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Requirements at Argonne National Laboratory to establish the best estimates and uncertainties for LMR design parameters have lead to an extensive evaluation of the available critical experiment database. Emphasis has been put upon selection of a wide range of cores, including both benchmark, assemblies covering a range of spectra and compositions and power reactor mock-up assemblies with diverse measured parameters. The integral measurements have been revised, where necessary, using the most recent reference data and a covariance matrix constructed. A sensitivity database has been calculated, embracing all parameters, which enables quantification of the relevance of the integral data to parameters calculated with ENDF/B-V.2 cross sections.

Introduction

A current program at Applied Physics Division of ANL is establishing a system to provide the best possible estimates of fast reactor performance parameters and uncertainties. Of immediate interest are the metallic-fueled cores for the IFR program and space-reactor cores, but it is intended that the system would also be applicable to a wide range of designs. The method adopted is least squares fitting, expanding the parameter space of the ENDF/B cross sections with integral data from critical assembly experiments by means of sensitivity coefficients.

A number of cores have been selected on the basis of including a wide range of compositions, spectra and measured parameters. The selection of reliable data with good uncertainty estimates, a variety of independent measurements and inclusion of data from different laboratories was considered of primary importance. All calculations were made with the best transport methods practicable, supplemented by Monte Carlo calculations in several cases where deficiencies were suspected.

This paper describes the integral database at the present stage and analyses made with ENDF/B-V.2 data. Sensitivity coefficients are used to show the most important cross sections impacting the integral parameters and the correlations between parameters.

The Integral Database

The database ranges from FLATTOP-Pu with a fissile loading of 6 kg to ZPPR-18 with a fissile loading of 3700 kg and includes the ZEBRA-8 zero-leakage test zones. At present, we include 6 hard-spectrum cores from LANL, 7 ZEBRA-8 zones plus Scherzo-556 and 11 ZPR/ZPPR cores from ANL. Calculations have been made for several other cores, presently in standby status pending calculation of sensitivities. Many of the data have been reported by Atkinson and Collins.[1] Since that time, the database has been expanded by inclusion of several more cores and parameters. In addition, experimental reaction rate data have been revised using latest constants and several calculations have been updated using Monte Carlo results.

Deterministic calculations were made with a 21 group energy structure favored by the core design group at ANL. Multigroup cross sections were processed individually for each core with 2082-group spectrum calculations for core and blanket regions, cell heterogeneity processing in 230 groups with special allowance for edge-region cells and collapse to 21 groups with one-dimensional reactor models. The smaller high-leakage cores were calculated with the TWODANT code[2] using high-order quadrature and anisotropic scattering. ZPR/ZPPR cores were calculated with a nodal transport code in xyz geometry[3] and detailed composition/geometry representation. Plate-cell streaming effects were included using anisotropic transport cross sections.

Calculations for several of the cores were made with the VIM Monte Carlo code: Jezebel, Godiva and the two FLATTOPs because of suspected effects due to anisotropic inelastic scattering and energy dependent fission spectra which are not treated in the ANL codes, Zebra-8A and 8C because of the strong heterogeneity effects (6 to 7%Δk).

The integral parameters in the database include k_{eff}, reaction rate ratios between F25, F49, F28 and C8 for most cores, a number of results for $^{10}B(n,\alpha)$ relative to F25, small sample worths of fissile and fertile materials and ^{10}B, sodium void reactivities, neutron spectra, control rod worths and reaction rate distributions. Inclusion of spatial variations in reaction rates and control worths was felt to be important for two reasons: (i) ENDF/B (and other) data show substantial variations in accuracy of prediction; (ii) the relative measurements can be quite precise and have a high weight in a data fitting scheme.

Correlations among integral parameters are important in a data fitting process. A covariance matrix has been constructed for the measured parameters. Correlations among calculated values must exist but are difficult to estimate. At present, we assume only total uncertainties. These are estimated from the results of Monte Carlo comparisons, from the size of heterogeneity, streaming, transport effects etc.

Table 1 summarizes the estimated uncertainties in the integral parameters. The calculational uncertainties are due to multigroup data processing and modeling. Nuclear data uncertainties are calculated from ENDF/B-V covariance data and sensitivity matrices. The ranges of calculation discrepancies are indicated in the last column. Experimental uncertainties are in most cases similar to, or smaller than, the calculational uncertainties. Nuclear data uncertainties are substantially larger than experimental uncertainties for k_{eff} and ^{238}U fission ratios but comparable in magnitude for many other parameters.

Sensitivities and Nuclear Data Covariances

Sensitivity coefficients in 21 energy groups have been generated for each integral parameter for all cross sections of importance. Those for the large cores were calculated by diffusion theory with the VARI3D code using rz and xy geometric models as appropriate. Sensitivities for the small cores containing few isotopes were calculated with the TWODANT code by direct variation of cross sections. A two-dimensional transport sensitivity option is being incorporated in VARI3D for future use.

Sensitivities to fission spectrum parameters were generated by direct calculations. For reactivity parameters, sensitivities to delayed neutron yields are also being calculated. Initial studies indicate that sensitivities to total inelastic scattering cross sections are inadequate. The codes have been developed to produce sensitivities for chosen groups of inelastic levels. In the case of ^{238}U, it appears that partitioning levels into rotational ground state band, vibrational bands and continuum may be a minimum extension.

Cross section covariance matrices were generated from the ENDF/B files using the NJOY code.[4] Difficulties were found in expanding data from a few points to the 21 groups where non-positive-definite matrices were obtained. These were remedied by minimal adjustments to the off-diagonal terms of the correlation matrices. At present covariances are available only for the principal uranium and plutonium isotopes and for several light and structure nuclides. Uncertainty estimates were made for the remaining cross sections and correlation information was added where it was considered of importance.

k-eff and Reaction Rate Ratios

The k_{eff} parameters have the highest weight in any fitting procedure because of the low uncertainties (measured and calculated) relative to the nuclear data uncertainties (Table 1). Fission ratios for ^{238}U are also important data. Calculation discrepancies for the cores are summarized in Table 2. The largest discrepancies with ENDF/B-V.2 data are found for the small hard spectrum assemblies, Scherzo and ZEBRA-8H, and these are shown in individually. Results for the LMR cores are rather similar and these are averaged. Results for the six ZEBRA-8 Pu cores are also averaged but have larger standard deviations because of the wider spread in spectra.

The most discrepant k_{eff}s by far are found for the LANL BIG-10 (10% enriched uranium core with depleted uranium reflector) and ANL U9 (similar to BIG-10 with 9% enrichment) with C-E of 1.6% and 1.4% respectively. These cores had been calculated with k_{eff} close to unity with ENDF/B-IV data. A discrepancy (+0.9%Δk) is found for Scherzo (an infinite uranium medium of 5.56% enrichment) followed by the FLATTOP core. Large discrepancies of 4% to 10% are found for the F28/F25 ratio in the hard spectrum cores. The LMR-type cores are rather consistently calculated with a discrepancy of -0.7%Δk. The mean discrepancy for the ZEBRA-8 cores is also -0.7%Δk with a wider dispersion. The F28/F49 ratio is about 1% low in the LMR cores and several percent high in the ZEBRA-8 cores. Most cores show overprediction of the ^{238}U capture ratio, 5% in the LMR cores but about 1.5% lower than this in the ZEBRA cores. This systematic difference has been noted previously and has been shown, by direct comparison, to be due principally to differences in measurement techniques.

Table 3 compares the importance of the principal cross sections for a selection of integral parameters in uranium cores. ZPPR-15D is a benchmark core for a 300 MWe LMR with 90% U235 fuel. The importance parameter is defined here as

$$I_i = \sum_j |S_{ij}| \Delta\sigma_j / \Delta M_i \qquad (1)$$

with S_{ij} the sensitivity coefficient, $\Delta\sigma_j$ the cross section uncertainty and Δm_i the combined experimental and calculational uncertainty for the integral parameter. At the bottom of the table we show the correlation for each parameter relative to ZPPR-15D. The correlation coefficient is defined as

$$C_{ij} = S_i^T C S_j / [(S_i^T C S_i)(S_j^T C S_j)]^{1/2} \qquad (2)$$

and follows from the covariance matrix of the integral data which is given by the error propogation law $C_Q = S^T CS$, with C the cross section covariance matrix.

Godiva is well calculated but discrepancies in k_{eff} and F28/F25 increase through Flattop-25, Scherzo and U9 (and BIG-10). Table 3 shows the increased importance of U238(n,n′), U238(n,γ) and the U235 fission spectrum for these cases. The importances are high for the F28/F25 ratio although the integral parameter uncertainty (Δm) is 5 to 15 times higher than for k_{eff}.

The critical eigenvalue is consistently predicted for the range of LMR cores from 1 tonne to 4 tonnes fissile loading and including conventional cores, radial heterogeneous and axial heterogeneous cores, provided transport calculations are made. The same conclusion was found by McKnight;[5] with ENDF/B-IV data the mean C/E was 0.985 with a standard deviation of 0.01 for 18 different cores. Analyses of the nuclear data importances as in Table 3, and the covariances shows that this should be the case. The k_{eff}'s for plutonium and uranium fueled LMRs have a correlation of about 0.5 due principally to the ^{238}U.

Measurements of fission in ^{241}Pu and ^{240}Pu made with fission chambers in the ZEBRA-8 series and in U9 are included in the database.[1] The ^{241}Pu fission ratios are calculated about 5% higher than experiment, while the ^{240}Pu fission ratios are calculated 20% to 40% higher. These latter results are not consistent with sensitivity analysis and interpretation of the chamber experiments is regarded as suspect.

Reaction Rate and Control Worth Distributions

In contrast to the eigenvalues, the accuracy of predictions of reaction rates and control worths as a function of position show remarkable differences between the small LMR cores and the larger more decoupled cores. This difference is correlated with the fundamental to first-harmonic eigenvalue separation. In the small cores, relative fission rates in ^{239}Pu, ^{235}U, ^{238}U and capture rates are predicted within the uncertainties of the measurement and analysis of 1 to 2%. The largest discrepancies in spatial predictions among the ZPPR cores were found in ZPPR-13C. This core, although of medium size (2500 kg fissile or about 700 MWe), had an eigenvalue separation of 1.3% which may be approached in some 1500 MWe designs.

The radial discrepancies in calculated fission rates for ZPPR-13C at the midplane are shown in Figure 1. It is worth noting that the discrepancies were about halved in going from Version 4 to Version 5.2 cross sections of ENDF/B. Axial distributions were well predicted with either data set. Relative control rod worths are also midpredicted with a maximum difference of 10%.[1] It is also signficant that extremely detailed modeling, allowing for small variation in composition about the average, was necessary for calculations in ZPPR-13.

The most important cross sections for the calculated integral parameters in ZPPR-13C are compared in Table 4 (Eq. 1). Here the radial fission rate is defined as the ratio of that in the inner fuel ring to that in the outer fuel ring. In contrast to k_{eff}, the most important reactions for the fission distribution are inelastic scattering and capture in ^{238}U followed by the total scattering in steel, sodium and oxygen. These cross sections are also important for the control banks and the importance cf most data shows a variation with radius. Table 5 shows the correlations between calculated parameters in ZPPR-13C. Correlations between spatially-varying parameters are very often quite strong but because they are both positive and negative, the discrepancies between experiment and calculation may be consistent with nuclear data uncertainties. In fact, least squares fitting produces consistent agreement for k_{eff} and among the spatially varying quantities with the uncertainties.

Sample Worths, Control Rod Worths, Sodium Void, Spectra

The worths of small samples of U235, Pu239 and U238 in the ZPR/ZPPR cores are calculated within a few percent of experiment following the cell studies of Smith and Schaefer.[6] Some recent results are shown in Table 6. Measurements made in a tube at the center of larger cores are in reasonable agreement with those in detailed in cell environments but many older measurements in high-leakage regions cannot be interpreted. Widely varying results are obtained for scattering materials and these data are regarded as unreliable. Similarly, the present situation for Pu240 samples is unsatisfactory. The results for worths in the similar cores BIG-10 (LANL) and U9(ANL) differ systematically by 2-3%, but within the estimated uncertainties. The uncertainties due to nuclear data are much larger in these two cases than in the LMR-type core, ZPPR-15.

Boron small sample worths and control rod worths have similar predictions provided that transport effects are adequately calculated. The C/E are always a few percent lower than for the fissile worths. Measurements of ^{10}B(n,α) relative to ^{235}U fission have been made in a number of cores using helium accumulation fluence monitors (HAFMs).[7] A selection of boron-related data is given in Table 7. Discrepancies are significantly greater than the nuclear data uncertainties except for control rod worths in ZPPR-13C. The discrepancies with experiment are greater in the uranium cores and the reaction rates are more discrepant than the worths. For the worths, the importance of ^{10}B(n,α) cross sections is small compared with that of other materials as can be seen in Table 4.

Our present data for sodium void, analyzed with Version 5.2 cross sections, are limited to a number of central zones in ZPPR-15 and the completly voided core, ZPPR-12V. The ZPPR-15 measurements, shown in Table 7, compare results in a plutonium-fueled core 15A, the core with zirconium replacing some steel 15B, zirconium replacing depleted uranium and steel in a zone (high-Zr zone), a 50%-uranium/50%-plutonium core 15C, and a 90% uranium fueled core 15D. The central sodium void reactivity (small leakage fraction) is overestimated in all cases. The data are consistent with least squares fitting of all the integral parameters. A comprehensive assessment of sodium void data with ENDF/B-IV data has been made by Beck.[8]

Spectrum measurements are correlated with other parameters while the techniques are independent and are potentially valuable data. Proton recoil measurements, covering the range 1 KeV to 1MeV, have been included in the database. However, present sensitivity analysis shows several large discrepancies with other integral data and the uncertainty estimates are in question.

Summary

The integral database in this review was selected mainly from past experience with ENDF/B-IV data. While the immediate objective was setting up a system for systematic prediction of LMR parameters, only a few cores of this type are included. Many LMR mock-up cores have been built at ANL but their main usefulness has been in testing calculation methods. After refined calculations, the comparison with experiment generally shows consistent biases. An exception is the prediction of parameters as a function of position in the decoupled cores. Sensitivity analysis and least squares fitting show that these discrepancies are consistent with those of other integral data.

Although much progress has been made over the past decade, calculation of heterogeneity effects in the plate-cell critical experiments limit the usefulness of some of the data. With the exception of k_{eff}, which can be calculated by Monte Carlo methods where necessary, the uncertainty in calculation modeling for some parameters is similar to that due to nuclear data uncertainties. Particular areas of concern are adjacent cells with widely differing enrichment, fuel/blanket-cells and fuel/control rod cells. Reaction rate ratios, reaction rate distributions, control worths and sodium void have increased uncertainties in a number of cases.

Several extensions of the database are desirable. The inclusion of more experiments from different laboratories seems important to guard against systematic errors. While simplified models are available in a number of cases, uncertainties arise because the full details of loadings and measurements are rarely available. On the other hand, considerable effort is required for detailed analysis of unfamiliar cores. Further international cooperation in specifying benchmark cores seems desirable. Some more obvious shortcomings in our database for LMR cores are in integral data for higher actinide isotopes and structural materials.

From the point of view of the data sensitivity/fitting methodology, further measurements designed to provide high sensitivity to particular materials would be valuable. These should be small cores with simple cell structure designed to minimize calculation difficulties. Further zero-leakage experiments as in ZEBRA-8 would also be ideal. With present experience and more powerful calculation methods, it should be possible to reduce the uncertainties on the measured criticality for this type of experiment.

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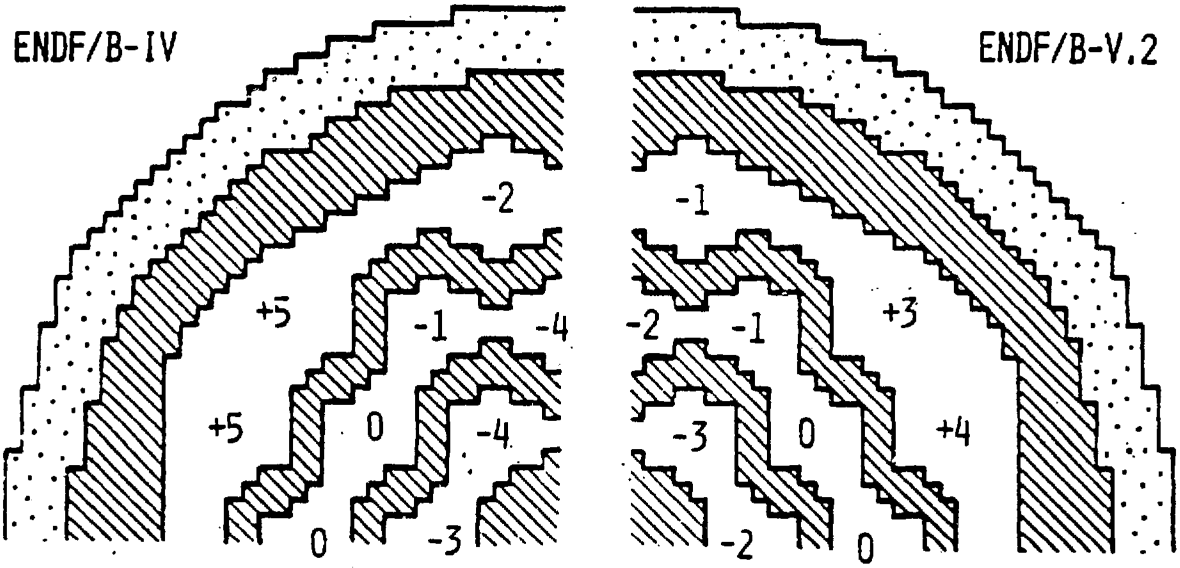

Figure 1. Percent Discrepancies between Calculated and Measured Fission Rates in ZPPR-13C.

Table 1. Uncertainties of Integral Parameters (1σ,%)

Parameter	Measurement Uncertainty[a]	Calculation Uncertainty	Nuclear Data Uncertainty[b]	Range of C/E-1,%
k_{eff} Criticals	$\geq$ 0.1	0.2 to 0.5	1 to 3	-2 to +1.5
ZEBRA 8	0.3 to 0.7			
Reaction Rate Ratios	1 (r)	2	2 to 5	-4 to +6
	2 to 3 (c)		10 (F28)	to +10 (F28)
Fission Distributions	1 to 2 (r)	1 to 2	1 to 2	-2 to +2
				-3 to +4 (13C)
Control Rod Worth	1 (r)	2	2 to 5	-5 to +1
	1 (c)			-11 (15D)
Control Rod Distribution	1 (r)	2	3 to 5 (13C)	-10 to 5
Material Worths:				
Fissile	1 to 5	3	2 to 7	-3 to +4
Boron	1 to 5	2	3 to 7	-10 to -5
Central Sodium Void	1 (r)	5	5 to 15	5 to 50
	1 (c)			
Spectrum	1 to 5 (r)	2?	1 to 5	-2 to +20
	2 to 15 (c)			

[a] r = random (statistical), c = correlated (systematic).

[b] Uncertainties in reactivity scale (βeff) are not included for worths.

Table 2. Discrepancies between Calculation and Experiment for k_{eff} and Reaction Rate Ratios (%)

Core	k_{eff}	F28/F25	C28/F25	F49/F25
U9	1.4	9.6	0.2	-2.0
BIG-10	1.6	7.2	-0.7	-2.2
Scherzo	0.9	9.9	2.0	1.3
Zebra-8H	0.3	8.4	4.7	---
Flattop-Pu	0.7	-4.0	---	---
Flattop-25	0.4	3.6	---	-0.7
Godiva	-0.3	4.0	---	-2.3
Jezebel-Pu	-0.8	-5.0	---	---
Jezebel	-0.2	-3.5	---	-4.2
	k_{eff}	F28/F49	C28/F49	F25/F49
ZPPR-12V	0.1	-5.2	4.4	1.0
ZPPR-12	-0.1	-3.5	6.7	2.6
Mean for LMR Cores (S.D.)	-0.7 (0.2)	-0.8 (1.5)	4.9 (1.1)	0.5 (0.5)
Mean for Zebra 8 Pu Cores (S.D.)	-0.7 (1.2)	5.2 (3.3)	3.4 (1.3)	-0.6 (2.0)

Table 3. Importance of Cross Sections for Uranium-fueled Cores

	k_{eff} Godiva	k_{eff} Flattop-25	k_{eff} Scherzo	k_{eff} U9	k_{eff}[a] ZPPR-15D	F28/F25 Flattop-25	F28/F25 Scherzo	F28/F25 U9
Δm	0.14	0.14	0.36	0.20	0.30	1.7	1.3	3.1
U235 n,f	13.1	11.5	4.0	7.2	5.3	0.8	1.7	0.7
n,γ	7.7	8.1	2.0	4.2	3.5	0.9	0.8	0.4
n,n′	8.9	3.1	0.6	1.1	0.3	1.4	0.5	0.3
n,n	2.0	0.6	0.0	0.1	0.1	0.1	0.0	0.0
ν	4.3	4.0	1.2	2.2	1.7	0.0	0.0	0.0
χ	2.2	3.7	4.5	5.3	1.6	1.7	4.2	1.5
U238 n,f	0.1	1.3	1.5	2.3	0.8	0.9	2.1	0.9
n,γ	0.1	1.8	5.1	6.8	4.0	0.1	2.0	0.6
n,n′	0.4	4.2	9.2	9.5	1.4	0.3	9.1	3.0
n,f	0.1	1.4	0.1	0.6	0.3	0.0	0.0	0.0
ν	0.1	1.0	1.3	3.3	0.7	0.0	0.0	0.1
χ	0.0	0.6	0.7	2.1	0.6	0.0	0.8	0.9
C/E	0.997	1.004	1.009	1.014	0.993	1.036	1.099	1.096
Correlation	0.297	0.403	0.618	0.743	1.000	0.074	0.248	0.266

[a] For ZPPR-15D importances for plutonium and steel in range 0.5 to 1.0 are not shown.

Table 4. The Importance of Cross Sections for Parameters in ZPPR-13C

	k_{eff}	Radial Fission Rate	Inner Ring Control Rods	Middle Ring Control Rods	Outer Ring Control Rods
Δm	0.30	1.4	5.9[a]	5.9[a]	5.9[a]
Pu239 n,f	10.1	1.43	0.90	0.74	0.63
n,γ	1.6	0.37	0.14	0.09	0.06
n,n′	0.3	0.18	0.05	0.03	0.04
ν	3.9	0.61	0.39	0.31	0.13
χ	2.3	0.66	0.03	0.06	0.31
U238 n,f	0.8	0.31		0.06	0.12
n,γ	3.8	1.99	0.62	0.37	0.38
n,n′	2.1	2.04	0.63	0.34	0.46
n,n	0.1	0.33	0.16	0.10	0.02
ν	0.8	0.14	0.04	0.05	0.09
χ	0.7	0.44	0.06	0.00	0.17
Pu240 and Pu241 all data	1.2	0.24	0.12	0.09	0.06
Steel, Na, O					
n,n′	1.0	0.63	0.16	0.08	0.16
n,n	0.7	1.87	0.84	0.57	0.20
n,γ	1.3	0.25	0.10	0.06	0.04
B10 n,α	---	---	0.07	0.08	0.09

[a] The control rod worth uncertainties include β_{eff}.

Table 5. Correlations for Calculated Parameters in ZPPR-13C

	(C/E-1%)	1	2	3	4	5	6	7	8
1. k_{eff}	-0.7	1.00							
2. Radial Fisison Rate	-4.8	0.43	1.00						
3. Azimuthal Fission Rate	+4.6	-0.42	-0.99	1.00					
4. Inner Ring Control Rods	-5.4	0.11	0.92	-0.93	1.00				
5. Middle Ring Control Rods	-2.1	-0.09	0.82	-0.82	0.97	1.00			
6. Outer Ring Control Rods	+0.7	-0.77	-0.85	0.84	-0.59	-0.39	1.00		
7. x-axis Control Rods	+3.7	-0.75	-0.87	0.87	-0.63	-0.44	0.99	1.00	
8. y-axis Control Rods	-4.4	0.01	0.86	-0.89	0.99	0.99	-0.50	-0.55	1.00

Table 6. Predictions of Plutonium and Uranium Worths

Core	Fuel	Material	C/E-1, %	Nuclear Data Uncertainty[a]
ZPPR-15A	Pu239	Pu239	3.6	1.9
	LMR	U235	2.2	4.7
		U238	2.3	5.3
ZPPR-15B	Pu239	Pu239	4.2	1.9
	LMR	U235	2.9	4.7
		U238	1.0	5.5
U9	U235	Pu239	-3.1	7.0
	9% enr.	U235	-3.1	7.0
		U238	-3.3	11.4
BIG-10	U235	Pu239	-0.2	6.9
	10% enr.	U235	-0.2	6.9
		U238	-1.2	13.6
ZPPR-15D	U235	Pu239	2.1	2.9
	LMR	U235	1.2	1.7
		U238	-1.5	4.5

[a] Excluding uncertainty in delayed-neutron data.

Table 7. Boron-related Integral Data

Core	Measurement	(C/E-1)%	Nuclear Data[a] Uncertainty 1σ%
BIG-10 U fuel	Sample Worth	-10.3	7.5
	$^{10}B(n,\alpha)/F25$	-13.4	3.2
ZPPR-15A Pu fuel	Sample Worth	-5.6	4.4
	Control Rod Worth	-5.4	2.5
	$^{10}B(n,\alpha)/F25$[b]	-12.1	N.C.
ZPPR-15D U fuel	Sample Worth	-9.8	3.2
	Control Rod Worth	-11.3	2.0
ZPPR-13C Pu fuel	Control Rod Worth (Ring 2)	-2.1	3.1
	$^{10}B(n,\alpha)/F25$ (Fuel ring 2)	-5.6	1.8

a Excluding delayed-neutron data for worths.

b Measured inside enriched-boron control rod.

Table 8. Central Sodium Void Measurements in ZPPR-15

Core	Fuel	Measured Reactivity ¢/kg(Na)	Uncertainty 1σ	C/E ¢/kg(Na)
15A	Pu/U	1.95	0.02	0.22
15B	Pu/U/Zr	2.08	0.02	0.15
High-Zr	Pu/U/Zr	1.74	0.03	0.29
15C	50% Pu/U/Zr 50% U/Zr	0.77	0.01	0.13
15D	10% Pu/U/Zr 90% U/Zr	0.23	0.01	0.12