{02} values shown in Table IV. The GE-San Jose and BAPL results agree well, but are 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 parameter measurements.

Table IV - Comparison of Calculated and Measured
Values of ρ^{02} for TUPE Cores

Core:	<u>15A</u>	<u>15B</u>	<u>Cutoff Energy</u>
Experiment	2.70 $\pm$.09	2.09 $\pm$.12	
Calculation:			
GE-San Jose (Ref. 17)	1.65	1.42	0.4 eV
BAPL RCP01/P7MG	1.69	1.43	0.4 eV
	1.56	1.33	0.625 eV

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

C. THUD Lattices (Th-U235-D₂O)

The THUD (Thorium-Uranium-Deuterium) lattice critical experiments were run at the Argonne National Laboratory in the late 1950's (Ref. 3). There were 45 uniform single-rod lattices with two types of fuel: U235O₂-ThO₂ rods with Th/U235 atom ratios of 15/1 and 25/1 (the same rods used in the TUPE criticals run at Babcock and Wilcox). The lattices were triangular arrays at four pitches (of 2, 3, 4, and 6 x 0.953 cm). At each pitch several lattices were run, differing in number of fuel rods and moderator critical height.

The D₂O purity, initially better than 99%, decreased by 2% over the 2½ year duration of the program. At the end, an independent analysis obtained a purity 1.6% below the last ANL determination, and this discrepancy was not explained.

To test overall consistency of interpretation, the initial choice was to analyze a specific lattice for which measurements were made at the beginning, middle, and end of the program (designated core 91, 233, and 456, respectively). This lattice had 745 fuel rods with Th/U235 of 25/1 at the 2 x 0.953 cm pitch. Core 456 was also analyzed with a D₂O purity 1.6% below the ANL determination. Composition data for the fuel were those used in the analysis of the TUPE lattices (Ref. 2).

The lattice was described explicitly in three dimensions by the RCP01 Monte Carlo program, including corner posts, grid sheets, cross shaped control rod guides and the tank.

Table V shows eigenvalues obtained from the full core analyses with ENDF/B-IV data. Within statistics, the three cores have consistent eigenvalues, averaging $1.0010 \pm .0013$ (σ). For core 456, a 1.6% reduction of D_2O purity reduced the calculated eigenvalue by $0.22 \pm 0.31\%$. It is noteworthy that neutron leakage out of the reactor tank was calculated to be ~10%. This suggests that questions of room return could be significant for these lattices.

Table V - Calculated Criticality of THUD Lattices
(Full Core RCP01)

Lattice Ident.	Date of Run	D ₂ O Purity (%)	Moderator Height (cm)	Calculated Net Leakage	Calculated $K_{eff} \pm \sigma^*$
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	$0.9987 \pm .0021$
				Average	$1.0010 \pm .0013$
456	12/59	95.6(?)	139.09	.271	$0.9965 \pm .0023$

* One standard deviation.

In order to do sensitivity studies, core 456 was analyzed with P7MG, which performed an explicit radial traverse of the homogenized lattice out through the reflector. Zero-leakage cell reaction rates were normalized to a Monte Carlo cell calculation.

For THUD 456, 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 ϕ^{25} (ratio of epithermal/thermal U235 fissions) although it has little effect on eigenvalue.

There is another ambiguity, which has to do with the composition of the 25/1 fuel. Different chemical analyses obtained values for the Th/U atom ratio of 25.33 and 24.65, as shown in Tables XLII and XLVI of Ref. 3. Although the former value seems to be preferred and has been used by B&W (Ref. 2 and private communication from Warren Wittkopf), there remains a significant uncertainty in this regard. K_{eff} results quoted here are for Th/U = 25.33. Use of the 24.65 value would raise K_{eff} by 0.75% for these THUD lattices. It would raise K_{eff} for the 25 $\sqrt{2}$ B and 25D TUPE lattices by 0.9%, worsening agreement with the 15/1-fueled TUPE lattices.

There were a limited number of integral parameter measurements for these cores - 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.

D. BNL U233-ThO₂ Exponential Experiments

To provide an extensive set of data for lattice parameters for the evaluation of various theoretical techniques and nuclear data, a series of exponential experiments were carried out at the Brookhaven National Laboratory. The assemblies were fueled with U233-ThO₂ elements, which were arranged in uniform lattices having a triangular pitch in light and heavy water. Measurements were made of the material buckling B_m^2 , reflector savings, dysprosium disadvantage factor, ratio of epicadmium to subcadmium capture in thorium (ρ^{02}), and the ratio of Th232 fission to U233 fission (δ^{02}). Much of the basic data for the BNL experiments has been compiled by Price (Reference 4), and the most recent survey of the data is presented in the paper by Windsor et al. (Ref. 5).

Recent calculations of the light water lattices having moderator-to-fuel (M/F) volume ratios ranging from 0.997:1 to 3.004:1 have been reported by Sehgal et al. (Ref. 19). This analysis, which used ENDF/B-IV cross sections in RABBLE/HAMMER cell calculations, produced values of K_{eff} shown in the third column of Table VI. Another set of calculations were reported by Shapiro et al. (Ref. 18) for the lattices whose volume ratios ranged from 0.997:1 to 4.2722:1. The analytic model used in this study was based on the CEPAC code and used ENDF/B-IV data and L factors for Th232 and U233 resonance

reaction rates which were corrected for resonance interference between Th232 and U233. These results are shown in the fourth column of Table VI. They typically are 0.5-1% higher than the corresponding results of Sehgal, but they also exhibit the same upward trend with increasing moderator-to-fuel volume ratio (Figure 4).

Other recent studies of the light water lattices have yielded differing results. Weiss and Malaviya (Ref. 20) have analyzed all eight unpoisoned light water lattices using the HAMMER computer code and ENDF/B-IV cross sections. Resonance self-shielding was accounted for using the Nordheim approximation. The results, which are seen in column five of Table VI, show that criticality was underpredicted by an amount varying from 0.1-1.3%. However, the trend in the calculated K_{eff} vs moderator-to-fuel volume ratio is opposite to that of References 18 and 19. The causes for this difference were not discussed.

Bhatt et al. (Ref. 17) have reported an analysis of those BNL exponential lattices with $(M/F) \leq 3.0043$. These calculations used BWR lattice physics methods similar to those applied to the TUPE lattices (Table III). The calculated critical eigenvalues, listed in column six of Table VI, are overpredicted by ~0.5% for $(M/F) \leq 2.0$. For the $(M/F) = 3.004$ lattice, the bias changes sign.

Another key comparison of the results reported from several of the studies mentioned above can be made of the predicted episcadmium-to-subcadmium capture ratios (ρ^{02}) for Th232. These calculations of ρ^{02} are compared with

Table VI - Calculated Values of K_{eff} for the BNL U233-Th232-H₂O
Exponential Experiments Using ENDF/B-IV

$V(\text{Moderator})$ $V(\text{Fuel})$	$B_m^2(\text{m}^{-2})$ (Experimental)	Calculated K_{eff}			
		(Ref. 19)	(Ref. 18)	(Ref. 20)	(Ref. 17)
0.997	75.88	0.9823	0.9918	0.9994	1.005
1.384	86.06	0.9895	0.9957	0.9915	1.005
1.7134	89.34	0.9962	1.0013	0.9907	1.006
2.1943	90.35	1.0005	1.0054	0.9889	1.002
3.0043	85.54	1.0037	1.0087	0.9871	0.994
4.2722	69.8	--	1.0117	0.9886	--
6.8449	32.2	--	--	0.9928	--
9.2747	-1.22	--	--	0.9970	--

FIGURE 4: BNL U233-ThO₂-H₂O Exponential Lattices, Comparison of K_{eff} Calculations Based on ENDF/B-IV

the measured values in Table VII. Generally, the calculations of ρ^{02} are in good agreement with each other, but they consistently underpredict the measured values.

The above comparison of K_{eff} values, which were calculated for the BNL light water U233-thorium lattices, depicts a method dependence which tends to confound the interpretation of these experiments for nuclear data testing purposes. In an attempt to clear up some of these discrepancies, the unpoisoned light water lattices and all of the heavy water lattices were analyzed. Three methods to compute K_{eff} were compared. In increasing order of sophistication, they were:

- (1) Single lattice cell Monte Carlo (using the RCP01 program) calculations which were corrected for neutron leakage using the MUFT7 program and the measured material bucklings. Resonance absorption in MUFT7 was handled by a heterogeneous collision probabilistic method. Computed reaction rates in the resonance range and other energy ranges for the unbuckled MUFT7 calculations generally were in good agreement with the corresponding Monte Carlo cell results.
- (2) Same as Method 1 except that one-dimensional, homogenized P7MG transport calculations with a small negative transverse buckling given by $B_z^2 = -\frac{1}{\ell_z^2}$, where ℓ_z was the measured relaxation length, were used to correct for neutron leakage.

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

$\frac{V(\text{Moderator})}{V(\text{Fuel})}$	B_m^2 (m ⁻²)	Measured ρ^{02}	Calculated Results			
			Ref. (19)	Ref. (18)	Ref. (17)	This Work
0.997	75.88	1.380 $\pm$ 0.042	1.308	1.307	1.283	1.271
1.384	86.06	0.928 $\pm$ 0.033	0.901	0.906	0.904	0.865
1.713	89.34	0.754 $\pm$ 0.024	0.716	0.720	0.729	0.698
2.194	90.35	0.607 $\pm$ 0.026	0.553	0.561	0.575	0.543
3.004	85.54	0.435 $\pm$ 0.013	0.406	0.411	0.431	0.396
4.2722	69.8	--	--	--	--	--
6.8449	32.2	0.218 $\pm$ 0.008	--	--	--	0.201
0.2747	-1.22	0.170 $\pm$ 0.007	--	--	--	0.158

This avoided the use of the measured radial bucklings. (Resonance absorption in P7MG was treated in a manner similar to MUFT7.)

- (3) Monte Carlo calculations (using the RCP01 program) which represented the entire lattice explicitly in two dimensions. The final K_{eff} values included a small correction for axial inleakage which was obtained from the P7MG transport program.

The results for the light water lattices using Method 1 (Table VIII, column 2) are in good agreement with (Ref. 19) and once again exhibit an upward trend with (M/F) volume ratio for values of (M/F) below 3.0. The results for the lattices with $(M/F) \geq 3.0$ become more uniform with the exception of the 9.27:1.0 lattice, which has a negative material buckling. The Method 2 (RCP Cell + P7MG) results appear to be nominally 0.8% 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 the 1.38:1.0 lattice, the 2D Monte Carlo calculations (Method 3) yield the most consistent set of K_{eff} values (Figure 5).

It appears that the greater overall consistency of interpretation that is achieved with the 2D Monte Carlo results as compared with those based on Methods 1 and 2 may be due to the elimination of approximations

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

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

* Monte Carlo statistical errors are one standard deviation.

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

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.

FIGURE 5: BNL U233-ThO₂-H₂O Exponential Lattices, Comparison of Three Methods (see text) to Calculate K_{eff} using ENDF/B-IV

The calculated values of ρ^{02} are compared with experiment and those yielded by other analyses in Table VII. Once again, ρ^{02} is underpredicted by ~8% which is consistent with the other studies. Sensitivities of the calculated ρ^{02} values to alternate thorium evaluations will be discussed in Section II.A.

The BNL U233-thorium-D₂O exponential lattices were also analyzed in a similar manner as described for the light water lattices above. Results are shown in Table IX and Figure 6. Using Method 1 (RCP01 Cell + MUFT7) the calculated values of K_{eff} form a nearly consistent set. However, criticality is nominally underpredicted by 1.5%. Those results based on Method 2 (Cell RCP01 + P7MG) and Method 3 (2D full core RCP + 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.

The calculated values of ρ^{02} for the D₂O lattices are compared with experiment in Table X. These predictions of ρ^{02} based on ENDF/B-IV generally are in good agreement with experiment in contrast to the ρ^{02} results for the H₂O lattices which fell 8% below experiment. For the $(M/F) = 81.2$ and 120.5 lattices, the ρ^{02} results appear to be out of line with the others. This may be due to a problem of interpretation of those experiments.

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

<u>V(Moderator)</u> <u>V(Fuel)</u>	Calculated K_{eff} *		
	Cell RCP01 + MUFT7 (Method 1)	Cell RCP01 + P7MG** (Method 2)	2D Full Core RCP01 + P7MG (Method 3)
3.005	0.9857 $\pm$ 0.0032	--	--
11.716	0.9806 $\pm$ 0.0020	0.9911	0.9906 $\pm$ 0.0029
16.051	0.9821 $\pm$ 0.0020	--	--
29.113	0.9822 $\pm$ 0.0019	0.9868	0.9846 $\pm$ 0.0028
37.828	0.9890 $\pm$ 0.0020	--	--
55.226	0.9792 $\pm$ 0.0020	0.9905	0.9795 $\pm$ 0.0025
81.212	0.9913 $\pm$ 0.0027	--	--
120.491	0.9892 $\pm$ 0.0033	--	--

* Monte Carlo statistical errors are one standard deviation.

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

FIGURE 6: BNL U233-ThO₂-D₂O Exponential Lattices, Calculated K_{eff} (Method 1) vs. M/F Volume Ratio

Table X - Comparison Between Calculated and Measured ρ^{02}
Values for the BNL U233-Th232-D₂O Lattices

$\frac{V(\text{Moderator})}{V(\text{Fuel})}$	Measured ρ^{02}	Calculated ρ^{02}	$\frac{\rho^{02}(\text{calc.})}{\rho^{02}(\text{meas.})}$
3.005	4.71 $\pm$ 0.18*	4.377	0.929 $\pm$ 0.038
11.716	0.794 $\pm$ 0.028*	0.759	0.956 $\pm$ 0.035
16.051	0.565 $\pm$ 0.017*	0.555	0.982 $\pm$ 0.030
29.113	0.297 $\pm$ 0.011	0.297	1.000 $\pm$ 0.037
37.828	0.234 $\pm$ 0.008	0.230	0.983 $\pm$ 0.034
55.226	0.166 $\pm$ 0.006	0.164	0.987 $\pm$ 0.036
81.312	0.104 $\pm$ 0.005	0.111	1.066 $\pm$ 0.048
120.491	0.089 $\pm$ 0.005	0.079	0.888 $\pm$ 0.056

* Weighted average of ρ^{02} .

E. ETA-I and ETA-II Lattices

The ETA-I and ETA-II critical experiments were carried out at the Bettis Atomic Power Laboratory in 1969 and 1970. These were D₂O-moderated tight lattices designed to test thorium and uranium cross sections in very hard neutron flux spectra. For ETA-I, the 26 inch diameter test lattice contained 2304 U²³⁵O₂-ThO₂ fuel rods, with Th/U²³⁵ atom ratio of 15/1. (These were the same rods that had been used ten years earlier in the TUPE and THUD experiments.) For ETA-II, there were 864 U²³⁵O₂-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. Parameters were measured by activation techniques, as follows (Ref. 6):

$\delta^{23}(\delta^{25})$ (a) cadmium ratio; U²³³(U²³⁵)-Al detector foil.

(b) thermal subtraction method, relative to Dyl64-Al detector foil, normalized in reflector.

ρ^{02} Thermal subtraction method, relative to Dyl64-Al detector, normalized in reflector. Ge(Li) count of 312 keV γ from fuel and ThO₂ pellets.

CR*, the ratio of thorium captures to uranium fissions.

(a) From same thorium and U²³³(U²³⁵) activations.

(b) Indirect, from ρ^{02} and $\delta^{23}(\delta^{25})$ as a check.

δ^{02} , the ratio of thorium fissions to uranium fissions.

Fuel and ThO_2 detector pellets. Ge(Li) counting of selected fission product γ 's.

Interpretation of the parameters requires an explicit radial analysis of the full core to obtain leakage corrections. Since spatial activation shapes were not measured, 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 using RCP01, with leakage corrections from P7MG, which performed a homogenized multigroup P_0 radial traverse. Results from the original analyses are compared with experiment in Table XI. For both lattices agreement with experiment is reasonably good, with ρ^{02} approximately 3% high. These analyses used the LWBR thorium cross sections (Ref. 12) which differ in several significant respects from the ENDF/B-IV file. The most notable differences affecting integral parameters are a thermal σ_a of 7.34b (versus 7.40b in ENDF/B-IV) and a fission cross section about 10% higher than ENDF/B-IV. The U235 deck had a fission resonance integral of 259b above 0.625 eV, compared to 268b for ENDF/B-IV material 1261. Its thermal fission cross section was 0.8% below ENDF/B-IV. Other important data (for U233, deuterium and oxygen) were not significantly different from the ENDF/B-IV set.

The ETA lattices have been reanalyzed with the same calculational methods and ENDF/B-IV data. These integral parameter results are also shown in Table XI. The major differences from the calculated parameters of Ref. 6 are:

- (1) Slightly reduced (1.5%) Th232 resonance capture (reflected in ρ^{02} and CR*).
- (2) 4.5% higher δ^{25} , of which 3.5% can be attributed to the higher U235 resonance fission integral of ENDF/B-IV. (This also lowers calculated CR* by about 1% and raises ρ^{02} by 1%.)
- (3) Approximately 10% lower δ^{02} is due mostly to the difference of σ_f^{Th232} .

Additional studies to examine alternative thorium data sets have been undertaken and are discussed in Part II of this paper.

F. LWBR Criticals

Of those critical assemblies constructed in support of the LWBR program, the detailed cell (Ref. 9) and one BMU (Ref. 8) core were analyzed with RCP01 and ENDF/B-IV data. For these calculations the cores 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 ThO₂ blanket rods. These were approximately 0.25-inch diameter on a 0.32-inch triangular pitch. The upper 14-inch of each rod was 5 w/o ²³³UO₂-ThO₂,

Table XI - Comparison of Measured and Calculated Integral Parameters for ETA-I (U235-Th-D₂O) and ETA-II (U233-Th-D₂O)

Integral Parameter	ETA-I Experiment	Calculation*		ETA-II Experiment	Calculation*	
		Original (Ref. 6)	ENDF/B-IV		Original (Ref. 6)	ENDF/B-IV
ρ^{02}	10.54 $\pm$.15	10.92 $\pm$.06	10.9 $\pm$.06	8.89 $\pm$.15	9.16 $\pm$.05	8.71 $\pm$.05
δ^{25}	1.74 $\pm$.02	1.78 $\pm$.01	1.86 $\pm$.01	2.96 $\pm$.08	2.99 $\pm$.02	2.90 $\pm$.02
δ^{02}	.0166 $\pm$.0009**	.0155 $\pm$.0002	.0141 $\pm$.0001	.0181 $\pm$.0014	.0185 $\pm$.0001	.0165 $\pm$.0002
CR*	.867 $\pm$.009	.832 $\pm$.003	.857 $\pm$.003	1.047 $\pm$.02	1.050 $\pm$.003	1.034 $\pm$.004

*Uncertainties on calculated results are from Monte Carlo statistics for one standard deviation.

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

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 can. 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 $^{233}\text{UO}_2\text{-ThO}_2$ rods. These were of approximately 0.625-inch diameter, on a 0.70-inch triangular pitch.

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 non-symmetric hexagon comprising ordinary and power-flattening regions. The outer blanket comprised a driver region with 2 w/o $^{233}\text{UO}_2\text{-ThO}_2$ rods and a reflector region of ThO_2 rods.

Eigenvalues obtained with RCP01 and ENDF/B-IV data are shown in Table XII. The particular detailed cell configuration which was calculated had a critical seed position of ~2.0 inches lower than the blanket.

Table XII - Eigenvalues of LWBR Criticals Calculated
with RCP01 and ENDF/B-IV Data

<u>Core</u>	<u>K_{eff} ± σ</u>
Detailed Cell	.9940 ± .0012
BMU-1B	.9963 ± .0014

G. Resonance Integrals for Thorium Capture

Measurements of the dilute resonance capture integral have usually been made by the cadmium ratio method relative to the dilute resonance integral of gold. In this method, resonance and thermal activation ratios are compared by irradiating dilute gold and thorium detector foils, bare and cadmium-covered, in a pseudo 1/E flux spectrum. Normalization depends on the thorium and gold thermal capture cross sections and the gold dilute resonance integral:

$$I_{Th232} = \frac{(A_{res}/A_{ther})_{Th232}}{(A_{res}/A_{ther})_{Au}} \times \frac{\sigma_{Th232}}{\sigma_{Au}} I_{Au} \quad (1)$$

The measured resonance and thermal specific activation (A_{res} and A_{ther}) of Equation (1) must be suitably corrected for cadmium cutoff energy, detector foil shielding and neutron flux spectrum.

Grenêche (Ref. 21) has recently reviewed the available integral experiments. On the basis of fourteen measurements he obtains a dilute resonance integral

$$I_{\text{Th232}} = 85.8 \pm 0.9b \text{ (experimental)} \\ \pm 1.6b \text{ (normalization)}$$

This represents all capture above 0.5 eV and is normalized as follows:

$$\sigma_{\text{Au}} = 98.8 \pm 0.3b \\ \sigma_{\text{Th232}} = 7.40 \pm 0.08b \\ I_{\text{Au}} = 1560 \pm 22b$$

The BNL-325 (Ref. 22) value of the thorium resonance integral is $85 \pm 3b$.

Complementing lattice experiments as a test of shielded resonance capture are measurements of effective resonance integrals for thorium metal and ThO_2 rods of various diameters. The methods, problems of interpretation and results have been summarized by Hellstrand (Ref. 23).

For thorium, the experiments were done by activation techniques in which a cadmium-covered rod was irradiated in a pseudo-1/E flux spectrum. Thorium captures were sampled by counting the capture activity of a ground-up portion of the ThO_2 rod or (for a metal rod) of a thorium metal detector foil. Normalization was explicitly to the dilute resonance integral of thorium:

$$I^*(S/M, T) = \left(\frac{A_{\text{res}}^*(S/M, T)}{A_{\text{res}}} \right)_{\text{Th232}} \times I_{\text{Th232}} \quad (2)$$

where I^* and A_{res}^* are the effective resonance integral and specific thorium resonance capture activation for a rod of surface/mass ratio

$S/M \text{ cm}^2/\text{gm}$ at temperature T . In some experiments, normalization was directly to the gold resonance integral via Equation (1).

In comparison to lattice measurements, the thorium activation counting techniques are similar, but there is the additional complication of determining the actual flux spectrum impinging on the rod. In this sense an effective resonance integral measurement is more difficult to interpret than a lattice experiment, although in principle it is more specific (i.e., not subject to interference from competing reactions).

On the basis of two experiments (Ref. 24, 25) for metal and three for oxide rods (Ref. 27, 23, 26), Hellstrand (Ref. 23) recommends the following room-temperature effective resonance integrals:

$$\text{Thorium metal} \quad I' = 5.05 + 15.5 \sqrt{S/M}$$

$$\text{ThO}_2 \quad I' = 5.85 + 16.2 \sqrt{S/M}$$

Here, S/M is the surface-to-mass ratio (cm^2/gm) of metal or of oxide. These expressions apply over the range $0.30 < \sqrt{S/M} < 0.90$, with an assigned uncertainty of $\pm 4.5\%$ and include all capture above 0.5 eV.

A connection with lattice measurements of thorium resonance capture can be established via the LWBR thorium capture data evaluation (Ref. 12). The LWBR data set produced calculated effective resonance integrals for ThO_2 rods which are well represented by the expression

$$I' = 5.74 + 15.54 \sqrt{S/M} \quad (300^\circ\text{K})$$

The calculated effective resonance integral is approximately 3% below the Hellstrand recommendation, and the dilute integral is 85.2b. The ENDF/B-IV thorium (as will be shown subsequently) produces approximately 3% less resonance capture than the LWBR set. On this basis, it is inferred that the ENDF/B-IV thorium would produce effective resonance integrals approximately .6% below the Hellstrand recommendation.

H. Consistency of Capture Measurements

There are only a very limited number of integral Th232 capture measurements potentially useful for data testing purposes. For room temperature ThO₂ rods, these are:

- (1) Effective resonance integrals of ThO₂ rods.
- (2) ρ^{02} measurements in the Th-U233 BNL exponentials (H₂O and D₂O moderated).
- (3) ρ^{02} measurements in the D₂O-moderated, hard-spectrum ETA-I (Th-U235) and ETA-II (Th-U233) lattices.

The consistency of these measurements can be seen from Figure 7, which shows experiment/ENDF/B-IV calculation ratios. The experiments range from 10% high to 3% low, with experimental uncertainties ranging from $\pm 2\%$ to $\pm 5\%$. In addition, there are several questions of interpretation which should be mentioned:

- (1) The measured ThO₂ rod resonance integrals are directly proportional to the dilute resonance integral I. Integral measurements of I are directly proportional to the thorium thermal capture cross section.
(Normalization at present is to $\sigma_a = 7.40b$, consistent with ENDF/B-IV.)

FIGURE 7: Comparison of Thorium Capture Predictions Based on ENDF/B-IV

- (2) ρ^{02} measurements do not depend on any such normalization. However, calculated ρ^{02} depends inversely on the thorium thermal σ_a . Without a firm value of σ_a , it is difficult to draw conclusions about resonance capture.
- (3) In the ETA cores, ρ^{02} calculations are somewhat sensitive to data other than Th232 capture itself (through leakage corrections and competing absorptions). For example, the ENDF/B-IV calculated δ^{25} is 7% above experiment. A 10% reduction of the U235 fission integral can remove about half of this difference. Such a change would lower calculated ρ^{02} by 1% and raise calculated CR* by about the same amount.

Altogether, these experiments, assuming that the ENDF/B-IV $\sigma_a^{Th232} = 7.40b$ is fixed, favor an amount of thorium resonance capture slightly above - or at least, not much below - ENDF/B-IV.

II. Testing of Alternative Data Sets for Thorium and Other Data Sensitivities

Part I of this paper established a data base to assess how well ENDF/B-IV cross sections do in predicting the neutron economies of thorium-uranium cores. Although, ENDF/B-IV does a reasonably good job, improvements are desirable in some areas. In what follows, calculated sensitivities of selected experiments covered in Part I to several alternate thorium data sets are reported. The experiments include the ETA-I and ETA-II cores, two TUPE lattices, the BNL exponential experiments, and the BMU-1B core. In addition, a comparison is presented of ENDF/B-IV and the Leonard thorium set,

which was made for the High Temperature Lattice Test Reactor (HTLTR) U233-Th lattices (Ref. 10). Other data sensitivities, notably to the fission neutron spectrum representation, were determined for the homogeneous U233-H₂O criticals and selected lattice experiments.

A. Testing of Alternate Thorium Evaluations

In addition to ENDF/B-IV material 1296, three alternate thorium data sets were used to analyze selected lattice experiments. These evaluations were:

- (1) The Leonard evaluation (Ref. 10) up to 50 keV, ENDF/B-IV above. Mat. 600.
- (2) The Derrien evaluation (Ref. 11). Mat. 445.
- (3) The LWBR data set, based on the 1970 evaluation by N. M. Steen (Ref. 12).

In each case, all data other than that for thorium were from ENDF/B-IV.

Table XIII shows dilute resonance capture integrals and 2200 m/s capture cross sections for the several thorium data sets. A more detailed comparison of the recent evaluation (Mat. 445 and Mat. 600) appears in Table XIV, which shows dilute resonance capture integrals in three ranges. Above 67.4 keV, the difference of smooth capture integral is small. The 3.2 barn difference below 454 eV is nearly all in the resonances and in fact mostly in the large resonances just above 20 eV.

Table XIII - Comparison of Resonance Integrals and Thermal Capture Cross Sections for Several Thorium Data Sets

	<u>I(>0.625 eV)</u>	<u>σ_c (.0253 eV)</u>
ENDF/B-IV	85.2	7.40
Leonard	79.0	7.62
Derrien	83.5	7.40
LWBR	84.8	7.34

In the middle range*, Derrien added additional capture (in file 3) above that contributed by the resolved and unresolved resonances. This was done to make up the $\sigma_c(E)$ adopted by Derrien, as shown in Figure 8 which is taken from Ref. 11. This extra capture was significant down to 450 eV. Since resonance shielding is quite strong in these lattices (the effective resonance integral is only approximately 12 barns), such added capture can be very important, particularly in file 3 where it is not shielded. For this same reason, the accuracy of the $\sigma_c(E)$ shown in Figure 8 becomes significant. As will appear below, 0.1b of unshielded resonance capture integral is worth 1% in ρ^{02} in the ETA-I lattice.

*NOTE: It appeared after some initial work that Mat. 445 had the unresolved resonance capture cross section duplicated in file 3. This duplication was eliminated by reducing the smooth capture cross section in MUFT groups 27-30 (the total reduction was 1.2568b of resonance integral).

Table XIV - Comparison of Dilute Capture Integrals
for Mat. 600 and Mat. 445

Energy Range	MUFT Groups	Resonance Integrals (barns)		
		Mat. 600	Mat. 445	Mat. 445 - Mat. 600
21.1 MeV - 67.4 keV	1-23	.674	.637	-.037
67.4 keV - 454 eV	24-33	6.312	7.630*	1.318
454 eV - 0.625 eV	34-57	<u>72.022</u>	<u>75.254</u>	<u>3.232</u>
		79.0	83.5	4.5

* Reduced by 1.257b in MUFT groups 27-30 to remove duplicated unresolved resonance capture from file 3.

NOTE:

Resonance Ranges			
Mat. 445	resolved	0 eV - 3008 eV	MUFT groups 30-57
	unresolved	3008 eV - 10 keV	MUFT groups 27-30
Mat. 600	resolved	5 eV - 4000 eV	MUFT groups 29-50
	unresolved	4 keV - 50 keV	MUFT groups 24-29

Table XV compares the resonance and background (file 3) MUFT-group smooth capture cross sections for materials 445 and 600. The extra capture in deck 445 is apparent - the cumulative difference in this range is 1.318b of resonance integral.

FIGURE 8: Thorium Capture Cross Section Between 1 keV and 500 keV

Table XV - Comparison of Dilute Capture Cross Sections
Between 454 eV and 67.4 keV

MUFT Group	σ_c (barns)				Mat. 445 - Mat. 600	
	Mat. 445 (Derrien)		Mat. 600 (Leonard)		σ_c (b)	I(b)*
	File 3	Resonance	File 3	Resonance		
24	.42120	0	.23604	.13628	.04888	.02444
25	.55843	0	0	.43024	.12818	.06409
26	.69254	0	0	.55563	.13692	.06846
27	.69321	.15016	0	.69241	.15096	.07548
28	.09306	.92594	0	.85301	.16598	.08299
29	.10753	1.1474	.00174	.89829	.35476	.17738
30	.26742	1.3581	.00588	1.1988	.42086	.21043
31	.42183	1.9689	.00755	1.9016	.48160	.24080
32	.51998	1.9417	.00970	1.8870	.56494	.28247
33	.22942	3.7643	.01245	3.7990	.18220	.09110
						1.31764

*
 $\Delta u = 0.5$

Cell reaction rates in ETA-I were calculated with RCP01, with leakage corrections obtained with P7MG. Resulting integral parameters are shown in Table XVI. The Derrien set is also shown with a 1.0b reduction of smooth capture integral (in MUFT groups 27-33).

A similar calculation was done for the ETA-II experiment with Leonard's thorium. Results are shown in Table XVII.

The following points are noteworthy:

- (1) The LWBR thorium produces 1.5% more resonance capture than ENDF/B-IV Mat. 1296.

Table XVI - Integral Parameters in ETA-I Calculated with
ENDF/B-IV and Various Thorium Data Sets

	Experiment	Calculation*				
		Mat. 1296 Th232	LWBR Th232	Mat. 600 Th232	Mat. 445/*** Th232	Mat. 445#**** Th232
ρ^{02}	10.54 $\pm$.15	10.9 $\pm$.06	11.2	10.1	11.6	10.5
δ^{25}	1.74 $\pm$.02	1.86 $\pm$.01	1.86	1.86	1.84	1.85
δ^{02}	.0166 $\pm$.0009	.0141 $\pm$.0001	.0158	.0141	.0142	.0140
CR*	.867 $\pm$.009	.857 $\pm$.003	.871	.812	.915	.830

* Calculations used ENDF/B-IV data, and thorium data as indicated.
Uncertainties in each case are the same as shown for Mat. 1296 Th232.

** Mat. 445/ has unresolved resonance capture removed from file 3 in
groups 27-30, totaling 1.2568b of resonance integral.

*** Mat. 445# has reduced smooth capture in groups 27-33 totaling 1.0b
of resonance integral (relative to Mat. 445/).

Table XVII - Integral Parameters in ETA-II Calculated with ENDF/B-IV
and Leonard Thorium Data Sets

	Experiment	Calculation	
		Mat. 1296 Th232	Mat. 600 Th232
ρ^{02}	8.89 $\pm$.15	8.71 $\pm$.05	8.15
δ^{23}	2.96 $\pm$.08	2.90 $\pm$.02	2.93
δ^{02}	.0181 $\pm$.0014	.0165 $\pm$.0001	.0164
CR*	1.047 $\pm$.02	1.034 $\pm$.004	.981

- (2) The Derrien data set produces high ρ^{02} and CR* relative to experiment. Removal of 1.0b of smooth (file 3) capture leads to much better agreement.
- (3) The Leonard thorium produces ρ^{02} and CR* significantly below experiment in both ETA-I and ETA-II. Lowering the thermal σ_a could improve ρ^{02} but has small effect on CR*.
- (4) The Leonard set produces a dilute resonance integral (79.0b) significantly below the value 85.8 ± 0.9 (exp), ± 1.6 (norm) obtained by Grenêche (Ref. 21) from integral experiments. Raising σ_a (.0253 eV) from 7.40b to 7.62b would raise the integral value by 3%, increasing the discrepancy.

TUPE lattices 15A and 15D were reanalyzed with the Leonard thorium data set (Mat. 600). Eigenvalues are shown in comparison with ENDF/B-IV (Mat. 1296) in Table XVIII. The effects of the reduced resonance capture and increased thermal capture of Mat. 600 nearly cancel in lattice 15D. The tighter 15A lattice shows more sensitivity to the reduced resonance capture.

Table XVIII -- Comparison of K_{eff} Values Calculated for the TUPE Lattices with Mat. 1296 and Mat. 600 Thorium Data Sets

Lattice	Mod./Fuel Vol. Ratio	Calculated K_{eff}		ΔK_{eff} (Mat. 600- Mat. 1296)
		Mat. 1296 Th232	Mat. 600 Th232	
15A	1.379	1.0002 $\pm$.0014	1.0058 $\pm$.0017	+.0056 $\pm$.0022
15D	2.945	1.0056 $\pm$.0014	1.0074 $\pm$.0019	+.0018 $\pm$.0024

The sensitivities of the 2D Monte Carlo (corrected for axial inleakage) results for the BNL light water lattices to the various thorium evaluations were calculated. Results are shown in Table XIX and are plotted vs (M/F) volume ratio in Figure 9. For each lattice K_{eff} from use of the LWBR thorium is higher than that based on 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 the core neutron leakage fraction and contributes to raise 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. The Leonard thorium set produces higher K_{eff} values for the tighter lattices due to reduced resonance capture. For values of (M/F) > 2.0, the higher Leonard thorium thermal capture cross section overcompensates the reduced resonance capture, resulting in lower values for K_{eff} . Core leakage fractions were similar from use of the Leonard and ENDF/B-IV thorium sets.

Use of the Derrien thorium set yielded values for K_{eff} (not plotted) which were relatively unchanged from those based on the ENDF/B-IV thorium.

FIGURE 9: BNL U233-ThO₂-H₂O Exponential Lattices, Sensitivity of K_{eff} to Thorium Evaluations

Table XIX - Comparison of K_{eff} Values Calculated for the
BNL Exponential Light Water Lattices Using
Different Thorium Evaluations

<u>V(Moderator)</u> <u>V(Fuel)</u>	Calculation*			
	Mat. 1296 Th232	LWBR Th232	Mat. 600 Th232	Mat. 445 Th232
0.997	0.9986 $\pm$ 0.0020	1.0072	1.0046	0.9982
1.384	0.9907 $\pm$ 0.0022	0.9948	0.9918	0.9885
1.713	1.0077 $\pm$ 0.0028	1.0134	1.0084	1.0071
2.1943	1.0040 $\pm$ 0.0019	1.0090	1.0036	1.0037
3.0043	1.0028 $\pm$ 0.0024	1.0078	1.0019	1.0034
4.2722	1.0055 $\pm$ 0.0025	1.0086	1.0028	1.0052
6.8449	1.0015 $\pm$ 0.0025	1.0037	0.9986	1.0015
9.2747	0.9969 $\pm$ 0.0023	0.9974	0.9934	0.9962

*Errors are Monte Carlo statistics at 1σ .

The sensitivity of the calculated parameter ρ^{02} to several of the thorium data sets considered above was determined. Results are summarized in Table XX, and values of $\rho^{02}(\text{calc.})/\rho^{02}(\text{meas.})$ are plotted for comparison in Figure 10. As yielded by RCP cell calculations discussed in Part I, the values of ρ^{02} based on the ENDF/B-IV thorium are ~8% below experiment. As expected with its reduced resonance capture and higher thermal capture cross section, the Leonard thorium yields values of ρ^{02} which are lower

FIGURE 10: BNL U233-ThO₂-H₂O Exponential Lattices, Sensitivity of ρ_{02} to Thorium Evaluations

Table XX - Comparison of ρ^{02} Values Calculated for the BNL Exponential Light Water Lattices Using Different Thorium Evaluations

$\frac{V(\text{Moderator})}{V(\text{Fuel})}$	Measured ρ^{02}	Calculated ρ^{02}		
		Mat. 1296 Th232	LWBR Th232	Mat. 600 Th232
0.997	1.380 $\pm$ 0.042	1.271	1.317	1.185
1.713	0.754 $\pm$ 0.024	0.698	0.728	0.656
2.1943	0.607 $\pm$ 0.026	0.543	0.563	0.504
3.0043	0.435 $\pm$ 0.013	0.396	0.424	0.372
6.8449	0.218 $\pm$ 0.008	0.201	0.209	0.187

still, they being 14% below experiment. The LWBR thorium produces better agreement with experiment than ENDF/B-IV through increased resonance capture and reduced thermal capture.

Similarly, values of ρ^{02} for several of the BNL D₂O moderated lattices were calculated using the LWBR and Leonard thorium evaluations. They are compared with the measurements and values based on the ENDF/B-IV thorium in Table XXI. The ρ^{02} values for the LWBR thorium are about 4% higher than those yielded by the ENDF/B-IV thorium and ~3% above experiment. Leonard's thorium yields ρ^{02} values which are generally 9% below experiment and about 7% below ENDF/B-IV. These results are compared further with other integral measurements related to thorium capture in Section II.B.

Table XXI - Comparison of ρ^{02} Values Calculated for Several BNL Heavy Water Exponential Lattices Using Different Thorium Evaluations

$\frac{V(\text{Moderator})}{V(\text{Fuel})}$	Measured ρ^{02}	Calculated ρ^{02*}		
		Mat. 1296 Th232	LWBR Th232	Mat. 600 Th232
11.716	0.794 ± 0.028	0.759 (0.956 ± 0.035)	0.793 (1.000)	0.724 (0.912)
29.113	0.297 ± 0.011	0.297 (1.000 ± 0.037)	0.308 (1.035)	0.275 (0.927)
55.226	0.166 ± 0.006	0.164 (0.987 ± 0.036)	0.171 (1.031)	0.150 (0.903)

*Numbers in parentheses are $\rho^{02}(\text{calc.})/\rho^{02}(\text{meas.})$.

The BMU-1B core was also analyzed with two alternate thorium data sets: the Leonard evaluation and the LWBR data set based on the Steen evaluation. All other data were from ENDF/B-IV. Major full-core reaction rates and eigenvalues are shown in Table XXII. Mat. 600 produces 2.9% less thorium resonance capture than Mat. 1296 (ENDF/B-IV). The LWBR deck produces 2.8% more. These differences are counteracted thermally by the increased thorium capture of Mat. 600 and the decreased capture of the LWBR set. The fact that the epithermal U233 fission rate is higher with LWBR thorium than with ENDF/B-IV (despite the higher epithermal capture of LWBR thorium) appears to be due to reduced neutron leakage.

Table XXII - Comparison of Major Reaction Rates and Eigenvalues for BMU-1B Obtained with ENDF/B-IV and Various Thorium Data Sets

		Mat. 1296 Th232	Mat. 600 Th232	LWBR Th232
Fast	Th fiss.	.0081 $\pm$.0000	.0081	.0088
	Cap.	.1991 $\pm$.0004	.1913	.2047
	U233 fiss.	.1692 $\pm$.0003	.1705	.1706
	Q(0.625 eV)	.5725 $\pm$.0010	.5786	.5652
Thermal	Th Cap.	.2220 $\pm$.0006	.2260	.2168
	U233 fiss.	.2213 $\pm$.0005	.2233	.2239
	K _{eff}	.9963 $\pm$.0014	1.0045 $\pm$.0016	1.0079 $\pm$.0021

Note: Mat. 1296 is ENDF/B-IV Th232.

Mat. 600 is Leonard's evaluation.

Uncertainties in each case are the same as shown for Mat. 1296.
These are one standard deviation from Monte Carlo statistics.

Another recent test of ENDF/B-IV and the Leonard thorium sets was part of a detailed study (Ref. 10) of the three High Temperature Lattice Test Reactor (HTLTR) U233 lattices (Table XXIII). This work was intended to assess the ability of methods and nuclear data to predict the temperature coefficient of reactivity for HTGR's. The basic assumption of this work was that the possible systematic uncertainties in the measured values of

Table XXIII - Characteristics of the HTLTR U233 ThO₂ Lattices

	<u>Lattice #2</u>	<u>Lattice #3</u>	<u>Lattice #5</u>
C/U-233*	10470	13990	9460
C/Th-232**	193	282	146
Fuel Rod Radius (cm)	0.5969	0.5969	0.9982
Square Lattice Pitch (cm)	1.905	1.905	4.763

* Ratio of carbon to U233 atoms.

** Ratio of carbon to Th232 atoms.

$k_{\infty}(T)$ were relatively temperature independent, and therefore the existing data base of k_{∞} versus T is adequate for verification of neutronic predictions of $\frac{1}{k_{\infty}(T)} \frac{dk_{\infty}(T)}{dT}$. The calculations were based primarily on ENDF/B-IV cross section data, and sensitivities to alternate cross section data for U233 were also determined.

Correlations between calculated and measured temperature coefficients of the HTLTR lattices provided an interesting comparison of thorium data sets. The particular correlation employed had the form

$$k_{\infty}^{\text{meas.}}(T) = k_{\infty}^{\text{calc.}}(T) [A+B(T-293)] \quad (3)$$

$$\left[\frac{1}{k_{\infty}(T)} \frac{dk_{\infty}(T)}{dT} \right]_{\text{meas.}} = \left[\frac{1}{k_{\infty}(T)} \frac{dk_{\infty}(T)}{dT} \right]_{\text{calc.}} + \left(\frac{B}{(A+B(T-293))} \right) \approx \left[\frac{1}{k_{\infty}(T)} \frac{dk_{\infty}(T)}{dT} \right]_{\text{calc.}} + B \quad (4)$$

since $A \sim 1.0$, $B \sim 10^{-5}$, and $T \sim 10^3$. The parameter A plays the role of a normalizing coefficient, and the parameter B expresses the bias in the calculated temperature coefficients. The dependence of the bias parameter B on different sources of cross section data were studied (Table XXIV). There were negligible effects on B from the use of the alternate U233 data, which was effectively a decrease in the thermal eta from 2.2972 to 2.284.

Table XXIV - Calculated Values* of the Temperature Coefficient Bias Parameter B for the HTLTR Lattices

	Lattice #2	Lattice #3	Lattice #5
ENDF/B-IV Data	+0.21±0.07×10 ⁻⁵	1.55±0.19×10 ⁻⁵	+0.41±0.09×10 ⁻⁵
Leonard Thorium (Mat. 600)	-0.18±0.07×10 ⁻⁵	1.08±0.19×10 ⁻⁵	+0.03±0.09×10 ⁻⁵
Leonard Thorium and Alternate U233	--	1.11±0.19×10 ⁻⁵	--

* All values are in units of °K⁻¹.

The values of B obtained using the alternate Leonard thorium were uniformly $0.4 \times 10^{-50} \text{K}^{-1}$ lower than those based on ENDF/B-IV and generally improved the agreement between the calculated and measured temperature coefficients of reactivity for the three $\text{U233O}_2\text{-ThO}_2$ fueled HTLTR lattices. Due to the reduced effective resonance integral, the Leonard thorium produces a smaller negative contribution to the temperature coefficient from the thorium Doppler effect. On this basis it was concluded (Ref. 10) that the Leonard thorium evaluation is preferred over ENDF/B-IV for predicting temperature coefficients of thorium fueled lattices.

Unfortunately, due to systematic uncertainties direct comparisons of calculated $k_{\infty}(T)$ with experiment are not fruitful from a data testing point of view.

B. Overall Comparison of Thorium Evaluations and Capture Measurements

In Figure 11, experiment/calculation ratios are displayed for the limited number of integral Th232 capture measurements for three of the thorium evaluations considered in this work. Errors which are shown are experimental. The ENDF/B-IV results are the same as in Figure 7 and were discussed in Section I.H. The results based on the LWBR thorium evaluation are slightly in better overall agreement with experiment. This is due to greater thorium resonance capture and a 1% smaller thermal capture cross section. The effects of a 3% higher thermal capture cross section and reduced resonance capture are readily apparent in the results produced by Leonard's thorium evaluation. Particular note is made of the bias of +13%

FIGURE 11: Comparison of Thorium Capture Predictions for Several Thorium Evaluations

vs +6% for ENDF/B-IV for the ThO_2 rod resonance integrals. Almost half of this increase is due to the higher σ_a^{Th232} , which is used for normalization of the experimental rod resonance integrals, adopted by Leonard. This again points out the need to firm up the value of σ_a^{Th232} before substantive conclusions can be drawn about resonance capture. Collectively, these comparisons suggest that thorium resonance capture should be slightly above - or at least not much below - ENDF/B-IV and that σ_a^{Th232} should not be increased - or at least not much - over 7.4b.

C. Sensitivities of Calculated Eigenvalues to Other Nuclear Data

Sensitivities of calculated eigenvalues to several nuclear data changes were determined for selected U233 homogeneous criticals. These changes included the hydrogen thermal absorption cross section, the uranium capture and fission resonance integrals, the uranium inelastic cross sections, the ENDF/B version of oxygen, and representations of the fission neutron spectra.

A reference eigenvalue was computed for each assembly with P7MG and ENDF/B-IV data. Then for each change in data δK_{eff} was determined relative to this reference value. The sensitivities of K_{eff} to the various parameters are summarized in Table XXV. The following points are noteworthy:

- (1) The uranium capture and fission resonance integrals were varied as shown in Table XXV. In each case this was achieved by a uniform percentage change of the smooth multigroup cross sections. Although there were significant sensitivities for the U235 systems (Ref. 1), this is not so for U233.

Table XXV - Sensitivities of U233 Critical Assemblies to Changes in Nuclear Data

Data Component	Change in Data Component	Change in Eigenvalue (δK_{eff})			
		H/U233=154(L2)*	381(L3)	1535(L5)	1986(L11)
<u>Hydrogen Cross Sections</u>	Reduced thermal absorption cross section from 0.332b to 0.330b.	+0.0004	+0.0009	+0.0026	+0.0030
<u>Uranium-233 Scattering Cross Sections</u>	Reduced the inelastic cross section by 20%.	-0.0004	-0.0001	0.0000	0.0000
	Inelastic cross sections reduced by 20% and the elastic cross section increased by an equivalent amount to maintain the same total cross section.	-0.0003	-0.0001	0.0000	0.0000
<u>Oxygen Cross Sections</u>	ENDF/B-IV $\rightarrow$ ENDF/B-III	-0.0041	-0.0031	-0.0008	-0.0001
	ENDF/B-IV $\rightarrow$ ENDF/B-I	-0.0062	-0.0044	-0.0012	-0.0002
<u>Fission Spectrum**</u>	Maxwellian spectrum $E=2.0$ MeV	+0.0036	+0.0029	+0.0009	+0.0003
	Maxwellian spectrum $E=2.1$ MeV	-0.0134	-0.0109	-0.0049	-0.0024
	Watt spectrum ($\bar{E}=2.0$ MeV)	-0.0001	+0.0001	+0.0005	+0.0004
Smooth Capture Integral Increased by 6.0b ($I_C=132\pm 6b$ ENDF/B-IV)***		-0.0017	-0.0007	-0.0002	--
Smooth Fission Integral Increased by 13.0b ($I_F=733\pm 13b$ ENDF/B-IV)***		+0.0016	+0.0009	+0.0005	--

*Experiment ID's correspond to those in Table I.

**All δK_{eff} are relative to the ENDF/B-IV fission neutron spectrum for U233.

***Resonance integrals above 0.625 eV.

- (2) Reducing the hydrogen 2200 m/sec absorption cross section from 0.332b to 0.330b increases the reactivity of the thermal assemblies by 0.3% with negligible effect on the high-leakage assemblies.
- (3) A 20% reduction of the inelastic cross sections produced negligible changes of reactivity.
- (4) Sensitivities to the ENDF/B version of oxygen are worth as much as 0.6% in K_{eff} for the high-leakage assemblies and are negligible for the large assemblies. The successive versions of oxygen (ENDF/B-I to ENDF/B-IV) show an increase in backscattering.
- (5) The fission neutron spectrum significantly affects fast neutron leakage. Eigenvalue sensitivities to mean energy (for a Maxwellian shape) and to the difference between Watt and Maxwellian shapes (for the same mean energy) are shown in Table XXV.

Eigenvalue sensitivity to selected cross section variations was calculated for TUPE cores 15A, 15D, and 25 $\sqrt{2}$ B, THUD456, and three BNL exponentials, with results shown in Table XXVI. The smooth epithermal multigroup cross sections were increased by a uniform percentage to obtain the changed resonance integrals indicated. Thermal $\sigma_f(E)$ and $\sigma_c(E)$ were increased 1%. As expected, these lattices are most sensitive to the effective thorium resonance integral. The next greatest sensitivity is generally to revisions of the fission neutron spectra.

Table XXVI - Sensitivity of Eigenvalues to Selected Data Changes

Data Type	$(K_{\text{eff}}/K_{\text{eff}}^{\text{base}} - 1)$							
	TUPE Lattices				THUD Lattice	BNL Exponential Lattices		
	Change	Core 15A	Core 15D	Core 25/2B	456	(M/F) - 0.997:1.0	3.0043:1.0	6.845:1.0
Th232 I_C	+1.0b	-0.0093	-0.0048	-0.0030	-0.0065	-0.0150	-0.0060	-0.0029
Th232 thermal $\sigma_C(E)$	+1.0%	-0.0011	-0.0011	-0.0016		-0.0013	-0.0021	-0.0019
U235 I_F	+5.0b	+0.0023	+0.0011	+0.0005	+0.0012	--	--	--
U235 I_C	+6.0b	-0.0023	-0.0015	-0.0006	-0.0015	--	--	--
U235 thermal $\sigma_F(E)$	+1.0%	+0.0024	+0.0031	+0.0044	+0.0034	--	--	--
U235 thermal $\sigma_C(E)$	+1.0%	-0.0013	-0.0010	-0.0009	-0.0010	--	--	--
U233 I_F	+13.0b	--	--	--	--	+0.0044	+0.0020	+0.0074
U233 I_C	+6.0b	--	--	--	--	-0.0024	-0.0009	-0.0060
U233 thermal $\sigma_F(E)$	+1.0%	--	--	--	--	+0.0027	+0.0038	+0.0014
U233 thermal $\sigma_C(E)$	+1.0%	--	--	--	--	-0.0001	-0.0004	-0.0002
U235 fission spectrum	ENDF/B-IV → Adams	-0.0041	-0.0044	-0.0021	-0.0009	--	--	--
U233 fission spectrum	ENDF/B-IV → Steen	--	--	--	--	-0.0034	-0.0041	-0.0013

From the study of U235 and U233 homogeneous criticals (Ref. 1) (parts of which are reproduced in this review) using ENDF/B-IV data, it was concluded that leakage was being underpredicted. For U235 systems, a suitable hardening of the fission spectrum and adoption of the Watt shape seemed to account for half the discrepancy. The other half seemed to be due to a I_F^{235} which was 10.0b too high. The sensitivities of the TUPE and THUD456 lattices to the more recent Adams U235 fission neutron spectrum are shown in Table XXVI and Figure 12 (TUPE only). (The basis for the spectrum can be found in the Proceedings of the Specialists Meeting on Inelastic Scattering and Fission Neutron Spectra, which was held at Harwell in April 1975.) This spectrum has a Watt shape and a mean energy of 2.016 MeV vs 1.985 MeV for ENDF/B-IV. Better agreement with experiment also was achieved for the U235 homogeneous criticals with Adams' spectrum (Ref. 28).

Steen (Ref. 29) has reevaluated the fission spectra for both U235 and U233. It was found that the Watt and his standard models represented the U235 data, which was the same as used by Adams, with about equal reliability. In the case of the standard model, it was possible to obtain a prompt fission neutron mean energy as high as 2.07 MeV. For U233, the same standard model represented best the existing data and yielded a mean prompt neutron energy of ~2.08 MeV. The effects of this spectrum on K_{eff} for the BNL exponential lattices have been calculated and are depicted in Figure 12. A substantial improvement is obtained.

The overall effect of Steen's new U233 fission neutron spectrum on K_{eff} for the homogeneous U233 criticals, the BNL H₂O moderated exponential experiments, and the two LWBR criticals considered in this

SENSITIVITIES TO FISSION SPECTRA

FIGURE 12: Sensitivities of K_{eff} to Alternate Fission Neutron Spectra

work is depicted in Figures 13 and 14. Figure 13 shows K_{eff} vs total neutron leakage fraction based on ENDF/B-IV. The BNL exponentials and the LWBR cores fit nicely into the pattern that was established for the homogeneous criticals. These same K_{eff} results are shown in Figure 14a when Steen's harder U233 fission neutron spectrum is employed. Much of the rising trend in K_{eff} vs leakage is eliminated with the result that most of these experiments, which are H₂O moderated, form a reasonably consistent set. However, the BNL D₂O moderated exponentials are not consistent with this picture since K_{eff} is already underpredicted by 1.5% using ENDF/B-IV. It is expected that a harder U233 fission neutron spectrum would worsen this underprediction.

In addition to the fission spectrum change, the effects of replacing the ENDF/B-IV thorium by the LWBR and Leonard evaluations, respectively, are depicted in Figure 14b and c. The consistency of the results 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} . As seen previously in Figure 9, Leonard's thorium tends to increase K_{eff} for the tighter BNL lattices and lower K_{eff} for the looser lattices. This re-introduces a slight rising trend in K_{eff} vs leakage for those thorium-bearing lattices in Figure 14c, but the overall consistency is not much disturbed.

FIGURE 13: K_{eff} vs. Neutron Leakage Fraction for U233 Systems

FIGURE 14: K_{eff} vs. Neutron Leakage Fraction: a) ENDF/B-IV and the Harder Steen U233 Fission Neutron Spectrum, b) Case a plus the Leonard Th232, and c) Case a plus the LWBR Th232

The LWBR thorium raises K_{eff} for the BMU-1B core by 1.2%. This is thought to be attributed to reduced leakage with the LWBR set since the overall thorium capture rate was virtually unchanged compared to that for ENDF/B-IV. The Leonard thorium evaluation also raised the BMU-1B K_{eff} significantly by 0.8%. In this case though, the effect was due mainly to the reduced resonance capture which was not compensated by the increased thermal capture. The implication here is that if Leonard's thorium resonance evaluation is firm, then an even higher σ_a^{Th232} is required to bring the BMU-1B core back into line with the other experiments. This is considered to be unlikely and suggests, as do the integral thorium capture measurements, that resonance absorption is underpredicted by the Leonard set.

III. Summary

This study was intended to provide a systematic review of selected U233 and thorium-uranium experiments using ENDF/B-IV data. A second aim was to test the performance of thorium data sets, which have recently been proposed, to predict measured integral parameters and to examine sensitivities to various nuclear data changes.

K_{eff} for critical homogeneous U233 systems, calculated with ENDF/B-IV data, show an upward trend of approximately 2% with decreasing H/U, and there is a similar trend for homogeneous U235 systems. These trends appear to be due mostly to an underprediction of fast leakage.

Based on full energy range, explicit geometry Monte Carlo calculations, K_{eff} for many of the H_2O moderated thorium-uranium lattices (TUPE's, THUD's, BNL exponentials) also tends to be overpredicted with ENDF/B-IV data. Since many of these cores have leakage fractions between 20-30%, this trend is not inconsistent with that for leaky homogeneous criticals and therefore partly may be associated with an underprediction of leakage. On the other hand, K_{eff} for the BNL D_2O moderated exponentials appears to be underpredicted by 1.5%.

In the area of measured integral parameters, it was judged that interpretation of ρ^{02} measurements for the TUPE and THUD lattices would require detailed study and are unpromising. For the BNL H_2O moderated exponential lattices, the ENDF/B-IV predicted values for ρ^{02} were generally ~8% below experiment, as were the predictions for the D_2O lattices by 3%. ρ^{02} for ETA-I was overpredicted by 3%, and ρ^{02} for ETA-II was 2% low. Overall, the consistency among predictions of integral thorium capture measurements based on ENDF/B-IV is reasonable (Figure 7).

Three alternate thorium evaluations due to Derrien, Steen (LWBR), and Leonard were tested besides ENDF/B-IV. The most unambiguous test of these cross section sets were the measured ρ^{02} values for the BNL exponential and ETA lattices. Calculated K_{eff} values were also sensitive to the thorium set used, but here the fission neutron spectrum was an additional factor. How well these evaluations predict thorium capture measurements is depicted in Figure 11.

The additional unshielded capture in the resonance and unresolved resonance ranges assumed in the Derrien evaluation is a questionable alternative. As a result, testing of this evaluation has not been pursued as far as that for the other evaluations and those results that were obtained have not been plotted in Figure 11.

The consistency among various experiment/calculation comparisons using the LWBR thorium set is similar to that for ENDF/B-IV. However, agreement with experiment is slightly better for the LWBR set.

The high thorium thermal capture cross section of 7.61b adopted by Leonard has a nontrivial implication as far as the measured dilute resonance capture integral is concerned. Based on the review by Grenêche, which assumed $\sigma_a^{\text{Th232}} = 7.4 \pm 0.08\text{b}$, the dilute integral would be raised to 88.5b. This would also serve to raise the measured shielded resonance integrals. It is noted in connection with the Leonard evaluation that measured integral parameters such as ρ^{02} and I^{Th232} are furthest discrepant from the differential data, which underpredicts them (Figure 11).

There is a good deal of evidence from these analyses to support hardening of the fission neutron spectra of both U235 and U233. Calculations of K_{eff} for several TUPE lattices are improved somewhat (Figure 12) by using the harder Adams spectrum for U235. Predictions of the parameter δ^{02} for the ETA-I lattice are 15% (Table XVI) below experiment and also could be improved with a harder fission spectrum. An even harder U235 fission neutron spectrum has resulted from an evaluation due to Steen. In a similar manner, Steen has

reevaluated the U233 fission spectrum. This spectrum is also significantly harder than the ENDF/B-IV U233 spectrum. Use of Steen's U233 fission spectrum virtually eliminates the bias trend in the predictions of K_{eff} vs neutron leakage for the U233 homogeneous criticals and the BNL H₂O moderated exponential lattices (Figure 14) and should also improve the low predicted δ^{02} value for the ETA-II lattice.

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