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**Monte Carlo Analysis of Pu-H₂O and UO₂-PuO₂-H₂O
Critical Assemblies with ENDF/B-IV Data
(AWBA Development Program)**

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cp
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MONTE CARLO ANALYSIS OF PU-H₂O AND
UO₂-PuO₂-H₂O CRITICAL ASSEMBLIES
WITH ENDF/B-IV DATA

(AWBA DEVELOPMENT PROGRAM)

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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 or more. 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 Office of the Deputy Assistant Secretary for 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 set of critical experiments, comprising thirteen homogeneous Pu-H₂O assemblies and twelve UO₂-PuO₂ lattices, was analyzed with ENDF/B-IV data and the RCP01 Monte Carlo program, which modeled the experiments explicitly. Some major data sensitivities were also evaluated. For the Pu-H₂O assemblies, calculated K_{eff} averaged 1.011. The large (2.7%) scatter of K_{eff} values for these assemblies was attributed mostly to uncertainties in physical specifications since no clear trends of K_{eff} were evident and data sensitivities were insignificant. The UO₂-PuO₂ lattices showed just one trend of K_{eff} , which indicated an overprediction of U238 capture consistent with that observed for uranium-H₂O experiments. There was however a ~ 1% discrepancy in calculated K_{eff} between the two sets of UO₂-PuO₂ lattices studied.

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1. Introduction

A number of plutonium benchmark critical assemblies have been analyzed with consistent ENDF/B-IV nuclear data and detailed Monte Carlo methods. These studies were undertaken to provide a basic test of the adequacy of the ENDF/B-IV data for use in AWBA (Advanced Water Breeder Applications) analyses of thorium-uranium fuel cycle reactor concepts.

The emphasis of this work is of necessity on K_{eff} since, in general, the only reliable information available for these assemblies is the critical configuration. The basic analysis tool was the RCP01 Monte Carlo program, which represented the benchmark assemblies explicitly in three dimensions and described resonance cross section profiles in fine detail. This was supplemented by the one-dimensional multigroup P_L program P7MG, which was used primarily to study nuclear data sensitivities.

Both homogeneous aqueous assemblies and UO_2 - PuO_2 lattices were studied.

a. The set of homogeneous systems comprised the following:

- The seven assemblies designated recently as data-testing benchmarks by the Cross Section Evaluation Working Group (CSEWG).

These are denoted PNL6-PNL12.

- A one-dimensional slab of $Pu-H_2O$ and an infinite medium of Pu^{239} in H_2O (both inferred from criticality experiments).
- Four older CSEWG benchmarks, denoted PNL1, 3, 4 and 5. (PNL2 corresponds to the newly specified PNL6A). These assemblies had been analyzed previously with ENDF/B-III, and were re-analyzed with P7MG in the current testing of ENDF/B-IV. It was previously found

that P7MG produces K_{eff} values in good agreement with RCP01 for these benchmarks (which are modeled as bare spheres in void) and this has been verified for PNL1 and PNL3 in the current calculations.

These benchmark assemblies span a wide range of hydrogen/plutonium atom ratios (125-3695) and leakage (0-38%). The Pu240 content ranges from zero to 42.9% and the spectrum hardness (as measured by $\delta^{49} = \text{Pu239 fission above 0.625 eV} / \text{Pu239 fission below 0.625 eV}$) ranges from 0.01 to 0.20. The calculated K_{eff} values show an overall spread of 2.7%, ranging from 0.55% low to 2.15% high (compared to measured $K_{eff} = 1.00$). Most values are high and the grand average is 1.011.

b. The set of UO_2 - PuO_2 assemblies comprised:

- Six triangular-pitch lattices of UO_2 -2 w/o PuO_2 and UO_2 -4 w/o PuO_2 rods.
- Six square-pitch lattices of UO_2 -2 w/o PuO_2 rods.

For these assemblies, the hydrogen/plutonium ratio ranges from 150-1100, neutron leakage fraction from 10%-30%, and Pu240 content from 8%-24%.

The calculated K_{eff} values range from 0.4% high to 1% low. The only significant trend in these results is a dependence on U238 capture rate, and this is consistent with a long-standing problem, the overprediction of U238 capture observed in slightly-enriched uranium assemblies.

The calculated K_{eff} values were compared with results obtained recently by other laboratories. The different methods show generally reasonable agreement, with a few exceptions.

II. Calculational Methods

ENDF/B cross sections were multigroup processed with ETOMX and ETOTX, which are Bettis versions of ETOG (Ref. 1) and ETOT (Ref. 2). P3 thermal scattering kernels for hydrogen bound in H_2O were processed with FLAN2, the Bettis version of FLANGEII (Ref. 3), from ENDF/B $S(\alpha, \beta)$ 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 H_2O . 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. 4), with job libraries generated by RCPL1 (Ref. 5). 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 (including 299 energies below 0.625 eV if necessary). S-wave resonances were treated explicitly except that only one set of unresolved parameters was allowed over the unresolved range. Above thermal energies, RCP01 used a Σ_A/Σ_T estimator. 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 assembly was represented in all essential detail.

Auxiliary calculations--mostly data sensitivity studies--were done with P7MG (an extension of P3MG, Ref. 6), 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 RCP01 cell calculations, as were flux-weighting factors for a single fast group (10 MeV-821 KeV).

P7MG employed a resonance treatment (Ref. 7) 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 0.625 eV to 5530 eV (to which this method is limited at present) resonance capture rates were found to agree well with RCP01.

III. Analysis of Homogeneous Aqueous Assemblies

A. Physical Description of the Assemblies

Specifications for the CSEWG benchmarks were taken from Ref. 8 and are based on information in Ref. 9; specifications for the infinite medium and the one-dimensional slab were obtained directly from Ref. 9. Table 1 summarizes the characteristics of the critical assemblies and shows the original references. Atomic number densities are shown in Table 2.

TABLE 1
Characteristics of the Pu-H₂O Assemblies

<u>I.D.</u>	<u>H/Pu</u>	<u>% Pu240</u>	<u>Ref.</u>	<u>Benchmark Model</u>
PNL6B	125	4.55	13	Sphere with thin stainless steel vessel, in void
PNL10	210	8.35	15	Cylinder with thin stainless steel vessel; partial H ₂ O reflector
PNL11	623	42.9	16	Cylinder with thin stainless steel vessel; partial H ₂ O reflector
PNL8A	758	4.55	13	Sphere with thick stainless steel vessel, in void
PNL9	910	4.56		Cylinder with thin stainless steel vessel, in void
PNL7B	980	0.54	14	Sphere with thin stainless steel vessel; full H ₂ O reflector
PNL12B	1067	4.54	13	Sphere with thin stainless steel vessel; full H ₂ O reflector
1D Slab	422	4.65	12	One-dimensional slab
Inf. Med.	3695	0	10,11	Infinite medium of Pu239 in H ₂ O
PNL5	554	4.15	14	Bare sphere in void
PNL1	668	4.58	13	Bare sphere in void
PNL4	873	4.18	14	Bare sphere in void
PNL3	1154	4.18	14	Bare sphere in void

NOTE: The older CSEWG benchmark PNL2 corresponds to PNL6.

[illegible]

A few comments on the RCP01 and P7MG modeling of the assemblies are as follows:

Infinite medium of Pu239 in H₂O

Plutonium concentration $7.19 \pm 0.15 \text{ kg/m}^3$.

One-dimensional slab

Thickness $16.91 \pm 0.4 \text{ cm}$.

PNL1,3,4,5

Model: Sphere of fissile solution in void. Radii were adjusted experimentally to account for omission of the vessel.

	<u>Radius (cm)</u>
PNL1	19.509
3	22.70
4	22.70
5	20.1265

PNL6B

Model: Fissile solution in thin spherical stainless steel vessel, surrounded by void.

Radii are: 19.318 cm (fissile solution)

19.440 cm (vessel)

[A simpler model (PNL6A) omits the vessel and has an experimentally adjusted radius, $r = 19.5085 \text{ cm}$.]

PNL7B

RCP01 Model: Fissile solution in thin spherical stainless steel vessel with fill tube, surrounded by H₂O. See Figure 1. For P7MG, a sphericized model (PNL7A) was used, omitting the fill tube. Radii were the same as for PNL7B, but the plutonium atomic number densities were adjusted experimentally to account for omission of the fill tube.

	<u>N atoms/b-cm</u>
Pu239	65998-4
Pu240	35689-6

PNL8A

Model: Fissile solution in thick spherical stainless steel vessel, surrounded by void.

Radii are: 19.318 cm (fissile solution)

20.1004 cm (vessel)

PNL9

RCP01 Model: Fissile solution in thin cylindrical stainless steel vessel, surrounded by void.

For P7MG, this was represented by a radial traverse through the fissile solution. Transverse B² values in four energy groups were adjusted to match axial leakage rates obtained in an axial traverse.

RCP01 Model of Assembly PNL7B

FIGURE 1

PNL10

RCP01 Model: Fissile solution in thin cylindrical stainless steel vessel, with partial H₂O reflector. Includes drain tube. See Figure 2.

For P7MG this was represented (crudely) by an axial traverse through the fissile solution with reflector below and void above. Transverse B² values in four groups were adjusted to match radial leakage rates obtained in a radial traverse. Used only for sensitivity studies.

PNL11

RCP01 Model: Fissile solution in thin cylindrical stainless steel vessel, with partial H₂O reflector. Includes drain tube. Same configuration as PNL10 except for fissile solution composition and height. See Figure 2. For P7MG this was represented by a radial traverse through the fissile solution. Transverse B² values in four energy groups were adjusted to match axial leakage rates obtained in an axial traverse.

PNL12B

RCP01 Model: Fissile solution in thin spherical stainless steel vessel with fill and drain tubes, surrounded by H₂O. See Figure 3.

For P7MG, a sphericized model (PNL12A) was used, omitting the fill and drain tubes.

RCP01 Models of Assemblies PNL10 and PNL11

FIGURE 2

RCP01 Model of Assembly PNL12B

FIGURE 3

B. Calculated Results

Table 3 lists K_{eff} values calculated with ENDF/B-IV. The P7MG results shown are thought to be as good as the RCP01 results. (In several other cases, they were reasonably close to RCP01 but were used only for data variation studies). For comparison purposes, K_{eff} values obtained previously with ENDF/B-III for PNL1-5 are also shown.

Uncertainties listed for the RCP01 results reflect Monte Carlo statistics only (at one standard deviation). Compared to measured $K_{eff} = 1.0$, the ENDF/B-IV calculated K_{eff} values range from 0.55% low to 2.15% high. Most values are high, and the grand average is 1.011.

Calculated two-group reaction rates can be found in the Appendix.

TABLE 3

Summary of Calculated K_{eff} Values for Pu-H₂O Assemblies*

Assembly I.D.	H/Pu Ratio	ENDF/B-IV		ENDF/B-III	
		RCP01 $K_{eff} \pm \sigma$	P7MG K_{eff}	RCP01 $K_{eff} \pm \sigma$	P7MG K_{eff}
PNL6B	125	1.0138 $\pm$.0012			
PNL10	210	1.0090 $\pm$.0021			
PNL11	623	1.0050 $\pm$.0012			
PNL8A	758	1.0215 $\pm$.0022			
PNL9	910	1.0026 $\pm$.0018			
PNL7B	980	1.0134 $\pm$.0016			
PNL12B	1067	1.0135 $\pm$.0018			
1D Slab	422		1.0166		
Inf. Med.	3695	.9945 $\pm$.0005			
PNL2		(corresponds to PNL6)		--	1.0057
PNL5	554		1.0118	1.0070 $\pm$.0029	1.0078
PNL1	668	1.0181 $\pm$.0033	1.0191	1.0162 $\pm$.0025	1.0142
PNL4	873		1.0059	1.0025 $\pm$.0024	1.0028
PNL3	1154	.9990 $\pm$.0043	.9981	.9967 $\pm$.0030	.9955

*The ENDF/B-III P7MG calculations used the older L-factor resonance treatment in MUFT. For ENDF/B-IV, the more sophisticated treatment based on detailed resonance profiles was used (see Section II).

A number of these assemblies have been analyzed recently at other laboratories with ENDF/B-IV data. Principal results of these studies are summarized in Table 4. Included are K_{eff} values obtained with the Monte Carlo programs MCNP [by R. E. Prael of Los Alamos (Ref. 17)], VIM and RECAP [by P. F. Rose, et al of Brookhaven (Ref. 18)] and KENO-IV [by R. M. Westfall of Oak Ridge (Ref. 19) and by U. Jenquin, et al of Battelle Northwest (Ref. 20)]. The Oak Ridge and Battelle Northwest studies also used the XSDRN program.

TABLE 4

Comparison of k_{eff} Results Obtained by Different Methods for the Pu-H₂O Assemblies

Assembly I.C.	RCP01 (Present Study)	MCNP (LASL)	VIM (BNL)	RECAP (BNL)	KENO-IV* and XSDRN	
					(BNL)	(ORNL)
PNL1	1.0181 (.33)	1.0170 (.21)				
3	.9990 (.43)	1.0007 (.23)		.9961 (.30)		
4	1.0059	1.0056 (.23)				
5	1.0118	1.0120 (.22)		1.0088 (.33)		
6	1.0138 (.12)	1.0109 (.20)		1.0105 (.34)	1.0137	1.0197
7	1.0134 (.16)	1.0133 (.23)			1.0197	
8	1.0215 (.22)	1.0224 (.21)			1.0254	1.0194
9	1.0026 (.18)	1.0101 (.24)	.9968 (.29)	.9982 (.21)	.9972 (~.6)*	1.0043 (.40)
10	1.0090 (.21)	1.0119 (.26)			1.0080 (~.6)*	1.0086 (.60)
11	1.0050 (.12)	1.0014 (.20)	1.0090 (.30)		1.0170	1.0145 (.30)
12	1.0135 (.18)	1.0092 (.22)			1.0207	1.0210
1D Slab	1.0166	1.0216 (.22)			1.0211	
Inf. Med.	.9945 (.05)	.9938 (.15)				

For Monte Carlo results, % uncertainties (1 σ) are shown in parentheses.

For PNL6, 7, 8, and 12, the MCNP results are for the same CSEWG benchmark model as the RCP01 results of Table 3 (i.e., PNL6B, 7B, 8A, and 12B).

*KENO-IV results have uncertainties shown; other results are from XSDRN.

Agreement among the various methods is reasonably good, allowing for Monte Carlo statistics, with a few specific exceptions. For PNL11 and PNL12, KENO-IV and XSDRN are significantly above RCP01 and MCNP. The large spread of K_{eff} for PNL11 is very likely due to sensitivities associated with calculating the large amount of Pu240 capture.

C. Analysis of Results

In an attempt to evaluate the benchmark K_{eff} results (in order to draw conclusions about adequacy of the ENDF/B-IV data) the RCP01 K_{eff} values were examined for trends. Although there may be some methods effects remaining in the RCP01 calculation, they are judged not to be significant. This view is supported by the generally good agreement of RCP01 with results obtained by other accurate methods such as MCNP, VIM and KENO-IV.

Table 5 shows calculated reaction rates and other parameters useful in looking for trends in the K_{eff} values. These include:

- (1) Net leakage from the core (all absorption outside the fissile material plus leakage into void).
- (2) δ^{49} = ratio of Pu239 fission above 0.625 eV to Pu239 fission below 0.625 eV. This is a measure of overall spectrum hardness.
- (3) The thermal (0-0.625 eV) spectrum-averaged hydrogen capture cross section in the fissile material. This is a measure of the thermal spectrum hardness.

TABLE 5

Calculated Reaction Rates and Other Parameters
Used in Searching for Trends (Pu-H₂O Assemblies)

ID	(1) Net Leakage	(2) δ^{49}	(3) $\frac{\sigma_A^H}{\sigma_A}$ (b)	(4) Thermal Hydrogen Capture	(5) Pu240 Capture		
					Fast	Thermal	Total
PNL6B	.3832	.2036	.185	.0103	.0440	.0044	.0484
PNL10	.3826	.1098	.211	.0221	.0465	.0092	.0557
PNL11	.1369	.0320	.258	.1386	.0979	.0900	.1879
PNL8A	.3529	.0375	.255	.0968	.0148	.0055	.0203
PNL9	.2978	.0307	.261	.1308	.0332	.0186	.0518
PNL7B	.3514	.0283	.260	.1245	.0015	.0006	.0021
PNL12B	.3161	.0262	.262	.1428	.0108	.0057	.0165
1D Slab	.3824	.0612	.237	.0492	.0225	.0053	.0278
Inf. Med.	0	.0118	.277	.4986	0	0	0
PNL5	.3667	.0481	.246	.0669	.0171	.0048	.0219
PNL1	.3654	.0417	.252	.0840	.0162	.0055	.0217
PNL4	.3219	.0329	.257	.1117	.0128	.0051	.0179
PNL3	.3140	.0268	.264	.1512	.0103	.0051	.0154

(1) Leakage into void plus all absorption outside the fissile material.

(2) δ^{49} = ratio of fast/thermal Pu239 fission.

(3) $\frac{\sigma_A^H}{\sigma_A}$ is the thermal-spectrum-average hydrogen capture cross section (barns).

(4) Thermal hydrogen capture rate in the fissile material.

(5) Pu240 capture rates.

(4) Thermal hydrogen capture rate in the fissile material, to characterize the competition between thermal absorption in plutonium and hydrogen.

(5) Pu240 capture rates (fast and thermal). In assembly PNL11, Pu240 captures nearly 19% of the neutrons.

Plots of K_{eff} versus leakage, thermal hydrogen absorption, δ^{49} , and total Pu240 absorption are shown in Figures 4, 5, 6 and 7, respectively.

The large (1.1%) error flag for the infinite medium of Pu239-H₂O reflects the effect of the quoted experimental uncertainty of 2.1% in Pu239 content. In like manner, the uncertainty in one-dimensional slab thickness (16.91 ± 0.4 cm) accounts for the Pu239-concentration uncertainty and is worth 1.6% in K_{eff} . The effects of dimension and Pu239-concentration uncertainties have not been evaluated for the other assemblies. However, from the observed scatter of the K_{eff} values, they seem to be significant.

There is an apparent dependence of calculated K_{eff} on leakage (Figure 4), but this hinges entirely on the infinite medium result, and in any case is hardly larger than the uncertainty. This trend appears also with thermal hydrogen absorption (Figure 5), which is strongly correlated with leakage.

It is difficult to discern any other trends outside the $\sim 2\%$ scatter of the K_{eff} values. The old (PNL1,3,4, and 5) and new (PNL6-12) benchmarks show comparable spreads of calculated K_{eff} .

K_{eff} Versus Net Leakage from the Fissile Solution for Pu-H₂O Assemblies

FIGURE 4

K_{eff} Versus Thermal Hydrogen Absorption for Pu-H₂O Assemblies

FIGURE 5

K_{eff} Versus δ^{49} for Pu-H₂O Assemblies

FIGURE 6

K_{eff} Versus Total Pu240 Capture for Pu-H₂O Assemblies

FIGURE 7

The effects of some major data variations were evaluated, as shown in Table 6 and Figure 8. These include variations of the Pu239 fission and capture resonance integrals and thermal cross sections, the hydrogen thermal capture cross section, and the Pu239 fission spectrum. Sensitivities for other assemblies can be estimated from these data by interpolation.

On the whole, the data sensitivities are insignificant compared to the 2% random scatter of calculated K_{eff} which is attributed to loading and dimension uncertainties.

Some comments about the individual data variations of Table 6:

- (1) The Pu239 fission resonance integral was increased by 5.0b.
(The value in BNL325 (Ref. 21) is $I_F = 301 \pm 10b$.) The maximum change of K_{eff} is +0.2%, in PNL6, where the spectrum is hardest.
- (2) The Pu239 capture resonance integral was reduced by 5.0b
($I_C = 200 \pm 20b$ in BNL325). The maximum change of K_{eff} is +0.16%, again in PNL6.
- (3) The Pu239 thermal fission cross section was multiplied by a factor such that the 2200 m/s value increased by 2.0b
($\sigma_F = 742.5 \pm 3.0b$ in BNL325). The maximum change of K_{eff} was +0.18%, in the infinite medium.
- (4) The Pu239 thermal capture cross section was reduced by a factor such that the 2200 m/s value decreased by 2.0b ($\sigma_C = 268.8 \pm 3.0b$ in BNL325). The maximum change of K_{eff} was +0.21%, in PNL6.

- (5) The mean energy of the Pu239 fission spectrum was increased by 0.069 MeV (from 2.085 MeV to 2.154 MeV). The shape was Maxwellian in both cases. The maximum change of K_{eff} was -0.84%, in PNL6.
- (6) The Pu239 fission spectrum was changed from the Maxwellian to a Watt shape with the same mean energy. The maximum change of K_{eff} was -0.23%, in PNL6.
- (7) The hydrogen thermal capture cross section was reduced by a factor such that the 2200 m/s value decreased by 0.002b ($\sigma_c = 0.332 \pm 0.002b$ in BNL325). The maximum change of K_{eff} was +0.30%, in the infinite medium.

TABLE 6

Summary of Data-Variation Results for K_{eff} (Pu-H₂O Assemblies)

ID	$\Delta K_{eff}/K_{eff}$						(7) Hydrogen $\Delta\sigma_C =$ -.002b
	Pu239						
	(1)	(2)	(3)	(4)	(5)	(6)	
	$\Delta I_F =$ +5.0b	$\Delta I_C =$ -5.0b	$\Delta\sigma_F =$ +2.0b	$\Delta\sigma_C =$ -2.0b	Fission Spectrum $\Delta E =$ +.069 MeV	Max. + Watt	
PNL6B	+.002012	+.001615	+.000813	+.002067	-.008439	-.002319	+.000116
PNL10	+.001006	+.000875					
PNL11					-.003394	-.000191	
PNL8A							
PNL9	+.000362	+.000231			-.006625	-.001097	
PNL7B					-.007037	-.001518	
PNL12B			+.001304	+.001581			+.001402
1D Slab							
Inf. Med.			+.001759	+.001038			+.002954
PNL5							
PNL1			+.001137				
PNL4							
PNL3			+.001411				

- (1) Pu239 fission resonance integral increased by 5.0b.
 (2) Pu239 capture resonance integral reduced by 5.0b.
 (3) Pu239 thermal fission cross section increased by 2.0b.
 (4) Pu239 thermal capture cross section reduced by 2.0b.
 (5) Pu239 fission spectrum changed from a Maxwellian with $E = 2.0 \times 10^5$ MeV to a Maxwellian with $E = 2.154$ MeV.
 (6) Pu239 fission spectrum changed from Maxwellian to Watt, same E .
 (7) Hydrogen thermal capture cross section reduced from 0.332b to 0.330b.

Effect of Selected Data Variations on K_{eff} for Pu-H₂O Assemblies

FIGURE 8

A systematic analysis of the trends in K_{eff} was obtained by a least squares fit. Calculated values of K_{eff} (Table 3) were fit to the equation

$$y^j = b_0 + b_1 x_1^j + b_2 x_2^j + \dots + b_n x_n^j + \epsilon^j$$

where

y^j = calculated K_{eff} for the j^{th} assembly

$x_1^j, \dots, x_n^j$ = selected reaction rates (or other parameters) for the j^{th} assembly

$b_0, \dots, b_n$ = least-squares fitted coefficients, and

ϵ^j = residual difference of y^j from the best-fit surface.

Selected least-squares-fit results are shown in Table 7, which includes the following information:

- (1) The significance of the fit coefficients as measured by
 $T_i = b_i / \sigma(b_i)$.
- (2) The % of the total sum-of-squares of differences from the mean K_{eff} accounted for by the fit.
- (3) Residual standard deviation (root-mean-square deviation, per degree of freedom, from the best-fit surface).

The results in part A of Table 7 include only the new CSEWG benchmarks PNL6-PNL12 and the infinite medium of Pu239-H₂O.

The following comments apply to the individual cases in Table 7, part A:

- Case 1. There is a statistically significant trend with leakage (as is apparent in Figure 4). This accounts for 62% of the total sum-of-squares of deviations from the mean. The residual scatter has a standard deviation of .0055 per degree of freedom.
- Case 2. Thermal hydrogen absorption in the fissile material, which is highly correlated with leakage, does nearly as well (Figure 5).
- Case 3. Use of both leakage and thermal hydrogen absorption does not improve the fit.
- Case 4. Correlation with spectrum hardness (as measured by δ^{49}) is very poor (see Figure 6).
- Case 5. Use of leakage and δ^{49} does not improve the fit.
- Cases 6-8. There is no significant trend with Pu240 absorption (see Figure 7).

TABLE 7

Least Squares Fit Results

Calculated $T_i = b_i/\sigma(b_i)$							Total Sum-of-Squares Accounted for (%)	Residual Std. Dev. per Degree of Freedom
	b_1	b_2	b_3	b_4	b_5	b_6		
Case	Leakage	Thermal H Absorption	δ^{49}	Pu240 Absorption				
				Fast	Thermal	Total		
A) PNL6-PNL12 plus Pu239-t ₂ O Infinite Medium								
1	3.13*						62.0	.0055
2		-2.53*					51.6	.0063
3	1.18	- .13					62.1	.0061
4			.75				8.6	.0086
5	2.76		-.49				63.7	.0059
6	2.39		-.44			.08	63.8	.0066
7	2.38		-.39	-.03			63.7	.0066
8	2.42		-.44		.21		64.1	.0066
B) All Assemblies (Table 1)								
1	2.56*						37.4	.0069
2		-2.44*					35.1	.0070
5	2.17		.11				37.4	.0072

*Significant at the $\alpha = .05$ level.

Including the older CSEWG benchmarks PNL1,3,4,5 and the one-dimensional slab does not change the overall picture. It does however increase the random scatter component, as shown in Part B of Table 7. This is illustrated for three cases numbered to correspond to those in part A. For Case 1, the total sum of squares accounted for by the leakage trend is now only 37.4% and the residual standard deviation is .0069.

In no case was there any indication that the residual distribution was non-normal.

In summary, calculated K_{eff} values for the Pu-H₂O assemblies scatter by more than 2%. They show only one possible trend (with leakage), and this depends entirely on the infinite medium result. The scatter is attributed mostly to uncertainties of inventory, and is large enough to obscure the major data sensitivities that were examined.

IV. Analysis of UO₂-PuO₂ Fueled Rod Lattices

A. Physical Description of the Lattices

The physical characteristics and RCP01 modeling of the UO₂-PuO₂ assemblies are summarized in this section. There were six triangular-pitch lattices and six square-pitch lattices. In every case the lattice was surrounded by a water reflector.

(1) UO₂-2 w/o PuO₂ and UO₂-4 w/o PuO₂ Lattices With Triangular Pitch

Characteristics of the six triangular-pitch lattices (Ref. 22) are shown in Table 8. The number of rods necessary to

achieve criticality was determined from approach-to-critical data in which up to 96% of the critical mass was loaded and the actual critical size was determined from inverse multiplication data. This extrapolation is considered accurate since at 96% loading the lattices are generally within 0.5% of critical.

A side view of the RCP01 representation of a typical fuel rod in these lattices is shown in Figure 9. Figure 10 shows the radial RCP01 representation of lattice 36, with each fuel rod described explicitly. The fuel rods were fixed in position by lucite templates, and each lattice was effectively fully reflected with water. The UO_2 - PuO_2 masses per fuel rod were approximately 1128 grams and 1084.5 grams for the 2 w/o PuO_2 and 4 w/o PuO_2 lattices, respectively. The PuO_2 powders used in the fuel consisted of particles whose diameters ranged from 0 to 44 μm with an average particle diameter of $\sim 25 \mu\text{m}$. Approximately 6 grams of UO_2 (natural) occupied the bottom 0.5 cm of each rod. Detailed descriptions of the fuel for the triangular-pitch lattices are given in Table 9.

TABLE 8
Triangular Pitch Lattice Parameters

<u>Lattice^a I.D.</u>	<u>Lattice Pitch (cm)</u>	<u>H/Pu Atom Ratio</u>	<u>$\frac{V_{\text{mod}}}{V_{\text{fuel}}}$</u>	<u>Critical No. of Rods</u>	<u>Fuel</u>
27	2.032	238	1.21	320	UO ₂ -2 w/o PuO ₂ (8% Pu240)
29	3.520	1113	5.63	179	UO ₂ -2 w/o PuO ₂ (8% Pu240)
36	2.032	238	1.21	520	UO ₂ -2 w/o PuO ₂ (24% Pu240)
38	3.520	1113	5.63	365	UO ₂ -2 w/o PuO ₂ (24% Pu240)
39	2.159	153	1.50	253	UO ₂ -4 w/o PuO ₂ (18% Pu240)
40	3.520	578	5.65	124	UO ₂ -4 w/o PuO ₂ (18% Pu240)

^aThe benchmark IDs conform with those of Ref. 9, except for lattice 40, which differs in pitch and number of rods.

RCP01 Axial Representation of the Triangular Pitch Assemblies

FIGURE 9

BENCHMARK 36 UO_2 - 2w/o PuO_2

Third-Core Radial Slice for Assembly 36

FIGURE 10

TABLE 9
Description of UO₂-PuO₂ Fuel Rods

<u>Lattice I.D. ></u>	<u>27,29</u>	<u>36,38</u>	<u>39,40</u>	<u>30-35</u>
Fuel Radius (cm)	0.6414	0.6414	0.6318	0.6414
Clad Radius (cm)	0.7176	0.7176	0.7176	0.7176
Fuel Rod Atom Densities atoms/(barn-cm)				
Pu238	4000-7	--	2300-5	4000-7
Pu239	3974-3	3044-3	6300-3	3974-3
Pu240	3344-4	9940-4	1513-3	3344-4
Pu241	2640-5	1680-4	3950-4	1600-5
Pu242	1200-6	2700-5	9600-5	1200-6
U235	1504-3	1503-3	1458-3	1504-3
U238	2073-1	2071-1	2011-1	2073-1
Am241	4700-6	1700-5	3600-5	1510-5
Ø16	4401-1	4258-1	4220-1	4401-1
Clad Atom Density				
Zr	4226-1	4226-1	4226-1	4226-1
Moderator Atom Densities				
H	6671-1	6668-1	6666-1	6671-1
Ø	3336-1	3334-1	3333-1	3336-1
B @ 1 ppm by wt	--	--	--	5558-7

(2) UO₂ - 2 w/o PuO₂ Lattices With Square Pitch

Characteristics of the six square-pitch lattices (Ref. 23) are shown in Table 10. For each pitch, the lattice was taken critical with borated and with unborated moderator. A side view of a typical lattice is shown in Figure 11, and Figure 12 shows the radial RCP01 representation of lattice 30.

Two aluminum "eggcrate" grids 1.00" thick were used to maintain lattice spacing (Figure 13). In the RCP01 Monte Carlo analyses, these eggcrate regions were homogenized with the surrounding water. The lattices were effectively fully reflected by water on the sides and bottom. The top reflector was six inches thick for assemblies 30, 31, 33 and 35; it was 2.25 inches and 0.9 inch thick for assemblies 32 and 34, respectively.

A detailed description of the fuel for assemblies 30-35, taken from Reference 9, also appears in Table 9. The PuO₂ powder consisted of particles with an average diameter of ~ 25 μ m.

These lattices have been designated as provisional CSEWG benchmarks.

TABLE 10
Square Pitch Lattice Parameters

<u>Lattice^a</u> <u>I.D.</u>	<u>Lattice</u> <u>Pitch</u> <u>(cm)</u>	<u>H/Pu</u> <u>Atom</u> <u>Ratio</u>	<u>$\frac{V_{mod}}{V_{fuel}}$</u>	<u>Critical No.</u> <u>of Rods</u>	<u>Boron</u> <u>(wppm)</u>
30	1.778	185	0.95	469	3.5
31	1.778	185	0.95	761	688.5
32	2.209	391	2.02	195	4.1
33	2.209	391	2.02	761	1093.5
34	2.514	564	2.91	161	6.0
35	2.514	564	2.91	689	768.0

^a The lattice IDs conform with Ref. 9.

RCP01 Axial Representation of the Square Pitch Assemblies

FIGURE 11

BENCHMARK 30 UO_2 -2w/o PuO_2

Quarter-Core Radial Slice for Assembly 30

FIGURE 12

FUEL TYPE	PITCH	GRID	DIM. A	DIM. B
UO ₂ -2WT% PuO ₂ (8% ²⁴⁰ Pu)	2.210	UPPER LOWER	.081 .081	1.562
UO ₂ -2WT% PuO ₂ (8% ²⁴⁰ Pu)	1.778 2.515	UPPER LOWER	.318 .318	1.778

DIMENSIONS IN CENTIMETERS

Aluminum "Eggcrate" Descriptions for Assemblies 30-35

FIGURE 13

B. Calculated Results

A summary of the calculated K_{eff} values and their 1σ statistical uncertainties is given in Table 11. The second column shows calculated K_{eff} obtained with homogeneous fuel represented in each fuel rod. It is necessary to correct these results for the finite PuO_2 particles relative to homogeneous fuel. These corrections, which were taken from Reference 24 and are listed in column three of Table 11, are very much dependent on the flux spectrum and Pu240 content of the lattices. In the harder flux spectra, there is a positive reactivity effect from increased shielding of capture in the 1.06 eV Pu240 resonance and the 0.3 eV Pu239 resonance. This nearly cancels the negative reactivity from increased shielding of fission in the 0.3 eV Pu239 resonance and results in a small overall correction, as seen for assemblies 30 and 31. The corrected K_{eff} values appear in the last column of Table 11.

For comparison, the K_{eff} results for assemblies 30-35 are compared in Table 12 with similar calculations made by P. F. Rose et al at BNL using the RECAP-12 program, which is an earlier version of RCP01. Also shown are results obtained by R. M. Westfall et al with the KENO-V multigroup Monte Carlo program (Ref. 19). For lattice 33 there is also a K_{eff} value calculated by R. L. Childs et al (Ref. 25) with the PX-KENO pointwise Monte Carlo program. Although there are some systematic differences, overall agreement is adequate.

TABLE 11
Calculated K_{eff} for UO_2 - PuO_2 Assemblies

Lattice I.D.	Calculated K_{eff} ($\pm 1\sigma$) ^a	ΔK_{eff} Correction for PuO_2 Particle Effects	Corrected K_{eff} ($\pm 1\sigma$) ^a
27	0.9919 $\pm$ 0.0022	-0.0013	0.9906 $\pm$ 0.0022
29	0.9957 $\pm$ 0.0026	-0.0044	0.9913 $\pm$ 0.0026
30	0.9965 $\pm$ 0.0022	-0.0008	0.9957 $\pm$ 0.0022
31	0.9979 $\pm$ 0.0021	-0.0008	0.9971 $\pm$ 0.0021
32	1.0009 $\pm$ 0.0023	-0.0024	0.9985 $\pm$ 0.0023
33	1.0022 $\pm$ 0.0023	-0.0024	0.9998 $\pm$ 0.0023
34	1.0056 $\pm$ 0.0024	-0.0030	1.0026 $\pm$ 0.0024
35	1.0070 $\pm$ 0.0024	-0.0030	1.0040 $\pm$ 0.0024
36	0.9913 $\pm$ 0.0018	-0.0007	0.9906 $\pm$ 0.0018
38	0.9938 $\pm$ 0.0027	-0.0038	0.9900 $\pm$ 0.0027
39	0.9935 $\pm$ 0.0023	-0.0008	0.9927 $\pm$ 0.0023
40	1.0028 $\pm$ 0.0023	-0.0026	1.0002 $\pm$ 0.0023

^a1 σ statistical uncertainty

TABLE 12

Comparison of Results for Assemblies 30-35

Lattice I.D.	Calculated K_{eff}			
	RCP01 ^a	RFCAP-12	KENO-V (Ref. 19)	PX-KENO (Ref. 25)
30	0.9965 $\pm$ 0.0022	0.9912 $\pm$ 0.0021	.9920 $\pm$.0042	
31	0.9979 $\pm$ 0.0021	0.9935 $\pm$ 0.0030	.9972 $\pm$.0037	
32	1.0009 $\pm$ 0.0023	0.9992 $\pm$ 0.0021	1.0073 $\pm$.0041	
33	1.0022 $\pm$ 0.0023	1.0037 $\pm$ 0.0021	1.0070 $\pm$.0036	1.0007 $\pm$.0027
34	1.0056 $\pm$ 0.0024	0.9989 $\pm$ 0.0021	1.0089 $\pm$.0045	
35	1.0070 $\pm$ 0.0024	1.0012 $\pm$ 0.0021	1.0056 $\pm$.0033	

^aErrors are 1 σ statistical uncertainties.

C. Analysis of Results

The calculated values of K_{eff} for these lattices range from 0.4% high to 1% low. This wide range of K_{eff} values suggests that it may be useful to examine the results for systematic effects. In searching for systematic effects, some variables of interest include H/Pu atom ratio, U238 capture, plutonium composition, Pu240 content, and neutron leakage. For the purpose of identifying certain correlations, important reaction rates have been edited and are shown in the Appendix. The following observations are made:

- (1) K_{eff} vs. H/Pu Atom Ratio (Figure 14) - H/Pu values range between 150 and 1200 for these lattices, but no distinct trend with H/Pu is discernible.
- (2) K_{eff} vs. Neutron Leakage (Figure 15a) - The lattices cover a reasonably wide range of neutron leakage fractions (10%-30%). K_{eff} results, however, appear to be random with respect to leakage. This contrasts with the trend observed for homogeneous aqueous assemblies and is to be expected due to the presence of U238 fast fission in these lattices.*

*For example, an underprediction of leakage due to a too-soft fission neutron spectrum is accompanied by a corresponding underprediction of U238 fission. The two effects tend to cancel (for K_{eff}), as observed for example in U235-H₂O and U235-U238-H₂O assemblies.

K_{eff} vs. H/Pu Atom Ratio for UO_2 - PuO_2 Assemblies

FIGURE 14

K_{eff} vs. Neutron Leakage for UO_2 - PuO_2 Assemblies

FIGURE 15a

K_{eff} vs. Pu240 Capture for UO_2 - PuO_2 Assemblies

FIGURE 15b

(3) K_{eff} vs. Pu240 Capture Fraction (Figure 15b)

No overall trend in K_{eff} vs. Pu240 capture is apparent. For the subset of lattices with UO_2 -2 w/o PuO_2 (8% Pu240) rods the only significant parameter that varies is the moderator-to-fuel volume (V_m/V_f) ratio. Yet the spectrum hardening associated with decreasing V_m/V_f , which could emphasize a problem with Pu240 capture, produces no discernible trend.

(4) K_{eff} vs. Pu239 Epithermal-to-Thermal Ratio (δ^{49})

No trend is apparent in the calculated results (Figure 16).

(5) K_{eff} vs. U238 Capture Fraction (Figure 17)

Capture in U238 ranges from 1% to 19% in these lattices. Overall there is a systematic decrease of K_{eff} with increasing U238 capture fraction (shown for capture above 0.625 eV in Figure 17). Furthermore, K_{eff} values for the triangular pitch lattices (27, 29, 36, 38, 39, 40) are systematically lower than those of the square pitch lattices (30-35) even though both sets of lattices exhibit the same trend with U238 capture. Reasons for this systematic difference are not known. It is noteworthy, however, that the zero-U238-capture intercept of the square pitch lattices is more nearly consistent with the Pu-H₂O assemblies (see Figure 18).

K_{eff} vs. Epithermal-to-Thermal Pu^{239} Fission Ratio (δ^{49})
for UO_2 - PuO_2 Assemblies

FIGURE 16

K_{eff} vs. U238 Fast Capture Fraction for UO_2 - PuO_2 Assemblies

FIGURE 17

K_{eff} vs. Net Leakage for the Pu-H₂O Assemblies. Also shown are the Zero-U238-Capture Projections of calculated K_{eff} (from Figure 17) for the UO₂-PuO₂ Lattices

FIGURE 18

An obvious sensitivity to examine first is to U238 capture. In the first instance, the U238 shielded resonance integral was reduced by 0.75 barn. This is just the magnitude necessary to bring ENDF/B-IV predictions of ρ^{28} in the TRX critical assemblies (Ref. 26) into agreement with experiment*. The change was achieved by a nearly uniform reduction of the U238 smooth multigroup capture cross sections between 40.87 keV and 167.0 eV. The effects of this change are to raise K_{eff} for the tight lattices (30,31) by $\sim 0.8\%$. The observed trend of K_{eff} vs. U238 fast capture fraction is entirely consistent with the slope expected from a 0.75b excess of shielded U238 resonance capture integral (see the dashed lines in Figure 17).

Several other data variations, similar to those for the Pu-H₂O assemblies, were examined, as follows (Table 13):

- (1) The Pu239 fission and capture resonance integrals were decreased by and increased by 5.0 barns, respectively. This was again achieved by a uniform percentage change in the smooth multigroup cross sections. As expected, the relative importance of these changes is highest in the tight lattices, but the ΔK_{eff} generally fall below 0.2%.

*The TRX assemblies are CSEWG benchmarks. They are H₂O moderated simple rod lattices of slightly-enriched uranium. ρ^{28} is the ratio of U238 capture above 0.625 eV to that below 0.625 eV.

TABLE 13
Nuclear Data Sensitivities

Cross Section Change	Calculated Relative K_{eff}		
	30	31	38
1) ENDF/B-IV Base Case	1.0000	1.0000	1.0000
2) $I_C(U238)$ reduced by 0.75b	1.0078	1.0083	1.0016
3) $I_f(Pu239)$ decreased by 5.0 barns	0.9987	0.9986	0.9996
4) $I_C(Pu239)$ increased by 5.0 barns	0.9991	0.9991	0.9998
5) $\sigma_c^{Th}(Pu239)$ decreased by 2.0b at 2200 m/s	1.0015	1.0014	1.0009
6) $\sigma_f^{Th}(Pu239)$ increased by 2.0b at 2200 m/s	1.0008	1.0009	1.0011
7) Maxwellian Fission Spectrum $E' = 2.1$ MeV for ENDF/B-IV $E' = 2.085$ MeV	0.9980	0.9994	0.9972
8) $\sigma_c(H)$ decreased to 0.330b from 0.332b at 2200 m/s	1.0004	1.0003	1.0006

- (2) Pu239 capture cross sections in the thermal group were reduced by a factor 0.992585, which reduces σ_c^{239} (2200 m/s) from 269.7b to 267.7b. Otherwise the shape remained unchanged. Values of ΔK_{eff} for this change were of the order of +0.10% to +0.15% with the higher value corresponding to the tighter lattices, which have harder flux spectra through the 0.3 eV resonance of Pu239.
- (3) A Uniform increase in the Pu239 fission cross sections, which raised σ_f^{239} (2200 m/s) to 743.55b from 741.55b produced a ΔK_{eff} of $\sim 0.1\%$ in all three lattices studied.
- (4) The ENDF/B-IV Pu239 fission spectrum (a Maxwellian with $E = 2.085$ MeV) was replaced by a Maxwellian with $E = 2.1$ MeV. It turns out that in the tight lattices with their larger leakage fractions (assemblies 30 and 31) the effects of increased leakage on K_{eff} are nearly compensated by increased U238 fission. In the thermal lattice 38 the effect of increased leakage is actually more pronounced.
- (5) Sensitivity to the hydrogen thermal absorption cross section was found by reducing the 2200 m/s value from 0.332b to 0.330b. This change produced almost negligible ΔK_{eff} .

In summary, estimates of the uncertainties in calculated values of K_{eff} due to reasonable experimental uncertainties in nuclear data reveal that the strongest sensitivity is to the U238 effective epithermal capture integral. A decrease of 0.75b in the U238 effective resonance capture integral can account for the observed trend of K_{eff} with U238

capture fraction. This is the only significant trend found among the K_{eff} values for these assemblies. Such a reduction of calculated U238 capture is precisely consistent with the nominal 5% overprediction of ρ^{28} in TRX lattices (and the associated underprediction of K_{eff}). The systematic K_{eff} difference (nearly 1%) between the square-pitch lattices and the triangular pitch lattices remains unexplained, although it is thought to be due to deficiencies in the physical specifications of the assemblies. The square-pitch lattices, which are provisional CSEWG benchmarks, appear to be the more consistent with the homogeneous Pu-H₂O assemblies.

V. Summary and Conclusions

Two sets of plutonium benchmark critical assemblies were analyzed with consistent ENDF/B-IV nuclear data and detailed Monte Carlo methods.

a) Thirteen Homogeneous Aqueous Assemblies

These span a wide range of hydrogen/plutonium ratio (125-3695) and leakage (0-38%). The Pu240 content ranges from zero to 42.9% and the spectrum hardness (as measured by $\delta^{49} = \text{Pu239 fission above } 0.625 \text{ eV} / \text{Pu239 fission below } 0.625 \text{ eV}$) from 0.01 to 0.20. The calculated K_{eff} values show an overall spread of 2.7%, ranging from 0.55% low to 2.15% high (compared to measured $K_{eff} = 1.0$). Most values are high and the grand average is 1.011.

The large scatter of calculated K_{eff} values is predominantly random. There is one possible trend, which appears versus leakage, but this hinges entirely on two assemblies: the infinite medium of

Pu239-H₂O, and PNL11, which happens also to have large Pu240 absorption. The remaining assemblies show a relatively small range of leakage (from 30-38%).

This same trend also shows in plots of calculated K_{eff} versus thermal hydrogen absorption rate in the fissile material, which is highly correlated with leakage. From the observed data sensitivities, it seems likely that leakage is the more important factor. There are no signs of correlations with δ^{49} (flux spectrum hardness), or Pu240 absorption.

The large random scatter of calculated K_{eff} values for these assemblies is apparently due mostly to uncertainties of inventory. This is borne out by the infinite medium and the 1D slab configurations for which experimental uncertainties (stemming mostly from plutonium content) are quoted. These uncertainties are worth $\pm 1.1\%$ and $\pm 1.6\%$ respectively in K_{eff} . For the newer CSEWG benchmarks (plus the infinite medium), the overall residual scatter shows a standard deviation of 0.6%. These uncertainties are much larger than for corresponding U233 and U235 assemblies (Ref. 27).

A number of data sensitivities were investigated. However, the large scatter of calculated K_{eff} values makes it difficult to draw specific conclusions about possible data inadequacies; that is, differential data uncertainties would produce K_{eff} differences much smaller than the random scatter of calculated K_{eff} .

A comparison of calculated K_{eff} values obtained by different methods (RCP01, MCNP, VIM, KENO-IV, XSDRN and RECAP) show reasonably

good agreement in most cases. In general, the method differences are not large compared to the scatter of K_{eff} attributed to inventory uncertainties. Differences are significant in several cases, however, most importantly for PNL11, which has a large amount (19%) of PU240 capture.

b) Twelve UO₂-PuO₂ Lattices

For these assemblies, the hydrogen/plutonium ratio ranges from 150-1100, neutron leakage fraction from 10%-30%, and Pu240 content from 8%-24%. The U238 capture fraction ranges from 1%-19%.

The calculated K_{eff} values vary from 0.4% high to 1% low. The only significant trend in these results is a dependence on U238 capture fraction. K_{eff} decreases with increasing U238 capture, which implies that U238 capture is being overpredicted with ENDF/B-IV. This is precisely consistent with the 5% overprediction of ρ^{28} observed for the U235-U238-H₂O TRX lattices with ENDF/B-IV.

Very little change in K_{eff} was noted from perturbing the Pu239 resonance integrals. Other results generated included sensitivities to the Pu239 thermal cross sections, the Pu239 fission spectrum, and the hydrogen thermal capture. The ΔK_{eff} 's from these sources were generally below 0.2%.

References

1. D. E. Kusner, S. Kellman, and R. A. Dannels, "ETOG-1, A Fortran IV Program to process Data from the ENDF/B File to the MUFT, GAM, and ANISN Formats," WCAP-3845-1 (ENDF 114), December 1969.
2. C. L. Beard and R. A. Dannels, "ETOT, A Fortran IV Program to process Data from the ENDF/B File to Thermal Library Format," WCAP-7363, March 1971.
3. H. C. Honeck and D. R. Finch, "FLANGEII (Version 71-1). A code to Process Thermal Neutron Data from an ENDF/B Tape," DP-1278, October 1971.
4. N. R. Candelore, R. C. Gast, and L. A. Ondis II, "RCP01 - A Monte Carlo Program for Solving Neutron and Photon Transport Problems in Three-Dimensional Geometry with Detailed Energy Description," WAPD-TM-1267, August 1978.
5. A. V. Dralle, N. R. Candelore and R. C. Gast, "RCPL1 - A Program to Prepare Neutron and Photon Cross-Section Libraries for RCP01," WAPD-TM-1268, August 1978.
6. H. Bohl, Jr., et al, "P3MG, A One-Dimensional Multigroup P-3 Program for the Philco-2000 Computer," WAPD-TM-272, 1963.
7. E. Schmidt and L. D. Eisenhart, "A Successive Collision Calculation of Resonance Absorption," WAPD-TM-1468, July 1980.
8. Cross Section Evaluation Working Group Benchmark Specifications, BNL 19302 (ENDF-202), November 1974.

9. U. P. Jenquin and S. R. Bierman, "Benchmark Experiments to Test Plutonium and Stainless steel Cross Sections," NUREG/CR-0210, PNL-2273, June 1978.
10. R. H. Masterson, et al, "The Limiting Critical Concentration for Pu239 and U235 in Aqueous Solutions," HW-77089, 1963.
11. C. R. Richey, "Reexamination of the Value of the Minimum Critical Concentration of Plutonium-239 in Water," Nucl. Sci. Eng. 55, 244 (1974).
12. R. C. Lloyd, et al, "Criticality of Plutonium Nitrate Solutions in Slab Geometry," Nucl. Tech. 18, 225 (1973).
13. R. C. Lloyd, et al, "Criticality Studies with Plutonium Solutions," Nucl. Sci. Eng. 25, 164, 1966.
14. F. E. Kruesi, et al, "Critical Mass Studies of Plutonium Solutions," HW-24514DEL, 1952.
15. R. C. Lloyd, et al, "Criticality of Plutonium Nitrate Solution Containing Soluble Gadolinium," Nucl. Sci. Eng. 48, 300 (1972).
16. R. C. Lloyd and E. D. Clayton, "The Criticality of High Burnup Plutonium," Nucl. Sci. Eng. 52, 73 (1973).
17. R. E. Prael, "Summary of Thermal Reactor Benchmark Calculations Using MCNP with ENDF/B Version IV Data" in LA-8232-PR.
18. P. F. Rose, et al, "Improvement of Reference nuclear Data for Commercial Power Reactor Analysis and Design," EPRI NP-556, October 1977.

19. R. M. Westfall, et al, in a Review of Multigroup Nuclear Cross Section Processing - Proceedings of a Seminar-Workshop, Oak Ridge, March 1978, ORNL RSIC-41.
20. U. P. Jenquin, et al, "Integral Data Evaluation of Stainless Steel, PU239, PU240, and H₂O for Homogeneous Plutonium Systems," PNL-3071, August 1979.
21. S. F. Maghabghab and D. I. Garber, "Neutron Cross Sections," BNL-325, Third Edition, June 1973.
22. V. O. Uotinen, J. H. Lauby, L. C. Schmid, and W. P. Stinson, Nucl. Tech. 15, 257, August 1972.
23. R. I. Smith and G. J. Konzek, "Clean Critical Experiment Benchmarks for Plutonium Recycle in LWR's," EPRI NP-196, Vol. 1, April 1976.
24. R. C. Liikala, V. O. Uotinen, and U. P. Jenquin, Nucl. Tech. 15, 272, August 1972.
25. R. L. Childs, et al, "Sensitivity and Uncertainty Analysis for the Mixed-Oxide Thermal Lattice U-L212," EPRI NP-1248, December 1979.
26. J. Hardy, Jr., "Monte Carlo Analyses of TRX Slightly Enriched Uranium-H₂O Critical Experiments with ENDF/B-IV and Related Data Sets," WAPD-TM-1307, 1977.
27. J. J. Ullo and J. Hardy, Jr., "An Analysis of U233 and U235 Critical Experiments with ENDF/B-IV Data," WAPD-TM-1299, Bellis Atomic Power Laboratory (1977).

TWO-GROUP CALCULATED REACTION RATES

TABLE A1

Major Absorption Rates in Plutonium Isotopes
(Pu-H₂O Assemblies)

Assembly	Pu239				Pu240		Pu241			
	Fission		Capture		Capture		Fission		Capture	
	Fast	Thermal	Fast	Thermal	Fast	Thermal	Fast	Thermal	Fast	Thermal
Inf. Med.	.00405	.34204	.00245	.14225						
1D Slab*	.02031	.33200	.01219	.15561	.02246	.00532	112-3	.00103	230-4	360-3
PNL1	.01417	.33995	.00847	.15362	.01625	.00552				
3	.00907	.33849	.00546	.14755	.01028	.00513				
4*	.01113	.33880	.00675	.15043	.01276	.00506				
5*	.01614	.33579	.00974	.15406	.01713	.00485				
PNL6B	.05930	.29122	.03438	.15268	.04395	.00439	390-3	94-3	80-4	33-3
7B	.00971	.34239	.00580	.15029	.00149	643-3				
8A	.01279	.34110	.00766	.15311	.01479	.00554	793-4	.00265	163-4	464-3
9	.01038	.33831	.00625	.14891	.03323	.01859				
10	.03429	.31230	.02018	.15331	.04649	.00918	637-3	.00320	131-3	.00112
11	.00812	.25411	.00493	.11250	.09789	.08995	.00411	.08078	847-3	.02821
12B	.00897	.34216	.00539	.14893	.01083	.00569	561-4	.00138	116-4	484-3

*P7MG results. Others are RC201.

TABLE A2

Hydrogen and Nitrogen Absorption Rates
in the Fissile Solution, and Net Total Leakage
(Pu-H₂O Assemblies)

Assembly	Hydrogen Absorption in Fissile Solution		Nitrogen Absorption in Fissile Solution		Net Total Leakage
	Fast	Thermal	Fast	Thermal	
Inf. Med.	.00683	.49857	--	--	0
1D Slab*	.00412	.04919	.00272	.00897	.38243
PNL1	.00440	.08399	834-3	.00453	.36542
3	.00488	.15124	.00107	.00982	.31398
4*	.00468	.11169	.00415	.02927	.32192
5*	.00428	.06692	.00387	.01734	.36669
PNL6B	.00347	.01033	.00661	.00514	.38322
7B	.00429	.12449	950-3	.00821	.35143
8A	.00453	.09684	863-3	.00541	.35288
9	.00482	.13075	894-3	.00708	.29780
10	.00347	.02211	.00280	.00478	.38260
11	.00525	.13859	.00205	.01602	.13693
12B	.00449	.14283	734-3	.00700	.31609

*P7MG results. Others are RCP01.

TABLE A3

Total Absorption of Minor Constituents of the Fissile Solution (< 1%)
(Pu-H₂O Assemblies)

<u>Absorption Type</u>	<u>Inf. Med.</u>	<u>ID Slab*</u>	<u>PNL1</u>	<u>PNL3</u>	<u>PNL4*</u>	<u>PNL5*</u>	<u>PNL6B</u>	<u>PNL7B</u>	<u>PNL8A</u>	<u>PNL9</u>	<u>PNL10</u>	<u>PNL11</u>	<u>PNL12B</u>
Pu238 Cap.		11-4									72-5	70-3	
Fiss.		0									52-6	3-4	
Pu240 Fiss.		85-4	55-4	31-4	40-4	58-4	25-3	42-5	43-4	13-3	27-3	62-3	33-4
Pu242 Cap.		9-5					14-4		35-5		71-4	38-2	34-5
Fiss.		0					0		51-7		12-5	5-4	45-7
AM241 Cap.												62-2	
Fiss.												5-4	
Gd. Abs.												32-2	
Fe Abs.				24-4	23-4	18-4	77-5	24-4					88-5
O Abs.	379-2	306-2	278-2	295-2	330-2	313-2	334-2	258-2	275-2	298-2	267-2	337-2	264-2

*P7MG results. Others are RCP01.

TABLE A4
Pu239 and Pu240 Core Reaction Rates
(UO₂-PuO₂ Assemblies)

<u>Lattice</u>	<u>Pu239 Fission</u>			<u>Pu239 Capture</u>		<u>Pu240 Capture</u>	
	<u>Fast</u>	<u>Thermal</u>	<u>δ^{49}</u>	<u>Fast</u>	<u>Thermal</u>	<u>Fast</u>	<u>Thermal</u>
27	0.0249	0.2450	0.1016	0.0144	0.1163	0.0237	0.0070
29	0.0084	0.2681	0.0313	0.0048	0.1161	0.0091	0.0082
30	0.0306	0.2384	0.1283	0.0179	0.1153	0.0287	0.0068
31	0.0351	0.2336	0.1503	0.0204	0.1156	0.0314	0.0066
32	0.0171	0.2593	0.0659	0.0099	0.1187	0.0177	0.0076
33	0.0219	0.2542	0.0861	0.0128	0.1205	0.0223	0.0073
34	0.0131	0.2660	0.0493	0.0074	0.1193	0.0139	0.0079
35	0.0165	0.2628	0.0629	0.0096	0.1208	0.0184	0.0077
36	0.0218	0.2226	0.0977	0.0128	0.1063	0.0458	0.0245
38	0.0070	0.2424	0.0290	0.0040	0.1051	0.0176	0.0283
39	0.0169	0.2423	0.0696	0.0169	0.1146	0.0414	0.0203
40	0.0116	0.2686	0.0431	0.0063	0.1174	0.0180	0.0234

TABLE A5

U238 and U235 Core Reaction Rates
(UO₂-PuO₂ Assemblies)

<u>Lattice</u>	<u>U238 Fission</u>	<u>U238 Capture</u>		<u>U235 Fission</u>		<u>U235 Capture</u>	
		<u>Fast</u>	<u>Thermal</u>	<u>Fast</u>	<u>Thermal</u>	<u>Fast</u>	<u>Thermal</u>
27	0.0218	0.1107	0.0351	0.0094	0.0513	0.0043	0.0088
29	0.0099	0.0370	0.0437	0.0031	0.0653	0.0014	0.0111
30	0.0259	0.1353	0.0332	0.0117	0.0482	0.0053	0.0083
31	0.0280	0.1552	0.0312	0.0132	0.0449	0.0061	0.0077
32	0.0163	0.0756	0.0391	0.0064	0.0578	0.0029	0.0099
33	0.0192	0.0975	0.0365	0.0082	0.0534	0.0038	0.0092
34	0.0135	0.0588	0.0413	0.0049	0.0614	0.0022	0.0105
35	0.0154	0.0734	0.0395	0.0061	0.0582	0.0028	0.0099
36	0.0236	0.1245	0.0412	0.0104	0.0603	0.0049	0.0103
38	0.0105	0.0409	0.0514	0.0033	0.0769	0.0015	0.0131
39	0.0182	0.0876	0.0216	0.0071	0.0313	0.0033	0.0054
40	0.0092	0.0332	0.0267	0.0027	0.0396	0.0012	0.0067

TABLE A6
Core Neutron Leakage Fractions
(UO₂-PuO₂ Assemblies)

<u>Lattice</u>	<u>Core Neutron Leakage^a</u>
27	0.2842
29	0.1906
30	0.2596
31	0.2057
32	0.2890
33	0.1416
34	0.2734
35	0.1178
36	0.2210
38	0.1217
39	0.2868
40	0.2295

^aDefined to be the net neutron leakage fraction from the fueled region of the lattice assembly.