238+100 FAST REACTOR

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ANNUAL TECHNICAL PROGRESS REPORT
LMFBR SAFETY PROGRAMS
GFY 1970

AEC Research and Development Report

Atomics International
North American Rockwell

P.O. Box 309
Canoga Park, California 91304

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LMFBR PHYSICS PROGRAMS
GFY 1970**

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Program: Civilian Power, LMFBR

AEC Task: 5-B, Reactor Physics, Fast-Reactor Physics Experiments

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Principal Investigators: T. H. Springer, R. J. Tuttle, H. N. Royden,
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I. PROJECT OBJECTIVES

The objectives of this project are to (a) determine reactivity, temperature, and Doppler coefficients of various materials in a variety of fast-reactor spectra; (b) investigate effects due to different geometric arrangements of such materials, including the variation of the surface-to-mass ratio; (c) provide experimental results for checking theoretical predictions; and (d) develop improved experimental and theoretical methods for treatment of problems in the field of fast-reactor physics.

II. TECHNICAL PROGRESS DURING FISCAL YEAR 1970

A. SUMMARY

Major emphasis at the Epithermal Critical Experiments Laboratory (ECEL) was placed during GFY 1970 on experimental and analytical studies of control-rod reactivity and heating effects as they pertain to full-scale FBR application. The experimental studies were done in Core 17, a U^{235} plate-fueled spherical core whose spectrum closely simulated that of conceptual FBR power plants. Some comparative investigations were also made in Core 18, a sodium-voided version of Core 17. Special attention was paid to a comparison between the calculated and measured effects of the control-rod systems studies so that present analytical techniques for dealing with rather geometrically complex FBR control rods could be evaluated and modified to be more useful to the reactor designer.

Fabrication of the major hardware items required for assembling Core 20, the pin-type cylindrical mockup of an FBR, was completed and production of the 15%-enriched UO_2 pellets was begun by an outside supplier.

Detailed information on the above items in addition to other work carried on during GFY 1970 is given below.

B. EXPERIMENTAL MEASUREMENTS AND THEIR ANALYSIS

1. Control-Rod Worth Studies

A comprehensive study of reactivity self-shielding of tantalum in Core 17 was completed. These measurements covered a wide range of sample sizes and geometries and have proved to be a useful set of experiments for comparing various calculational methods. The samples used in this study are listed in Table 1 along with the results of the measurements of the total and specific worths. A graphical presentation of the specific worth as a function of a sample-size parameter is given in Figure 1.

The reactivity worths of tantalum samples up to 0.75-in.-diam were measured by the oscillator technique; the large 1.75-in.-diam sample and the series of 1, 3, 6, 12, and 18 pins were measured by determining the reactor excess reactivity with and without the sample in place. For clusters up to 18 pins a large cavity (Core 17A) was formed at the center of the test region and a tubed can, or calandria, inserted to hold the pins.

A cross-sectional view of this calandria is shown in Figure 2. The can was 4-in. long. In the single-pin measurement one pin was placed in the inner ring. Next, three pins were located symmetrically in the inner ring which was then filled completely for the 6-pin measurement. These pins were removed and 12 pins inserted in the outer ring for the next configuration listed in the table. Finally all 18 locations were filled with tantalum pins. Additional measurements made after filling the space in the can between the tube with sodium showed no significant difference from the sodium-voided case. This fact is due to the small amount of sodium in the calandria and the relatively long mean free-path of neutrons in sodium.

Calculations have been carried out using first-order perturbation theory, exact perturbation theory, and eigenvalue differences. While the atomic thickness

Figure 1. Specific Worth of Tantalum vs $N\bar{l}$ in Cores 17 and 17A

TABLE 1
SUMMARY OF TANTALUM WORTH MEASUREMENTS

Sample Description			$N\bar{l}$ (atoms/barn)	ρ (¢)	ρ_m (m¢/gm)
Diameter (in.)	Length (in.)	Mass (gm)			
0.450 (0.001 wall tube)	3.820	1.566	0.565×10^{-3}	- 0.0092 ± 0.0003	-5.87 ±0.18
0.495 (0.002 wall tube)	4.020	3.283	1.021×10^{-3}	- 0.0177 ± 0.0003	-5.39 ±0.10
0.510 (0.003 wall tube)	4.005	4.845	1.465×10^{-3}	- 0.0261 ± 0.0005	-5.38 ±0.10
0.505 (0.005 wall tube)	4.007	8.158	2.491×10^{-3}	- 0.0430 ± 0.0003	-5.28 ±0.04
0.063	4.025	3.389	8.710×10^{-3}	- 0.0164 ± 0.0004	-4.84 ±0.12
0.123	3.996	12.842	16.90×10^{-3}	- 0.0564 ± 0.0005	-4.39 ±0.04
0.252	4.005	53.592	33.82×10^{-3}	- 0.2117 ± 0.0005	-3.955 ±0.008
0.438	4.003	63.269	57.99×10^{-3}	- 0.5894 ± 0.0006	-3.61 ±0.01
0.752	4.001	484.80	96.77×10^{-3}	- 1.585 ± 0.002	-3.27 ±0.01
1.775	4.010	2706.8	204.5×10^{-3}	- 7.633 ± 0.001	-2.82 ±0.02
0.751 (1 pin)	3.995	483.1	96.68×10^{-3}	- 1.55 ± 0.10	-3.21 ±0.21
3 pins		1448.2	109.6×10^{-3}	- 4.59 ± 0.10	-3.17 ±0.07
6 pins		2895.6	149.3×10^{-3}	- 8.89 ± 0.10	-3.07 ±0.03
12 pins		5796.6	167.2×10^{-3}	-16.52 ± 0.10	-2.85 ±0.02
18 pins		8692.2	225.5×10^{-3}	-22.51 ± 0.10	-2.59 ±0.01

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Figure 2. 18-Pin Control-Rod Calandria

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($N\bar{l}$) is an accurate parameter for the first-order perturbation calculations, the sample mass must also be matched in the exact perturbation and eigenvalue-difference calculations. This is because the latter two methods account for the perturbation in the flux due to the sample, which is dependent on the mass of tantalum present. The exact perturbation calculations use the unperturbed adjoint flux with the perturbed real flux, and provide accurate predictions in the range of $N\bar{l}$ where first-order perturbation theory is no longer adequate and where eigenvalue-differencing is not applicable due to limitations in the precision of the eigenvalue calculations.

The initial series of calculations of the Ta worths used perturbation theory over the entire range of $N\bar{l}$ values (see Figure 1). It was initially concluded that the calculation was overestimating by about 25% the worth of the samples at high $N\bar{l}$ values. Subsequent analytical work has shown, however, that the exact perturbation and eigenvalue-difference results improve the agreement between calculation and experiment. We have concluded, therefore, that eigenvalue-difference calculational techniques are valid (within $\pm 10\%$) for full-scale FBR core-design work.

Early measurements at the ECEL had shown that europium had a high specific-reactivity worth in fast-reactor spectra. These results were verified and extended to much larger samples in Core 17. The samples of Eu_2O_3 used in these measurements and the reactivity values obtained are listed in Table 2.

TABLE 2
SUMMARY OF EUROPIUM WORTH MEASUREMENTS

Sample Description			$N\bar{l}$ (Eu atoms/barn)	Total Worth (ϵ)	Specific Worth (m ϵ /gm)	
Diameter (in.)	Length (in.)	Mass (gm Eu_2O_3)			Eu	Eu_2O_3
0.355	3.910	6.047	2.878×10^{-3}	-0.1064 ± 0.0006	-20.37 ± 0.11	-17.59 ± 0.09
0.545	3.945	13.907	4.223×10^{-3}	-0.2398 ± 0.0014	-19.96 ± 0.12	-17.24 ± 0.10
0.438	3.505	26.628	10.87×10^{-3}	-0.4455 ± 0.0006	-19.44 ± 0.03	-16.79 ± 0.02
0.843	3.872	97.624	18.22×10^{-3}	-1.634 ± 0.005	-19.38 ± 0.06	-16.74 ± 0.05
1.685	3.795	131.455	12.50×10^{-3}	-2.22 ± 0.10	-19.6 ± 0.9	-16.9 ± 0.8

The specific reactivity, ρ_m , has been listed for Eu as well as for Eu_2O_3 for direct comparison with other elemental specific worths. The effect of the oxygen is expected to be small. As a potential control-rod material the oxide is preferable to the metal because of the high cost of the latter.

These measurements are of considerable significance in FBR design in that they show europium oxide to have certain advantages over the two present candidates for control-rod absorbers, tantalum and boron carbide. A europium-oxide rod of the same design as the 18-pin cluster shown in Figure 2 with the same worth as a tantalum rod would require less than one-fifth the absorber mass. The gamma-ray heating in such a rod would be reduced even further because of the lower atomic number of Eu_2O_3 compared to Ta. This reduced heat load would permit use of a simpler more compact rod design, therefore providing more in-core clearance. While the cost of europium-oxide material for a rod would be about three times that for a tantalum rod, this would be mitigated by savings resulting from less frequent replacement, reduced internal heating, and lower control-rod weight.

Self-shielded cross-sections for europium have been prepared and are being used in reactivity calculations.

2. Control-Rod Heating Studies

Because of the importance of gamma-ray heating in the design of tantalum control rods, several trials were made to measure the gamma-ray dose in the 18-pin tantalum cluster previously described. For these measurements thermoluminescent dosimeters (TLD) were placed in split pins in the cluster and irradiated. Because of its relatively flat response to the gamma-ray energy, Li^7F was chosen in preference to CaF_2 . Three dosimeter types were tried: powder, extruded rods, and microtomed discs of Li^7F dispersed in Teflon. The dosimeters were placed between the halves of two pins cut transversely and inserted in the inner and outer rings of the 18-pin cluster. The powder was uniformly spread over the mating faces of the joined halves, while the discs (1/4-in.-diam) were distributed symmetrically, four to a pin, to cover the pin cross-section. The rods, 1-mm-diam by 6-mm-long, were placed in holes drilled in the pins, one at the centerline and one near the edge. Irradiations were made with the tantalum cluster and a similar lead cluster in order to determine the relative

contributions to the total dose of gamma-rays from the reactor and gamma-rays from neutron capture in the tantalum. Reactivity measurements showed that the neutron absorption in the lead cluster was negligible, while calculations of the average gamma-ray absorption for the tantalum and lead clusters showed them to be the same within about 2%. Calibration irradiations using a Co^{60} -irradiation facility were made along with the reactor irradiations.

The TLD reader (a commercial instrument consisting essentially of a controlled heater and a photomultiplier to detect the emitted light) was not intended for use with any of the TLD forms used, and performed with varying degrees of success. Reading the loose powder was hampered by poor and nonuniform heating of the powder and by high background readings from the heater. The Teflon discs were similarly hampered by high background because of the small mass of the dosimeter and the small thermoluminescent signal. Only the rods gave dependable glow curves.

Thus results for the powder and the discs which would have required small corrections for departure from the Bragg-Gray cavity conditions were unusable. The rods require a correction that is of the order of 2X and is dependent on the secondary-electron energy spectrum.

The effect of fast neutrons on the dose recorded by Li^7F is not well known. Measurements have been reported that indicate an "erasing" effect in which the fast neutrons reduce the recorded dose due to gamma-rays. These measurements were performed with low neutron doses and may not be applicable to the higher doses in the present measurements. The dose due to fast-neutron scattering is deposited by recoiling Li^7 and F ions and, because these are heavy particles, will be recorded considerably differently by the TLD than is a similar dose due to secondary-electrons from gamma-rays.

3. Ancillary Reactivity-Worth Measurements

In addition to the extensive series of reactivity-worth measurements discussed in the above sections in connection with control-rod worth, several other standard measurements were made in Core 17 and Core 17A to ascertain what deleterious effect if any the cavity in the core center had on sample worth. These results are shown in Table 3 along with some previously unreported measurements for Core 17. For Inconel and stainless steel the results are identical

within the statistical uncertainties which in one case or the other are rather poor. Only the PuO_2 and Ta represent valid comparisons, and they show that a small spectrum-change exists between the two cores.

TABLE 3
COMPARISON OF WORTHS OF SELECTED SAMPLES IN
CORES 17 AND 17A

Sample	Mass (gm)	Specific Worth (10^{-3} μ /gm)	
		Core 17	Core 17A*
Plutonium Oxide	66.20	+13.00 ± 0.01	+12.36 ± 0.01
Inconel-750	81.56	—	-0.443 ± 0.005
Tantalum	163.27	- 3.610 ± 0.003	-3.431 ± 0.003
Hafnium	178.99	—	-2.814 ± 0.002
Dysprosium	4.21	—	-4.0 ± 0.2
Stainless Steel	77.85	- 0.358 ± 0.003	-0.32 ± 0.04
Inconel-600	6.96	- 0.51 ± 0.07	—

*Core 17A has a large cavity for 18-rod tantalum-cluster measurements.

The anomalous results discussed in the GFY 1969 Annual Report concerning the reactivity worth of oxygen were investigated during GFY 1970 in Core 17. Basically the series of experiments consisted of determining the worth of a sample of a metal and then of its oxide and subtracting algebraically. The old oxide samples were suspected of having absorbed water vapor during fabrication; consequently a new set of samples was prepared under more carefully controlled conditions. The experiments were repeated but no substantial change in the results was noted as can be seen in Table 4.

4. Spectrum Measurements

The fission rates of U^{235} and Pu^{239} as a function of position in Core 17 were measured. These measurements were made using solid-state detectors

TABLE 4
COMPARISON OF NEW AND OLD VALUES FOR THE
REACTIVITY WORTH OF OXYGEN IN CORE 17

Samples From Which Value is Derived	Specific Worth ($\$/\text{gm} \times 10^{-4}$)	
	New	Old
PbO/Pb	- 2.24 $\pm$ 0.15	- 5.2 $\pm$ 1.2
PbO ₂ /Pb	+ 2.61 $\pm$ 0.77	+ 3.46 $\pm$ 0.70
MgO/Mg	+40.69 $\pm$ 0.81	+44.0 $\pm$ 0.72
Al ₂ O ₃ /Al (powder)	+ 0.40 $\pm$ 0.44	-
Al ₂ O ₃ /Al (solid)	- 2.96 $\pm$ 0.23	- 2.70 $\pm$ 0.23
Al ₂ O ₃ /Al (solid)	- 3.94 $\pm$ 0.30	- 3.08 $\pm$ 0.30

calibrated by means of alpha-particle counting. Traverses were made with the 18-pin tantalum cluster in place and the cavity empty. Preliminary results subject to revision for reactor-power calibration and corrections for isotopic impurities are shown in Figures 3 and 4. The calculated fission rates are for an unperturbed core with only a small central cavity.

The importance of fission neutrons as a function of position was measured in Cores 17 and 18 using a small Cf²⁵² spontaneous fission source. The results were normalized by using the calculated neutron-production rate in the reactor to equate the measured and calculated production of neutron importance. The normalized experimental points are compared with the calculations in Figures 5 and 6. Figure 5 shows the calculated distribution for Cf²⁵² neutrons, which have a slightly harder spectrum than those of U²³⁵. It is clear that the calculated importance at the center exceeds the measured values by about 31%. Assuming the same discrepancy to hold for neutrons of all energies, this would lead to a discrepancy of 31% between calculated and measured central reactivity worths.

Figure 3. Uranium-235 Fission Rate in ECEL-17A

Figure 4. Plutonium-239 Fission Rate in ECEL-17A

Figure 5. Normalized Neutron Importance in Core 17

Figure 6. Normalized Neutron Importance in Core 18

A simple test was made of the effect of discrepancies between a neutron spectrum measured by a proton-recoil spectrometer and one calculated in a fine-structure mode by AILMOE or MC². The point-data making up the proton-recoil spectrum were collapsed to form group fluxes corresponding in energy to calculated fluxes based on the fine-group structure. These two sets were then used in two perturbation calculations to determine the change in the calculated worth of a selected sample. Although a visual comparison of the fine-structures of the measured and calculated spectra shows numerous discrepancies, the reactivity worth of a sample of Ta calculated with the analytical spectrum does not vary by more than 0.2% from the worth calculated with the measured spectrum.

C. ANALYTICAL INVESTIGATIONS

1. TRIX Code Development and Testing

Two modifications were made to the TRIX code. The first one involves a provision for inputting tables of level widths at energy points, and was made to accommodate the new ENDF/B data format. The data can be read from cards or from a file in the resonance-parameter library stored on a disk. The option was used for Pu²⁴¹ data in the calculation of reactivity and Doppler worths of measured PuO₂ samples.

In the second modification a version of TRIX was created which will weight resonance integrals across energy groups using an input spectrum. The spectrum is specified in up to 50 energy regions each of which may be pointwise data or an exponent for the form E^{-x} . The region boundaries are independent of the group boundaries for multigroup cross-sections. The input data in each region may be independently normalized. Throughout the code the flux is computed assuming that the logarithm of the flux is linear in the logarithm of energy between points where the flux is specified.

For unresolved resonances each energy group is subdivided based on an input parameter. Because of the abrupt change in the energy derivative of the cross-section at inelastic-scattering level thresholds, an additional subdivision boundary was placed at each threshold energy. In each subdivision the logarithm of the integral is assumed to be linear in the logarithm of energy and to pass

through the values calculated at the energies of the two-point Gaussian integration formula. The integral of the flux-weighted resonance integral is evaluated analytically.

Flux-weighted negative energy-resonance integrals are evaluated using two-point Gaussian integration between points where the flux is specified and/or at energy group boundaries. Flux-weighting integrals of the $1/v$ tails of positive energy resonances are evaluated analytically.

The new version permits the calculation of effective resonance cross-sections for multiple values of optical thickness more efficiently and with more sophistication than the GRISM code currently uses for flux-weighting. In addition the incorporation of theoretical improvements is greatly facilitated. Flux-weighting has been found to be an important consideration in generating accurate multigroup cross-sections for fast-spectrum assemblies.

2. Calculated vs Measured Reactivity Worths

The reactivity worths of a number of samples measured in Cores 14 through 17 have been calculated as follows. The spectra at the center of the test regions were obtained from diffusion-theory calculations of the fluxes in the assemblies. The basic cross-section data was the AIENDF of 1967. The basic data were formed into multigroup ($\Delta u = 0.5$) cross-sections, including intragroup flux-weighting and resonance self-shielding. The same basic data and methods were used for all cores. The sample worths were calculated using first-order perturbation theory with the central spectra. The effective cross-sections of the samples were calculated using the most recent choices of basic data.

For strong absorbers the contributions to reactivity worth from other than absorption reactions are not significant and were neglected. The $(n,2n)$ reactions were assumed to be negative absorptions at the energy of the reaction. The error introduced by this approximation is small for heavy absorbers.

Resonance self-shielded cross-sections were calculated with the TRIX code using parameters from AIENDF and were corrected by the difference between the infinitely dilute values of GRISM and TRIX. These calculations do not include high-energy shielding and fast-fission effects nor flux-weighting in the resonance region.

Ratios of calculated-to-measured worths of U^{238} are shown in Table 5. Small corrections for U^{235} contaminations were made to obtain the U^{238} worth along. The worth of oxygen was assumed to be zero. The ratios of calculation-to-measurement are generally lower than calculated worths of other isotopes. The reason is thought to be the choice of low capture cross-sections in the key region in the evaluation used.

TABLE 5
RATIO OF CALCULATED TO EXPERIMENTAL WORTH OF U^{238}

U ²³⁸ Sample	U ²³⁸ Mass (gm)	Outer Diameter (in.)	Length (in.)	Calculation/Experiment Ratio			
				Core 14	Core 15	Core 16	Core 17
Metal Cylinder	184	0.438	4.00	0.96	0.96	1.03	1.03
Metal Annulus	117	0.438	4.00	0.96	0.97	1.08	1.02
Metal Cylinder	60	0.250	4.00	0.98	—	—	1.05
Oxide Cylinder	69	0.395	4.00	—	—	—	1.09

For U^{235} the high-energy cross-sections come from the KEDAK data file. Corrections for U^{238} impurities were made. Comparison between calculation and experiment for metal cylinders is shown in Figure 7. Inclusion of the fast effect will increase the calculated worths more at low modulus values (large samples) than at high values. The calculations are high by 10 to 20%.

The calculated-to-measured worth ratios for the PuO_2 samples are shown in Table 6. Oxygen was assumed to have zero worth in the calculations.

Cross-section changes with temperature were calculated with the TRIX code using 1/E spectrum weighting. Worth changes were calculated with first-order perturbation theory (CTRWORTH).

Results for U^{235} metal samples are shown in Table 7. The U^{238} impurity is seen to dominate the U^{235} effect in most cases.

Calculated Doppler worths for U^{238} in Cores 14 and 17 are shown in Figure 8. Results for PuO_2 samples are shown in Table 8.

Figure 7. Specific Worths of U^{235} in Metal Cylinder
93% Enriched

TABLE 6
RATIO CALCULATION-TO-EXPERIMENT FOR PuO₂ SAMPLES

Item	Sample No.				
	2,3,4,5	6	7	8	9
Mass, gm	66 to 67	61.8	31.4	10.1	62.1
Length, in.	3.6 to 3.8	3.5	1.9	0.565	3.5
Outer Diameter, in.	0.37	0.36	0.38	0.36	0.36
Weight Percent Pu ²³⁹ O ₂	91.4	57.8	84.3	1.0	40.7
Weight Percent Pu ²⁴⁰ O ₂	7.9	31.7	13.3	3.7	41.9
Weight Percent Pu ²⁴¹ O ₂	0.66	7.1	2.0	94.0	10.3
Weight Percent Pu ²⁴² O ₂	0.04	3.4	0.4	1.3	6.9
Calculation/Experiment, Core 14	1.02	1.10	—	—	1.10
Calculation/Experiment, Core 15	1.01	—	—	—	—
Calculation/Experiment, Core 16	1.00	1.10	1.29	1.39	1.08
Calculation/Experiment, Core 17	1.06	1.10	1.28	—	1.10

TABLE 7
CALCULATED DOPPLER EFFECT IN U²³⁵ FOR VARIOUS CORES

U ²³⁵ Sample	U Isotope	Mass (gm)	Change in Reactivity, at 300 to 700°K ($\epsilon \times 10^{-5}$)			
			Core 14	Core 15	Core 16	Core 17
Metal Cylinder, OD 1/8 in.	235	12.85	7.8	3.4	1.23	1.04
	238	<u>0.93</u>	<u>-19.2</u>	<u>-7.8</u>	<u>-2.38</u>	<u>-1.45</u>
	Total	13.78	-11.4	-4.4	-1.15	-0.41
Metal Cylinder, OD 1/4 in.	235	55.0	11.4	5.28	2.21	0.49
	238	<u>4.0</u>	<u>-19.5</u>	<u>-7.58</u>	<u>-2.08</u>	<u>-0.62</u>
	Total	59.0	- 8.1	-2.30	0.13	-0.13
Metal Cylinder, OD 0.44 in.	235	170.9	—	6.9	3.14	2.63
	238	<u>12.4</u>	—	<u>-7.8</u>	<u>-2.24</u>	<u>-2.10</u>
	Total	183.3	—	-0.9	-0.90	-0.53
Metal Annulus 0.44 x 0.25 in.	235	109.7	12.0	5.6	2.39	2.00
	238	<u>8.0</u>	<u>-19.5</u>	<u>-7.2</u>	<u>-2.13</u>	<u>-1.95</u>
	Total	117.7	- 7.5	-1.6	-0.26	0.05

Figure 8. U^{238} Doppler Effect Between 300 and 700°K

3. Central Reactivity-Worth Discrepancy

A large number of comparisons between calculated and measured central reactivity worths in a wide variety of fast reactors has shown an average overestimate by the calculations of 17% for strongly reactive materials. The materials included in this average are B^{10} , Ta, U^{235} , U^{238} , Pu^{239} , Pu^{240} , and Pu^{241} . Weakly reactive materials and light-element scatterers are poorly predicted and do not show any systematic effect. Calculations for B^{10} have the smallest dispersion and are closer on the average to the experimental values, while those for Pu^{240} have the greatest dispersion and appear to be significantly less reliable.

Measurements of delayed neutron yields have been reviewed to determine if a systematic error in the reactivity value of the dollar is responsible for the observed discrepancies. Evaluated fractional delayed-neutron yields were determined for Th^{232} , U^{233} , U^{235} , U^{238} , Pu^{239} , Pu^{240} , Pu^{241} , and Pu^{242} . These yields are larger than values customarily used and result in calculated values of β_c that are larger by about 7 to 10%. Use of these evaluated yields reduces the discrepancy to 8.6%.

TABLE 8
DOPPLER EFFECT IN VARIOUS PuO₂ SAMPLES

Sample No.	Pu Isotope	Mass (gm)	Change in Reactivity, at 300 to 700°K ($\epsilon \times 10^{-5}$)			
			Core 14	Core 15	Core 16	Core 17
1	239	53.8	8.1	3.9		
	240	4.7	-31.5	-11.4		
	241	0.4	1.1	0.4		
	242	0.0				
Total		58.9	-22.3	- 7.1		
6	239	31.5	7.4	3.1	1.2	0.9
	240	17.3	-30.0	-12.6	-4.2	-3.8
	241	3.9	9.8	4.0	1.0	0.9
	242	1.9	-12.6	- 4.8	-1.3	-1.0
Total		54.6	-25.4	-10.3	-3.3	-3.0
7	239	23.3			1.45	1.11
	240	3.7			-2.73	-2.52
	241	0.6			0.25	0.22
	242	0.0			-0.16	-0.15
Total		27.6			-1.19	-1.34
8	239	0.1		0.2		
	240	0.3		- 9.4	-1.3	
	241	8.4		22.5	8.4	
	242	0.1		- 2.7	-0.5	
Total		8.9		10.6	6.6	
9	239	22.3	6.7	2.6	0.8	0.6
	240	23.0	-29.2	-12.7	-4.5	-4.1
	241	5.6	12.9	5.3	1.6	1.2
	242	3.8	-15.7	- 6.4	-1.7	-1.6
Total		54.7	-25.3	-11.2	-3.8	-3.9

4. Evaluation of Experiments to Measure the Capture-to-Fission Ratio

An analytical study of integral methods for measuring the effective capture-to-fission ratio in fast-reactor critical assemblies was completed. This study consisted of determining the sensitivity of the results of three different experimental methods for measuring α to errors in certain quantities that are derived analytically. The degree of sensitivity was based upon an analysis that used hypothetical experimental data with reactor calculations having different characteristics. Of the three methods the one used by Redman and Bretscher shows the least sensitivity to errors in the calculations.

D. REVIEW OF DOPPLER MEASUREMENTS

A systematic review of measurements of the nuclear Doppler effect in fast-critical assemblies has been under way for several months. Its first goal is to compare measurements made in similar spectra at different laboratories by analyzing all of them with the same method, and thus to determine whether they are consistent with each other. Once consistency is established, correlation with spectrum and comparisons with theory can be undertaken with greater confidence.

Detailed comparisons of experimental results from different facilities have been inconvenient to make for several reasons such as lack of reactivity normalization and differences in temperature ranges of the experiments. The main reason is probably the inability to express results of a Doppler measurement as a single number or pair of numbers. This results from the fact that the Doppler coefficient of reactivity decreases with temperature, so that its average value depends on the temperature range. Good fits to experimental results are provided by power-law expressions of the form

$$\rho = A + BT^{1-\gamma} \quad , \quad \gamma \neq 1 \quad ; \quad \dots (1a)$$

$$\rho = A + B \ln T \quad , \quad \gamma = 1 \quad ; \quad \dots (1b)$$

where ρ is measured sample reactivity, T is absolute sample temperature, and A , B , and γ are fitting constants. Attempts to compare measured values of the slope constant B are futile, however, because it is such a strong function of the exponent γ : B can vary by a factor of 10 for a 10% change in γ , with no change in quality of fit to the data.

The form chosen to fit Doppler data for this survey is the following:

$$\frac{\rho}{\rho_s} = \frac{\rho_o}{\rho_s} + \frac{CT_o}{1-\gamma} \left[\left(\frac{T}{T_o} \right)^{1-\gamma} - 1 \right] ; \quad \dots (2)$$

here, ρ_s is the measured total room-temperature reactivity of the Doppler sample, T_o is the reference temperature (300°K), and the fitting constants are ρ_o , C , and γ . When this form is used the variation of C with γ is much less than that of the previously defined coefficient B ; for a 10% change in γ , C typically changes by about 5%. This form also approaches the logarithmic form smoothly as γ approaches 1, which the simpler-appearing Equation 1a on the previous page does not. C has a simple physical interpretation; it is the relative reactivity change per unit temperature at the reference temperature, $(d\rho/dT)_o$. Normalization of reactivity changes to the total sample reactivity essentially eliminates differences due to use of different samples and reactors. (The Doppler dependence on S/M is quite weak.) Direct comparisons of the coefficient C measured at different facilities are now possible. These should be done for the same value of γ because of the slight remaining variation of C with γ ; this is an acceptable procedure as long as both measurements of γ agree within statistical uncertainty.

The existing DOPFIT code, written by R. J. Tuttle and used to analyze ECEL Doppler experiments for several years, has been converted for operation on the time-sharing computer and modified to calculate the Doppler coefficient C as discussed above. A method of determining the experimental uncertainty in γ , the Doppler shape parameter, has been developed, programmed, checked out, and added to DOPFIT. It is based on fitting a parabola to a plot of χ^2 (statistical goodness-of-fit parameter) vs γ , in which the other parameters of the fit (ρ_o and C) are adjusted for the best fit at each value of γ . The minimum of the parabola gives the best-fitting value of γ , and the curvature or sharpness of the curve determines the uncertainty. With this method the uncertainty in γ can be determined unambiguously from results of a single experiment. Previous error estimates have been based only on the scatter in gamma values from repeated experiments.

Analysis of Doppler experimental results obtained with ECEL, ZPR-3, and other fast-critical assemblies has now started using the new version of DOPFIT. Two assemblies having spectra similar to an LMFBR spectrum are ZPR-3-48 and ECEL-17. Data to some extent preliminary from Doppler experiments on natural UO_2 samples in these two assemblies have been analyzed with DOPFIT with the results shown in Table 9. The larger errors shown for ECEL-17 are due to the use of a smaller sample, which produces a smaller reactivity signal.

TABLE 9
COMPARISON OF ECEL-17 AND ZPR-3-48
DOPPLER MEASUREMENTS ON
NATURAL UO_2
SAMPLES

γ	$C(10^{-4}/^{\circ}\text{K})$	
	ECEL-17	ZPR-3-48
0.9	2.19 ± 0.19	2.20 ± 0.10
1.0	2.31 ± 0.22	2.33 ± 0.10
1.1	2.42 ± 0.23	2.48 ± 0.11
<u>Best-fit value of γ</u>		
ECEL-17: 1.5 ± 0.6		
ZPR-3-48: 0.94 ± 0.16		

As can be seen from Table 9 the ANL and AI results for natural UO_2 are in very good agreement. Analysis of other experiments is continuing. Comparison of ECEL-18 and ZPR-3-49 results may prove interesting; these assemblies are the sodium-voided versions of the assemblies compared above.

E. PREPARATION FOR FORTHCOMING EXPERIMENTS

The ECEL critical-assembly program is undertaking a series of studies of rodded test regions that provide a good geometrical simulation of conceptual LMFBR cores. During Government Fiscal Year 1970, work in this area centered on the nuclear design of a cylindrical test region composed of pin-type fuel elements laid out in a hexagonal array and on obtaining new hardware and material items for constructing the assembly. The nuclear and mechanical

designs of Na-voided (Core 20) and Na-filled (Core 20N) versions were completed and an application for an amendment to the facility operating license was submitted to the AEC. The application included a request for the possible use of PuO_2/UO_2 as a test-region fuel as well as UO_2 , and was supported by a supplement to the Safeguards Analysis Report in which were described the changes to be made in the existing matrix, the design and safety analyses of future assemblies, and analysis of the potential hazards associated with the use of plutonium.

The major hardware items consisted of the fabrication of a hexagonal matrix system and several pin-type hexagonal fuel elements. The fabrication of two hexagonal matrix systems was completed; one of the units is shown in Figure 9. One matrix system is to be installed in the center of each half of the reactor by removing a 9 x 9-in.-array of the existing 2 x 2 x 36-in.-long square matrix boxes (see Figure 10 for cross-sectional view of reactor matrix face). The seven central hexagonal matrix spaces are designed to accept pin-type fuel elements of the type shown in Figures 11 and 12. During GFY 1970 a total of four fuel elements that have a central hexagonal oscillator channel (2.25 in. across flats) were manufactured and brazed along with a total of 12 fuel elements consisting of a complete array of 271 fuel tubes, each 0.250-in.-diam. Two of the four fuel elements containing the oscillator channel are made up of 210 fuel tubes each 0.281-in.-OD, the remaining two contain 0.250-in.-OD fuel tubes. The 0.281-in.-OD-tubes are designed to accept fuel pins of PuO_2/UO_2 clad in 0.250-in.-OD tubing. For the first series of experiments in GFY 1971 these fuel elements will not be filled with Na. Subsequently the experiments will be repeated under Na-filled conditions.

Fabrication of 360 kg of 15%-enriched UO_2 fuel pellets was begun by a vendor, and by the end of the fiscal year a total of 120 kg of UO_2 powder was produced from UF_6 gas. The powder will be used to make pellets $0.215 \begin{Bmatrix} +0.000 \\ -0.006 \end{Bmatrix}$ in. in diameter by 0.40 ± 0.04 -in. long. These pellets will be inserted into the 3672 fuel tubes to form a cylindrical pin-type test region with an active core height of about 32 in. and an equivalent diameter of about 17.2 in. A 12-in.-high axial blanket of depleted- UO_2 pellets that are already on hand will be installed on each end of the pin-type test region.

In the transition zone of the hexagonal-matrix system and in the square-matrix boxes outside the hexagonal region will be placed standard plate-type fuel in order to form a fast-spectrum buffer zone. Outside the buffer zone will be a

Figure 9. Hexagonal Matrix System

Figure 10. Core-Loading Diagram, Core 20N

6-18-70

Figure 11. Pin-Type Hexagonal Fuel Element for Oscillator Measurements

7701-4030

END VIEW

FULL ASSEMBLY HAS 271 TUBES;
TEST ASSEMBLY HAS THE CENTRAL
61 TUBES REMOVED.

TUBE PATTERN

SIDE VIEW - CENTRAL ASSEMBLY

SIDE VIEW - FULL ASSEMBLY

Figure 12. Hexagonal Fuel Assemblies

7701-4526

cylindrical shell of plate-type slightly enriched (1.88%) U metal that will serve to decouple the fast-spectrum region from the thermal driver and also represent a "burned" radial blanket. Tables 10, 11, and 12 show some physical characteristics of the sodium-filled core relative to the various zones shown in Figure 10. Other materials required for the cores containing pin-type fuel elements were manufactured during the fiscal year. For example, the fabrication of 4,300 of the 1.88% enriched-U metal plates was completed by shearing some existing 5 x 18-in. metal-plate stock. Some 20%-enriched metal plates were also prepared to augment existing material for the buffer zone, and 10,000 U/Al-alloy plates were rolled out and cut to increase the fuel inventory for the driver region for Core 20.

To determine the void-fraction which will occur during the process of filling the pin-type hexagonal fuel elements with Na, a 2-by-2-by-36-in.-long pin-type test element was filled using a pouring technique. From weight and volume measurements it was determined that a 0.13 void-fraction occurred. This void-fraction would be acceptable for the full-size elements.

III. EVALUATION OF EFFORT DURING FISCAL YEAR 1970

The analyses carried out on experiments dealing with the reactivity worths of tantalum have proven to be very useful in reducing the uncertainty in the calculated-reactivity control associated with typical Ta FBR control rods. It has been shown that a single calculational technique for predicting the worths of all of the various Ta samples is not adequate, but by using different techniques applicable to different surface-to-mass regions one is able to predict the experimental results to an uncertainty of $\pm 10\%$.

This improvement between the calculated and experimental values leads to increased confidence in the calculation of the degree of control afforded by control rods in a typical FBR. New investigations into other absorber materials such as Eu_2O_3 have indicated the possibility of developing more efficient control rods that have reduced mass and heating rates.

Attempts to measure the heating rates in Ta control rods have not been particularly successful using the TLD detector method. Although some of the

TABLE 10
CORE 20N COMPOSITION

Region	Atom Densities (10^{24} atom/cm ³)										
	U ²³⁵	U ²³⁸	Oxygen	Sodium	Aluminum	Carbon	Hydrogen	Thorium	Iron	Chromium	Nitrogen
Test 1	-	-	0.0000084	-	-	-	-	-	-	-	-
Test 2	0.0009132	0.0051096	0.012046	0.010869	-	-	-	-	0.014559	0.0038035	0.0014972
Test 3	0.0010070	0.0056346	0.013284	0.010618	-	-	-	-	0.012818	0.0033488	0.0013182
Buffer 1	0.0010375	0.0052740	-	-	0.012349	0.008301	-	-	0.014843	0.003876	0.001705
Buffer 2	0.0011053	0.006985	-	0.0035027	0.013899	0.0076266	-	-	0.013354	0.003532	0.0019093
Decoupler 1	0.0007180	0.03692	-	-	0.004905	-	-	-	-	-	0.002330
Decoupler 2	-	-	-	-	0.004905	-	-	0.026435	-	-	-
Driver	0.00018889	0.000013745	-	-	0.014076	0.025066	-	-	(	0.0037211	)
Reflector	-	-	-	-	0.0063124	0.032154	0.064308	-	(	0.0024957	)

TABLE 11
CORE 20N ISOTOPIC ATOM DENSITIES, AXIAL REFLECTOR

Region	Atom Densities (10^{24} Atom/cm ³)									
	U ²³⁵	U ²³⁸	Oxygen	Sodium	Aluminum	Carbon	Iron	Chromium	Nickel	Hydrogen
Test 2	0.000012992	0.0058208	0.012046	0.010869	-	-	0.014559	0.003803	0.001497	-
Test 3	0.000014763	0.0066142	0.013284	0.010618	-	-	0.012818	0.00334	0.001318	-
Buffer 1	0.0000438	0.0060733	-	-	0.011148	0.0092584	0.016449	0.004296	0.001933	-
Buffer 2	0.0000414	0.0057191	-	-	0.020195	-	0.09867	0.002577	0.01370	-
Driver	-	-	-	-	0.0063124	0.032154	-	0.002496	-	0.064308

TABLE 12
NUCLEAR PARAMETERS OF CORES 20 AND 20N

Parameter	Value	
	Core 20	Core 20N
Fissile Inventory of Critical Core, kg U ²³⁵ :		
Test	46.01	46.01
Buffer	78.23	78.67
Decoupler	41.27	41.27
Driver	20.13	21.35
Fission Distribution, %:		
Test	3.6	3.4
Buffer	7.1	6.4
Decoupler	6.7	5.9
Driver	82.6	84.3
Central (Test-Region 2) Median Fission Energy, keV	127.0	78.4
Safety-Rod Worth (8 rods), % $\Delta k/k$	8.5	
Regulating-Rod Worth (2 rods), % $\Delta k/k$	0.35	
Reactivity-Insertion Rates, % $\Delta k/k$ -sec:		
Safety rod	0.02	
Regulating rod	0.01	
Fuel-Assembly Expansion Worth, % $\Delta k/k$	14	
Edge-Drawer Worth, % $\Delta k/k$	0.15	
Driver-Buffer Drawer Exchange Worth, % $\Delta k/k$ -drawer	0.1	

difficulties are at present related to problems in reading the small Li⁷F powder samples and the samples of Li⁷F dispersed in Teflon, the method may not be capable of achieving good accuracy. With the present TLD detector readout system, well-defined and reproducible glow curves are obtained with rod-type Li⁷F detectors, but analytic corrections for the rod thickness must be made and this correction produces somewhat large uncertainties. With the acquisition of another type of TLD reader attachment, improvements in capabilities in this area are expected.

The recently completed evaluation of delayed-neutron parameters along with a systematic and extensive review of the reactivity worth of a very large number of absorber samples that have been measured in a wide variety of foreign and domestic critical assemblies have proven most useful in obtaining an overview of the present central reactivity-worth discrepancy. It is particularly noteworthy that, even though many different cross-section sets and calculational codes were used by the various investigators the ratio of the calculated to the measured worth is remarkably consistent at around 1.17. The standard deviation about this ratio is ± 0.01 . By applying the evaluated delayed-neutron data this ratio could only be reduced to about 1.08, thus implying that another fundamental cause of the discrepancy exists. Calculations carried out relative to ECEL reactivity-worth measurements yield results in good agreement with the 1.17 ratio and also show that the sample size is not an important parameter relative to the discrepancy.

The systematic review of both foreign and domestic Doppler data has thus far shown that reasonably good consistency exists in the measurements of the Doppler effect of the same type of samples in different reactors with similar spectra. This seems to indicate that, as would be expected, the Doppler measurements are not dependent on the reactor being used. This review is expected to produce a consistent set of Doppler parameters for use by reactor designers.

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Program: Reactor Physics

AEC Task: 5-E, Theory and Computation for Reactor Analysis and Design

Project Manager: H. A. Morewitz

Reporting Period: Government Fiscal Year 1970

General Order: 7701

Subaccount: 14320

AEC Category: 04-01-61-02.1

Principal Scientists: L. B. Levitt, J. Spanier

I. OBJECTIVES

The basic objective of this project is to advance the state-of-the-art of Monte Carlo Applications to the analysis of fast reactors and fast-critical assemblies. This development is needed so that experimental programs as well as design studies may be optimized through the use of computer programs capable of describing complicated geometric configurations while calculating the effects of localized perturbations. These objectives will manifest themselves in the ultimate development of fast-reactor criticality codes and specialized codes to treat perturbations due to changes in temperature, density, and material composition. The objectives of this project are related to Tasks 9-3.3 and 9-4.5 outlined in WASH-1109, LMFBR Program Plan, Volume 9, Physics.

II. TECHNICAL PROGRESS DURING FISCAL YEAR 1970

Work during GFY 1970 concentrated in the following areas:

- 1) Completion and checkout of the VIM code for fast-critical assemblies.
- 2) Completion of a body of effort concerned with efficient adjoint sampling techniques.
- 3) Formulation of efficient methods for calculating perturbations by Monte Carlo.
- 4) Development of a new multistage procedure for systematic variance reduction in Monte Carlo.

Coding and checkout of the VIM code was completed by February 1970 and was followed by benchmark calculations of GODIVA, JEZEBEL, ZPR-3-48,

and ZPR-3-11. Novel features of VIM which were developed during GFY 1970 include (1) a simplified procedure for sampling the spatial distribution of source neutrons, (2) a new treatment of unresolved resonances which is more economical than others, (3) a data-packing scheme which permits complete point cross-section data sets for many isotopes to be stored simultaneously in high-speed core memory, and (4) the use of an estimator which allows a variable amount of absorption weighting at each collision. Comparison of the benchmark VIM calculations with more conventional Monte Carlo and S_N calculations showed good agreement and indicated that a non-multigroup Monte Carlo code such as VIM is a useful tool in analyzing fast-critical assemblies. Work on VIM was reported at the June 1970 meeting of the American Nuclear Society in Los Angeles.⁽¹⁾

The Monte Carlo fast-critical assembly code VIM-1 has been completely debugged and has satisfactorily passed every checkout test to which it has thus far been subjected, including several benchmark critical-assembly calculations. VIM-1 was subjected to extensive checkout using ZPR-3-48, ZPR-3-49, ZPR-3-11, JEZEBEL, and GODIVA as test cases. Analytic calculations using the CAESAR code were made for some of these assemblies, using a multigroup version of the same library used by VIM. These calculations with an estimated transport-theory correction were used as a basis for evaluating VIM results. To make this evaluation valid, variants of VIM were written to handle benchmark spherical and cylindrical mockups of these assemblies. These variants are identical with VIM-1 except for the geometric tracking and zone-location routines.

The ZPR-3-48 test case was run in five distinct ways:

- 1) Heterogeneous, as-built, using standard core drawers, control drawers, and safety drawers. (Total of 334 drawers, including 8 safety and 2 control drawers).
- 2) Heterogeneous, using standard core drawers only, but with additional peripheral drawers to compensate for fuel spiking in control and safety drawers.

- 3) Homogenized into three regions: core, axial reflector, and radial reflector; but using as-built compositions and retaining core and reflector outlines.
- 4) Homogenized as above but using compositions based on use of standard core drawers only.
- 5) Benchmark spherical mockup (a two-region spherical representation using compositions as given by Hess for benchmark calculations).

Table 13 contains a brief summary of eigenvalue calculations made with VIM-1. They should be regarded as preliminary since they were not made with the latest ENDF/B data. The calculations do, however, indicate that a non-multi-group fast-critical-assembly Monte Carlo code can now be used as a tool for analyzing fast-critical experiments, and that benchmark calculations can now be performed at moderate cost using standardized sets of heterogeneous input data. Overall computing times can be seen to vary considerably from one assembly to another. The spherical mockup of JEZEBEL requires a little over 4 min for 50,000 neutron histories on the CDC 6600, with a probable statistical error in k_{eff} of 0.004. At the other extreme the heterogeneous mockup of ZPR-3-48 will run at the rate of 30,000 histories per hour, with a probable statistical error of 0.005 in that time.

Table 14 gives a comparison of results for ZPR-3-48 using VIM-1 with a CAESAR diffusion-code run.

Note that no significant differences were observed in k_{eff} among the three Monte Carlo results but they were about 2% higher than the diffusion calculation (CAESAR).

While no significant differences were observed in k_{eff} , major differences were observed in core-to-blanket neutron-production ratios and the breeding ratio. Comparison with CAESAR diffusion-theory showed that in all cases the results of the spherical benchmark calculations were closer to those of CAESAR calculations than were the results of the heterogeneous representation or any of the others tried.

TABLE 13
VIM-1 EIGENVALUE CALCULATIONS

Assembly	Number of Histories	k_{eff}	(CDC 6600) Computer Running Time (sec)
GODIVA	50,000	1.012 ± 0.004	300
JEZEBEL	50,000	1.015 ± 0.004	240
ZPR-3-11 Benchmark (spherical mockup)	19,600	1.010 ± 0.005	775
ZPR-3-48 Benchmark (spherical mockup)	50,000	1.003 ± 0.004	3510
ZPR-3-48 (heterogeneous, using control and safety drawers as in the actual experiment)	25,600	1.004 ± 0.005	3150
ZPR-3-48 (homogenizing core)	25,600	1.001 ± 0.005	2280
ZPR-3-48 (heterogeneous, using standard core drawers only, adding extra drawers to compensate for fuel spiking in control and safety drawers)	25,600	0.991 ± 0.006	3200
ZPR-3-49 (heterogeneous, using actual experimental drawer loading)	25,600	1.001 ± 0.007	3110

TABLE 14
ZPR-3-48 COMPUTED RESULTS

Approximation	k_{eff}	$\frac{\sigma_f(\text{Pu}^{239})}{\sigma_f(\text{U}^{235})}$	Breeding Ratio	Core/ Blanket Neutron Production	Core/ Blanket Absorption	Core/ Blanket Flux	Leakage	Fissile/ Fertile Neutron Production
Heterogeneous As-Built Representation (VIM-1)	1.004	0.970	1.79	6.11	1.18	1.99	0.0296	2.88
Homogeneous Representation Based on As-Built Compositions (VIM-1)	1.001	0.975	1.82	5.48	1.15	1.95	0.0306	2.68
Spherical Benchmark (VIM-1)	1.003	0.971	1.69	6.38	1.32	2.26	0.0462	2.98
Diffusion Theory (CAESAR)	0.983	0.940	1.71	8.98	1.34	2.28	0.0450	3.79

Two categories of results appear to be emerging from this comparison:

- 1) Geometric effects, in which the major differences occur between the spherical representation and the other representations rather than between Monte Carlo and diffusion theory. The breeding ratio falls into this category.
- 2) Effects in which the major differences occur between Monte Carlo and diffusion-theory approaches to the solution of the problem, rather than from differences in the geometric representation. The parameters, k_{eff} , central fission ratio of $\sigma_f \text{Pu}^{239} / \sigma_f \text{U}^{235}$, and ratio of fissile/fertile neutron production fall into this category. All of the Monte Carlo calculations are in good agreement, differing sharply from the diffusion results.

This tends to show that even when a spherical representation correctly predicts the eigenvalue it may be quite misleading on other important design parameters. Examining the core-to-blanket ratios and the leakage shown in Table 14 we can see further evidence of this.

Here we clearly see the close agreement between the two spherical representations on leakage, core/blanket flux and absorption, differing sharply from the nonspherical representation. On the other hand, on core/blanket neutron production, diffusion-theory predicts a significantly higher value than does any of the Monte Carlo calculations.

An explanation for this difference may be found by examining the integrated spectra. A major difference observed between all the Monte Carlo and CAESAR calculations is the much larger flux in the blanket above 1 Mev in the former. A possible explanation for this lies in the more detailed treatment of angular data by VIM-1. This results in a much greater U^{238} fission rate and is sufficient to explain the 2% eigenvalue difference observed between Monte Carlo (1.003) and diffusion-theory (0.983). The estimated transport-correction to diffusion-theory is only 0.006. The remainder of the difference between Monte Carlo and transport theory is what appears to be a result of the differences in treatment of the angular data.

Spectral indices and leakage spectra calculated for JEZEBEL and GODIVA are shown in Tables 15 and 16.

TABLE 15
JEZEBEL DATA

Leakage Spectrum				Central-Fission Ratios		
Group No.	Lower Lethargy Limit	Experimental (%)	VIM-1 (%)		Experimental	VIM-1
1	0.5	3.1	2.7	$\frac{\sigma_f(U^{238})}{\sigma_f(U^{235})}$	0.205 ± 0.008	0.207 ± 0.002
2	1.0	11.7	10.9			
3	1.5	17.7	19.5			
4	2.0	20.0	20.8			
5	2.5	16.5	18.5	$\frac{\sigma_f(Pu^{239})}{\sigma_f(U^{235})}$	1.49 ± 0.03	1.40 ± 0.004
6	3.0	13.6	12.3			
7	3.5	9.7	7.6			
	Total	92.3	92.3			

TABLE 16
GODIVA DATA

Leakage Spectrum				Central-Fission Ratios		
Group No.	Lower Lethargy Limit	Experimental (%)	VIM-1 (%)		Experimental	VIM-1
1	0.5	2.0	1.7	$\frac{\sigma_f(U^{238})}{\sigma_f(U^{235})}$	0.156 ± 0.005	0.177 ± 0.002
2	1.0	7.1	8.2			
3	1.5	13.6	16.2			
4	2.0	16.8	20.4			
5	2.5	18.0	19.0	$\frac{\sigma_f(Pu^{239})}{\sigma_f(U^{235})}$	1.42 ± 0.02	1.37 ± 0.004
6	3.0	18.8	15.2			
7	3.5	11.5	9.9			
8	4.0	8.0	5.2			
	Total	95.8	95.8			

The UNICORN⁽²⁾ and DOPCRS⁽³⁾ codes were converted from the IBM 360/50 to the CDC 6600 and then combined into the UNIDOP code for use on the CDC 6600. The dimensioning of the UNIDOP code was increased to allow calculations involving up to 210 resolved-resonances and up to 6500 energy points. The modified version of UNIDOP was used to generate Doppler-broadened point cross-sections in the resolved-resonance regions for U²³⁸, Pu²³⁹, and Pu²⁴⁰ using ENDF/B (Version 1, January 1969) resonance parameters. These cross-sections were used to update the VIM cross-section library tape which previously was based on AI resolved-resonance parameters. These AI parameters were used initially because they were in a format which allowed them to be used easily and quickly, and they could be processed by existing AI codes to produce point cross-section values usable by the VIM code during the initial checkout of the code.

VIM-1 cross-section library preparation for the ZPR-3-48 test case was completed. Smooth cross-sections for U²³⁵, U²³⁸, Pu²³⁹, Pu²⁴⁰, Pu²⁴¹, C, Na, Fe, Ni, Cr, Al, and Mo were obtained from ENDF/B tapes and reformatted for use in generating the VIM-1 cross-section tape.

A Monte Carlo sampling procedure was developed to sample fission-neutron energies from a spectrum of the form:

$$f(E) = \frac{2}{k^{3/2} \sqrt{\pi}} E^{1/2} e^{-E/k} ,$$

where E is in electron volts.

Stratified sampling of neutron-source energies has been incorporated into VIM-1 to ensure that the selected energies are an adequate representation of the input distribution. The number of energy bands to be sampled with equal frequency is input as NEF. The energy boundaries are determined as follows:

$$\int_0^E f(E) dE = \frac{2}{(kT)^{3/2} \sqrt{\pi}} \int_0^E E'^{1/2} \exp(-E'/kT) dE' = \frac{\gamma\left(\frac{3}{2}, \frac{E}{kT}\right)}{\Gamma\left(\frac{3}{2}\right)} = P\left(\frac{2E}{kT} / 3\right) ,$$

where $P(\chi^2/\nu)$ is the probability integral of the χ^2 -distribution.

A more general version of subroutine UNRES for the optional use of self-shielded smooth cross-sections in the unresolved resonance region was incorporated into VIM-1. The coding changes required for the addition of flux monitoring and the calculation of spectral indices to the heterogeneous and spherical versions of VIM-1 were made and checked out. The required input for VIM-1 was reviewed and a number of arrays are now computed in the code rather than input; this simplifies input data preparation for the user of the code. A statistics package was put into VIM-1 and checked out.

A new method for treating cross-sections in the unresolved resonance region has been devised. When properly implemented it will permit full use of available information without resorting to analytic approximations to account for heterogeneity effects, while requiring relatively little storage. The method appears to have enough promise to warrant its development. The procedure for processing the unresolved data into probability tables for Monte Carlo selection has been outlined and codes to execute this have been programmed but as yet have not been tried.

A seminar on the use of VIM-1 for ZPR and ZPPR assemblies was held at the EBR-2 site of the National Reactor Test Station in Idaho.

A detailed review of adjoint Monte Carlo methods was undertaken to aid in preparation of a review paper on Monte Carlo methods. Material from several major articles on this subject is being combined and restated in one common notation. A review has been made of recent work on Monte Carlo perturbation methods and the methods combined with some new ideas both for the review article and to form a basis for further work on perturbation methods during next fiscal year.

A method was developed for increasing the efficiency of non-multigroup adjoint Monte Carlo calculations, based on a transformation of the adjoint equations by means of a discontinuous importance function. While the technique is particularly useful for solving slowing-down problems below the threshold for inelastic scattering it applies in the presence of inelastic scattering as well. The technique was described in Reference 4 and further comments about its applicability will appear in Reference 5.

Accurate Monte Carlo estimates of sodium-void coefficients and for similar perturbation calculations require nonstandard Monte Carlo techniques. Various ideas for increasing the efficiency of Monte Carlo perturbation calculations have been investigated. These ideas are based on the introduction of some degree of correlation between the unperturbed and perturbed simulations. In the simplest case this is accomplished merely by controlling the random-number sequence itself. More sophisticated methods for introducing correlation involve combining the perturbed and unperturbed simulations into a single simulation in which different weights are used to reflect the influence of the perturbation. Adjoint calculations should play a major role in implementing such techniques.

A rather long-term effort aimed at systematic variance reduction has given rise to a new idea quite recently. The idea is to take advantage of the possibility of estimating very efficiently the dependence of the Monte Carlo variance on various parameters introduced to lower the statistical uncertainty. A method has been discovered for accomplishing this in several short initial stages of the Monte Carlo simulation. The basis for the idea is that the parametric dependence of the variance may be estimated in a perfectly correlated way. The method is described in Reference 6, which also describes a successful application of the theory to the optimization of exponential transformation in deep-penetration calculations. The idea for systematic variance reduction offers great potential for increasing the cost-effectiveness of a wide variety of Monte Carlo calculations.

DOCUMENTATION. The following reports and papers were issued during the report period:

"VIM-1, A Non-Multigroup Monte Carlo Code for Analysis of Fast Critical Assemblies," AI-AEC-12951 (May 15, 1970)

"Monte Carlo Eigenvalue Calculations of Fast Critical Assemblies Using VIM-1," Trans. ANS 13, 194-195, June 28, 1970

III. EVALUATION OF EFFORT DURING FISCAL YEAR 1970

The successful checkout of VIM-1 establishes that a non-multigroup fast-critical assembly Monte Carlo code can now be used as a tool for analyzing fast-critical experiments and that benchmark calculations can now be made with standardized sets of heterogeneous input data. Even large critical assemblies such as ZPR-3-48 need not be run longer than 1 hr on the CDC 6600 to evaluate major reactor parameters such as k_{eff} , integrated group fluxes, and central-fission ratios. We are now able to proceed to more difficult calculations of such quantities as central-rod worths, activation ratios, and void coefficients with the confidence that the basic data-handling, source generation, and collision procedures are correctly and efficiently doing the tasks for which they were designed. ANL Idaho is being assisted in using VIM-1 as part of their experimental analysis procedure. It is expected that the feedback from outside users will enable us to achieve maximum simplicity of input preparation as well as expert guidance in the choice of experiments involving reactivity perturbations to be studied by later versions of VIM.

The possibility that calculations of large critical assemblies may be more sensitive to the treatment of the angular data than first believed, as indicated in the study of ZPR-3-48 using VIM-1, shows clearly the value of Monte Carlo as an analytic aid in preparation of group data and in determining the degree of sophistication required in non-Monte-Carlo design studies, in addition to its use as an independent design tool.

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Program: General Reactor Physics		
AEC Task: 26-A, Cross-Section Analysis		
Project Manager: H. A. Morewitz		
Reporting Period: Government Fiscal Year 1970		
General Order: 7762	Subaccount: 13130	AEC Category: 04-04-01-03.1

Principal Scientists: H. Alter, C. L. Dunford

I. PROJECT OBJECTIVES

The objectives of this project are the production and maintenance of an up-to-date set of basic nuclear data, the production and evaluation of multigroup constants, and the improvement of present-day methods of neutronic calculations as related to micro- and macroscopic nuclear data. To accomplish these objectives, existing experimental and theoretical information on nuclear data will be surveyed, analyzed, and compiled. Automated methods will be provided to periodically update compiled data, and nuclear-model calculations will be developed and used to help fill gaps in the data. An automated system will be developed and maintained for the ready production of multigroup constants. Spectra-generating techniques for production of realistic multigroup constants will be developed and incorporated into the system. The data and methods produced are needed to improve reliability for calculating advanced reactor concepts. In particular the realization of these project objectives will be used in ensuring that the LMFBR design incorporates adequate margins for safety and economy. The accomplishment of the stated project objectives is related to successful implementation of the LMFBR Program Plan in the areas of acquisition of nuclear data (Task 9-1), cross-section evaluation (Task 9-1.2), and compilation and distribution of evaluated data (Subtask 9-1.2.2).

II. TECHNICAL PROGRESS DURING FISCAL YEAR 1970

A. INTERACTIVE COMPUTER GRAPHICS

Considerable effort has been expended during the past year to improve the operating characteristics of the SCORE system. In all places where it was possible, "type-in" data entry has been replaced by list selection. List selection

by the light pen is a more natural way of selecting from many alternatives and removes the requirement that the user remember what the alternative selections are. The use of list selection to replace type-in information has been applied to nuclide- and reaction-type selections.

In areas where response time to user action could be improved by making only minor modifications to a display, new incremental graphic routines were used. These subroutines allow the programmer to update small blocks of instructions at any place in the 2250 buffer memory without having to regenerate the orders for the entire display. A most remarkable increase in response time has been realized by the use of incremental update to change option lists on the data displays. The delay has been cut from one or two seconds to essentially none.

With the use of the full extent of overlay capability, SCORE can now be carried out with a maximum requirement of 125 K-bytes of memory. This is a reduction of about one-third in core requirement and this improves the economies of using the system. Some reorganization and recoding were required so that the new overlay structure did not cause an increase in normal response time to a user request.

The flexibility of the Legendre-coefficient calculations for angular-distribution data has greatly improved by permitting the evaluator to select the order of fit required. After it is selected, an expanded data display (Figure 13) appears showing the evaluated curve and the Legendre curve as well as a listing of all the coefficients.

The resonance-region analysis module has been revised to provide extended capabilities to the data evaluator. Three resonance-region models, Breit-Wigner, Reich-Moore, and Adler-Adler, are now available. A new resonance-library format has been designed using the direct-access retrieval method. Parameters for 25 different nuclides for each of the three resonance models may be stored in this data set. Each spin sequence (g-value) for a nuclide is stored as a separated nuclide.

In addition the resonance library can store a maximum of ten resolution and ten Doppler functions for each model. The evaluator may select any combination of these when analyzing resonance-region data.

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DIFFERENTIAL INELASTIC SCATTERING NO. 8

E = 3.97000E 00 Q = -2.98000E 00

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Figure 13. Differential Inelastic Scattering Cross-Section

An improved version, written at Idaho Nuclear, of the automated fitting code SAP for single-level and Reich-Moore multilevel analysis has been included in the SCORE system. The current program replaces a preliminary version of that same code. At the present time there are no automated fitting procedures for the Adler model, but the outline of methods for accomplishing that task have been completed.

To aid in the checkout of the interactive graphics program, a simulation program was developed. This program is designed to eliminate the need for a 2250 while testing graphics subroutines. Interactive input is simulated by card input to the simulator. The output consists of hard copy of all displays which would normally be generated on the 2250 and a hexadecimal listing of the orders which would generate the display. This program has proven to be very useful when doing preliminary checkout, but is rather awkward to use for large interactive graphics systems. A useful byproduct of the completion of this graphic simulator system has been the generation of a program to translate a 2250 buffer load into orders for an SC 4020 or a CI 120 hard-copy display device. With minor modifications this subroutine can be used in SCORE to do the same task.

B. MICROSCOPIC CROSS-SECTION DATA EVALUATION

A re-evaluation of neutron cross-section data for uranium-235 in the energy range $15 \text{ keV} \leq E \leq 15 \text{ MeV}$ was completed. These data were checked, found to be free of mechanical error, and forwarded to the National Neutron Cross Section Center (NNCSC) at Brookhaven National Laboratory for placement on the revised ENDF/B data file. For this evaluation the energy grid ($E \geq 15 \text{ keV}$) associated with the original ENDF/B U²³⁵ smooth elastic-scattering cross-section was chosen as a base for interpolating all other cross-sections. The interpolation modes for the several cross-section reactions are given in Table 17.

For neutron energies above 15 keV, Davey's evaluated fission cross-section data^(7,8) were adopted. These data were similarly interpolated to the base energy grid.

The data of de Saussure,⁽⁹⁾ Weston,⁽¹⁰⁾ Diven,⁽¹¹⁾ and Hopkins⁽¹²⁾ were considered in evaluating alpha between 15 keV and 1 MeV. These data are plotted along with evaluated-data curves in Figure 14. The uncertainty on all these

Figure 14. Alpha for Uranium-235

TABLE 17
INTERPOLATION MODES FOR SEVERAL
U²³⁵ CROSS-SECTIONS

Reaction	σ	E
Total	linear	logarithmic
Capture	logarithmic	logarithmic
Fission	linear	logarithmic
Inelastic	linear	linear
n,2n; n,3n	linear	linear
Alpha	linear	logarithmic

data points is between 10 and 15%. The solid line on Figure 14 is the new recommended alpha curve for U^{235} . The dotted line indicates the Schmidt evaluation⁽¹³⁾ where it deviates from the new evaluated curve. The present alpha evaluation is summarized as follows:

<u>Energy Region (kev)</u>	<u>Description</u>
15 to 40	Schmidt Evaluation
40 to 60	Smooth joining of new and Schmidt
60 to 200	5 to 7% higher than Schmidt
200 to 400	Smooth joining of new and Schmidt
400 to 10,000	Schmidt Evaluation
10,000 to 15,000	Smooth continuation of Schmidt Evaluation

The alpha curve over the full energy range is given in Figure 15. These alpha values were combined with Davey's fission-data evaluation, between 15 kev and 10 Mev, to generate new values of the capture cross-section.

Following suggestions at the second BNL meeting (August 11, 12, 1969) of the Task Force on re-evaluation of ENDF/B fissile/fertile nuclide neutron cross-sections, modifications to the AI re-evaluation of uranium-235 were made. In particular, above 10 Mev the U^{235} fission cross-section was taken from the measured data of Henkel, Nobles, and Smith as corrected by Hansen and McGuire.⁽¹⁴⁾ These values replace the tables published in WASH-1074, pp. 77 and 78, 1967. The capture cross-section was then obtained by multiplying the fission data with alpha, and as before the remaining partial cross-sections were summed and subtracted from the original U^{235} total cross-section to obtain new values for elastic scattering.

Comparisons of the original and re-evaluated cross-section data for elastic scattering, capture, and fission are shown in Figures 16, 17, and 18. The Version 1 (original) data are represented by the open circles and Version 2 (re-evaluated) by the asterisks.

Phase I data testing for the isotopes of hafnium and rhenium contained in ENDF/B Version 1 was completed. For the hafnium isotopes the source of the major fraction of inaccuracies was the angular-distribution data of File 4.

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Figure 15. Full Energy Range, Uranium-235 Alpha

Figure 16. Elastic-Scattering Comparison, U²³⁵ ENDF/B

Figure 17. Radiative-Capture Comparison, U^{235} ENDF/B

Figure 18. Fission-Cross-Section Comparison, U^{235} ENDF/B

Legendre data, when used to generate differential elastic-scattering cross-sections, produced negative values at a number of energy points. Inadequate interpolation schemes appeared to be another source of errors encountered. A letter detailing the omissions and inaccuracies discovered as a result of this evaluation was sent to the NNCSC.

A review of the requests for measurements of reaction cross-sections was completed by the Fast Neutron Reaction Cross Sections and Thresholds Subcommittee of the Neutron Cross-Section Advisory Committee. The subcommittee review covered the pertinent portions of the U. S. Compilation of Request for Nuclear Cross Section Measurements, and appropriate status comments were supplied to aid the requestors. A recommendation for specific measurements to be carried out over the next five years to meet the high-priority needs of the U. S. applied-nuclear-energy program was submitted to the NCSAC.

1. Evaluation of Tantalum and Tungsten Isotopic Cross-Sections

A survey of the SCISRS I files for data relating to the evaluation of the tantalum isotopes was completed. This survey showed that:

- 1) Experimental data covering the neutron-energy range of interest are available for the total and radiative capture reactions only.
- 2) A large number of measurements have been made since the time of the last ENDF/B evaluation (1965).
- 3) The separate SCISRS files for natural tantalum (99.988% Ta¹⁸¹) and Ta¹⁸¹ should be merged into one file. This was done.

A review of tantalum referenced data on the CCDN file (European Data Center), references in the CINDA bibliography and search of the literature showed that several data sets (old and recent) are not yet available through SCISRS. These data are being requested and obtained directly from the originating laboratories. Upon receipt the format of the data will be restructured and then merged into the SCISRS files. This is an appreciable task since some of the data sets contain up to 8000 data points.

The tantalum evaluation by Hart (UKAEA) was requested and received. It will be converted to the ENDF/B format for comparison purposes using the computer program UKE. Similar survey and compilation operations for the tungsten isotopes are well along.

An evaluation of available Ta^{181} total, n-gamma, n-alpha, and n-2n cross-section experiments has been completed. This involved tabulation (and frequently estimation) of standards used for normalization, energy resolution of the impinging neutrons, statistical accuracy and systematic errors for the values determined, and sample thicknesses. Evaluations for the remaining Ta^{181} reactions as well as for the reactions in the several tungsten isotopes are continuing. Evaluation of the Ta^{181} (n,alpha) cross-section was completed. Few data were available and virtually none on the SCISRS tape. A recommended curve has been selected based on an eyeball average of sparse data. However, the fission-spectrum average of this curve is extremely sensitive to the low-energy tail where no data are available (Figure 19); consequently, theoretical cross-section calculations may be required. Documentation of this reaction evaluation was also completed.

The Ta^{181} (n,2n) cross-section was evaluated from several points of view. From the standpoint of the reactor neutronics there is only one component: the Ta^{181} (n,2n) reaction. From an engineer's viewpoint there are the Ta^{181} (n,2n) Ta^{180} ground-state and the Ta^{181} (n,2n) Ta^{180} meta-state reactions. As preliminary analysis shows that the Ta^{181} (n,2n) Ta^{180} meta-state cross-section approaches the nonelastic cross-section, we conclude that meta-state formation predominates.

The engineer is also interested in the decay radiation and daughter products of Ta^{180} meta-state. This information is not supplied in ENDF/B but is required to accomplish the evaluation from the experimenter's point of view. The experimenter must measure some quantity to deduce a cross-section. For the Ta^{181} (n,2n) reaction this can be electrons, positrons, photons, or neutrons. When one adjusts the results of two early electron-counting experiments to more-recent electron-yield data from Ta^{180} , they come into much better agreement with the photon- and neutron-counting experiments. One remaining problem is a recent electron-counting experiment by Borman et al at the University of Hamburg. A similar adjustment to this data is needed to obtain agreement but the electron-yield data assumed were not given. An inquiry to these workers for details on their experiment has been made.

A fourth point of view involves the interaction mechanism: compound-nucleus formation vs direct interaction. The importance of considering these

Figure 19. Influence of Cross-Section Tail on the Fission-Spectrum Integral

alternatives lies first in the desire to fill in data gaps. Below 12.5 Mev no measurements have been made. The threshold for the reaction is 7.68 Mev. Second in importance is the isotropy and energy distribution of the secondary neutrons. Direct interactions tend to retain the incident neutron energy and direction. Unless extensive calculations are made, our knowledge on this subject is limited to the estimate by Rosen and Stewart (LASL, 1957): direct interaction is about 10 to 15% of the total reaction. This is at least consistent with a 50% role in the $\text{Ta}^{181}(n, \alpha)$ reaction at higher energies. Our reliance on this limited information is somewhat tenuous.

Figure 20 illustrates the absolute cross-section measurements in the energy range where data from all experiments are given. Here all the β^- -counting measurements have been corrected to the same recent estimate (we have assumed that the Borman experiment, $\beta^-(68)$, required this adjustment). Examination shows that all the electron-measured cross-sections agree well. In fact the only disagreement is with the 1957 neutron-counting measurement of Ashby and the 1960 activating measurement of Poularikas. The latter is highly suspect for two reasons: (1) the Poularikas paper only mentions this work as an aside with no details; (2) the measurement occurs at an energy above the $\text{Ta}^{181}(n, 3n)$ Ta^{179} threshold. Consequently, we have omitted this measurement from further consideration. Study of the Ashby (60) neutron-counting experiment indicates a large number of corrections are used.

The $\text{Ta}^{181}(n, 2n)$ cross-section evaluation was temporarily set aside with the adoption of a recommended curve (Figure 21). To obtain this curve one set of data was shifted 2% in energy and several others were renormalized. Several sets of relative cross-section curves (magnitude not experimentally determined) were also used in the evaluation. The critical point in the evaluation is the apex of the curve where the cross-section relinquishes its initial behavior $\sigma \sim (E - E_0)^{1/2}$. We look for further adjustment from the evaluation of σ total and possibly from theoretical cross-section calculations.

The evaluation of Ta^{181} resonance parameters continues. In the "resolved" resonance region virtually no pointwise cross-section data exist. Resonance parameters deduced by various workers are based primarily on "area analysis" of neutron-transmission measurements. Though summary of the data in the resonance parameter format may be the desirable end product, it inhibits the

Figure 20. $\text{Ta}^{181}(n,2n)$ Reaction (Various Measurement Methods)

Figure 21. Ta^{181} (n,2n) Reaction

intercomparison of experiments for anomalies due to impurities, resolution, background, Doppler broadening, and general systematic errors.

2. Development of Evaluation Tools

Several approaches are underway to provide the tools needed for visual-data evaluation. What is desired is an economical computer program which will lucidly display a large amount of data from a variety of experiments. The data display should include error bars and allow overlaid fitted curves. The use of colors will certainly enhance the clarity. Possible approaches include:

- 1) CALCOMP mechanical color plots using the unpublished NNCSC programs SCIREF, SCIBIN, and SCIDAT with an out-of-house CDC-6600 computer.
- 2) Development of new programs to use the ORTHOMAT mechanical plotter with an in-house IBM-360/65 computer.
- 3) Modification of an existing CRT program to plot directly from SCISRS tape. Disadvantages: no colors, error bars, or large-size plots.
- 4) Use of the SCORE program (at a distant facility) coupled with polaroid photographs of the screen. Disadvantages: no colors or large-size plots; hard-to-read copy.

The adoption of Approach 1 or 2 plus the use of 3 and 4 appears to be a logical route.

Initially the tool described in Approach 4 was available for use. To implement it certain operations were required. The SCISRS files for natural tantalum and Ta^{181} , previously combined, were converted to the SCORE format. SCISRS and ENDF/B files for tantalum and tungsten were reblocked to conform to recent SCORE modifications and an initial SCORE run was made on the interactive graphics terminal. Approximately 3-1/2 hr were spent on the computer during which 125 K-bytes of core memory were allocated to the problem. This translates to a cost of approximately \$70.00 per evaluating hour. The initial experience suggests several ways by which the evaluator may optimize the time spent at the terminal. The brief experience particularly revealed a strong need for hard-copy production of desired pictures; reproduction by polaroid camera is

both poor and inefficient. The addition of hard-copy production is to be added in the next fiscal year.

To compare ENDF/B resonance parameters to experimental data the RESREG code is used. This code generates pointwise data directly from the ENDF/B tapes. A revised version of the RESREG code was checked out for use on the IBM 360. The revised version uses the energy-mesh scheme used in the UNICORN code. This code will prove useful later in checking out resonance parameters assembled for the tantalum and tungsten re-evaluations. It is also of interest to current Monte Carlo work at AI.

A code was written to separate the 27 materials on ENDF/B tape 114 by end-of-file marks. This will considerably shorten I/O time with codes such as RESREG.

To actually fit selected evaluated data with a continuous curve, several other tools are needed. Considerable tools are currently available with the SCORE program. The compound nucleus program COMNUC and the optical model program 2PLUS are also operational. An Unresolved Resonance Fitting Program UR was obtained from E. Pennington (ANL). Several versions of the JUPITOR code have also been obtained. The JUPITOR-1 code, as modified by Prince (BNL), has been made operational on an external CDC-6600 computer. It is also being converted for use with the in-house IBM 360/65. The JUPITOR-2 code from ORNL has also been received. Lack of documentation is currently inhibiting its use. An attempt to run a test case revealed that the input requirements have changed appreciably from those of JUPITOR-1.

C. BENCHMARK CRITICAL EVALUATION

Several industrial contractors and national laboratories participated in a special benchmark calculation. The purpose was to determine if a given critical-assembly configuration calculated by the participants using a single-reference multigroup library and given assembly specifications would yield results which were less divergent than those obtained when the several participants generated their own multigroup libraries. The benchmark critical assembly chosen was ZPR-3-48 and the participants used the ANISN transport-theory code for the calculation. Parameters calculated included the eigenvalue, k_{eff} ,

and the ratio of nuclide activity relative to $\nu\sigma_f^{235}$. Comparisons of the calculated k_{eff} 's and of the selected activity ratios are given in Table 18.

The results were grouped according to similarity of five-figure eigenvalues. However, because of valid questions as to significance of five figures, results are given to four figures for comparison purposes. To the original PNL(1) results are added data described as PNL(2) and PNL(3). Calculations [PNL(1)] were done using using a fast-running version of the ANISN code. Data for PNL(2) and PNL(3) were obtained using an unmodified version of ANISN, but with convergence criteria of 3×10^{-5} and 3×10^{-6} respectively. In Table 18 the AI values of the calculated activity ratios were arbitrarily chosen as a standard against which all other ratios are compared. If the values were identical the corresponding space is left blank; if not, the calculated value is given. From the groupings it appears that AI and ORNL used quite similar codes and computers; similarly for ANL and ANL(ID); B&W, BNL and CE; and PNL(1) and LRL.

The Los Alamos value was calculated using the transport-theory code DTF in place of ANISN and served as a control for the results calculated with ANISN. Though there is some slight scatter in the calculated results this scatter is significantly less than that obtained when many different methods and computer codes were used to process the microscopic cross-section data, generate multi-group libraries, and evaluate critical assemblies. Results for the calculated activity ratios are similarly close, with meaningful differences, as one might expect, recognizable in the LASL results. One concludes that with reasonable effort it is possible to factor out effects of code and computer differences in neutron cross-section evaluation.

In support of ENDF/B Phase II benchmark data testing, calculations for ZPR-3-11 and ZPR-3-48 using cross-section libraries prepared by MC² with the LASL data tape were carried out. These calculations used preliminary ENDF/B Version 2 data where applicable, and were made with both diffusion- and transport-theory codes. The results of the diffusion-theory calculations are given in Tables 19, 20, and 21.

TABLE 18
RESULTS OF BENCHMARK (ZPR-3-48) CALCULATIONS

Item	Reaction Type	AI	ORNL	ANL	ANL ID)	B&W	BNL	CE	LRL	PNL(1)*	LASL**	PNL(2)†	PNL(3)§
k_{eff}		0.9901	0.9901	0.9901	0.9901	0.9901	0.9901	0.9901	0.9902	0.9902	0.9903	0.9901	0.9902
C	σ_a	3.1379		3.1333	3.1382	3.1380	3.1380	3.1380	3.1376	3.1377	3.147	3.1380	3.1375
Mg		1.9497		1.9498	1.9498				1.9496		††		1.9496
Al		0.6733							0.6732	0.6732	0.6736		0.6732
Cr		2.9050				2.9051	2.9051	2.9051		2.9051	2.903	2.9051	2.9053
Mn		1.1654		1.1653	1.1653				1.1655	1.1655	1.165		1.1656
Fe		2.1545									2.153		2.1546
Ni		5.3090		5.3093	5.3093				5.3087	5.3087	5.315		5.3085
Mo		4.1117			4.1116	4.1118	4.1118	4.1118	4.1118	4.1119	4.109	4.1118	4.1122
U ²³⁵		5.1311									5.130		5.1312
U ²³⁸		0.6883									0.6883		
U ²³⁸	$\nu\sigma_f$	3.8373			3.3378	3.8374	3.8374	3.8374	3.8370	3.8370	3.844	3.8374	3.8368
Pu ²³⁹	σ_a	4.5530							4.5529		4.553	4.5531	
Pu ²³⁹	$\nu\sigma_f$	1.1219		1.1220	1.1220		1.1220	1.1220			1.122		
Pu ²⁴⁰	σ_a	1.8235							1.8233	1.8234	1.824		1.8234
Pu ²⁴⁰	$\nu\sigma_f$	3.0230		3.0232	2.0231	3.0231	3.0231	3.0231	3.0227	3.0228	3.026	3.0231	3.0227
Pu ²⁴¹	σ_a	0.6029									0.6028		
Pu ²⁴¹	$\nu\sigma_f$	1.5850									1.585		1.5851
Pu ²⁴²	σ_a	1.4287							1.4286		††		1.4286
Pu ²⁴²	$\nu\sigma_f$	2.4606		2.4609	2.4607	2.4607	2.4607	2.4607	2.4604	2.4605	††	2.4607	2.4604
Na	σ_a	3.7501		3.7502	3.7502	3.7502	3.7502	3.7502			3.751	3.7502	3.7503

*Modified (Fast) ANISN: $\epsilon = 3 \times 10^{-5}$

†Unmodified ANISN: $\epsilon = 3 \times 10^{-5}$

§Unmodified ANISN: $\epsilon = 3 \times 10^{-6}$

**DTF used in place of ANISN

*†No value calculated

TABLE 19
RESULTS FOR ZPR-3-11, ZPR-3-48 BENCHMARK
CALCULATIONS: PRELIMINARY ENDF/B
VERSION-2 DATA

	ZPR-3-11	ZPR-3-48
k_{eff}	0.962	0.970
β_{eff}	0.00701	0.00337
$\bar{l}(\mu\text{sec})$	0.0725	0.287
Critical mass (kg in core)	235.8	274.3

TABLE 20
COMPARISON OF CALCULATED CENTRAL REACTION RATIOS
WITH EXPERIMENT (RELATIVE TO U^{235} FISSION)

	ZPR-3-11		ZPR-3-48	
	Calculated	C/E	Calculated	C/E
A(B10)	0.906		1.343	
C25	0.198		0.274	
F28	0.034	0.90	0.0296	0.96
C28	0.116	1.04	0.138	1.00
F49	1.126	0.95	0.912	0.93
C49	0.112		0.225	
F40	0.325	0.96	0.226	0.93
C40	0.139		0.206	
F41	-		1.280	
C41	-		0.214	
A(Ta)	0.195		0.412	
F26	0.083	0.97	-	
C26	0.219		-	
F24	0.307	0.99	-	
C24	0.221		-	

TABLE 21
COMPARISON OF CALCULATED CENTRAL REACTIVITY
COEFFICIENTS WITH EXPERIMENT

	ZPR-3-11		ZPR-3-48	
	Calculated		Calculated	
	($\Delta k/k/\text{mole} \times 10^5$)	C/E	($\Delta k/k/\text{mole} \times 10^5$)	C/E
U ²³⁵	140.9	1.15	105.3	1.33
U ²³⁸	-7.51	1.14	-7.43	1.26
Pu ²³⁹	219.5	1.05	134.1	1.26
B ¹⁰	-71.9	1.00	-100.6	1.13
Ta	-18.7	0.95	-34.07	
Mn	-2.19	1.22	-2.10	1.78
Fe	-1.67	0.98	-1.00	1.45
Cr	-1.89	1.11	-0.81	1.65
Ni	2.87	1.20	-1.26	1.18
Na			-0.17	1.21
C			-0.24	4.8
Pu ²⁴⁰			21.9	1.13
Pu ²⁴¹			199.6	
Al			-0.52	1.24

Comparisons of multigroup constants generated by MC² and GRISM (AI microscopic data processing and multigroup generating system) revealed discrepant results. This was particularly true for resonance isotopes in the resolved-energy region. GRISM values were often 20 to 50% larger than those generated by MC². In contrast to this situation, results in the unresolved-resonance energy range above the resolved resonances agreed to within a few percent. The cause of discrepant results in the resolved-resonance energy range was traced to the p-wave unresolved-resonance calculation. In GRISM the s-wave unresolved-resonance calculation is made only for energies above the resolved resonances; however, the p-wave calculation is carried down to about 20 ev where the p-wave contribution is negligible. All contributing p-wave resolved resonances are deleted from the resolved-resonance input data to GRISM. MC² has provision for

carrying the unresolved-resonance calculation below the top of the resolved-resonance energy range but this is not done with present ENDF/B data which include p-wave resolved resonances. A report documenting the causes and resolution of this discrepancy, AI-AEC-MEMO-12933, was written and distributed.

Results of the transport-theory-code (S_4) calculations show an increase in k_{eff} from 0.962 to 0.968 for ZPR-3-11 and from 0.970 to 0.978 for ZPR-3-48. There were very minor differences for the central fission ratios; the central reactivity ratios were not determined. The validity of using first-order perturbation theory in calculating central reactivity coefficients was in question, since the calculated eigenvalues are between 3 to 4% below unity. It is assumed that whatever is causing this eigenvalue discrepancy is also adversely affecting the flux and adjoint spectra, which in turn relate directly to the perturbation calculations.

The results of the CAESAR-PERT (diffusion-theory) and APC-COMPOZ (transport-theory) calculations have been examined and the codes seem to be functioning properly and giving reasonable results. Further work on these problems will be deferred until the final ENDF/B Version-2 data and the modifications to ETOE and MC^2 are available.

D. COMPUTER PROGRAMS APPLICATION

A version of MC^2 in which the I/O time has been significantly reduced (as much as a factor of 8) was received from Rensselaer Polytechnic Institute and made operational on the local CDC-6600. Considerable effort was required to convert this CHIPPEWA-system chain program into the currently used SCOPE-system overlay program. The all-fine group option and the P1 ultrafine group with Legendre materials option were quickly checked out; however, the consistent P1 and B1 ultrafine options required corrections before successful runs were made. These required corrections were transmitted to other users of this version of MC^2 , i. e. Los Alamos (LASL), Babcock and Wilcox, and RPI. While a considerable savings in I/O time has been realized in using the RPI version of MC^2 , many improvements and corrections to the original MC^2 version had not been added to the RPI version. A slow and painstaking comparison with other versions uncovered the desired additions and corrections which were then added

to the RPI version. The MC² code was further modified to obtain such quantities as the ultrafine group energy, flux, and current as well as broad group-averaged microscopic cross-sections for use with an auxiliary processing code (CLIO). Thus the ultrafine group energy, flux, and current were obtained for use in GRISM, and broad group-averaged microscopic cross-sections in the CAESAR or ANISN format were calculated for use in those codes. The updated and modified RPI version of MC² is currently the only version in use at AI.

The preliminary ENDF/B Version-2 data for 12 materials were received from BNL along with new CDC-6600 versions of programs CHECKER and DAMMET. Program CHECKER was converted, compiled, and checked out on the IBM 360. Tapes 991, 992, and 997 (ENDF/B Version 2) were merged into one EBCDIC nine-track tape; all twelve materials were processed by CHECKER. Programs EDIT and ENDFAI were then modified to accept the preliminary Version-2 ENDF/B data, and graphical displays and data listings were obtained for the preliminary data. Both the CRT's and the listings as well as the CHECKER results were used to carry out a cursory Phase-I data review. Numerous errors in the data were found and appropriately documented, and the information forwarded to the NNCSC at BNL for corrective action. At the request of the NNCSC several thousand CRT plots were also sent to aid in the Phase-I data review.

The preliminary ENDF/B Version-2 data could not be processed by ETOE for use by MC² because of a number of format changes. An ETOE binary-data tape was made by LASL using modified preliminary ENDF/B Version-2 data and a modified ETOE. This data tape was received from LASL and successfully used by the AI MC² after minor modifications to the code.

Using MC² and the LASL data tape a 26-group cross-section library was prepared for the evaluation of the ZPR-3-11 critical assembly. The MC² code and the LASL data tape were then taken to the CDC-6600 at Kirtland Air Force Base where multigroup libraries for the other four critical assemblies assigned to Atomics International for Phase-II ENDF/B data evaluation were generated. The MC² calculations for both core and blanket compositions were completed for ZPR-3-48, ZPR-3-12, and ZEBRA-2. Multigroup constants for the ZEBRA-3 blanket were also run but the ZEBRA-3 core calculation failed. The cause of the failure was traced to the insufficient number of significant figures in the data statements in subroutine ALRAGO of MC². This caused negative transfer

elements in the elastic-scattering matrix for copper. A more precise set of data statements was obtained, and the program then correctly processed the data for copper.

Two cross-section plotting codes were written. One overlays plots of group cross-sections from various sources for any cross-section type; the data are normalized to an arbitrary standard source. The other overlays plots of ENDF/B File-3 smooth cross-section data for the old and the new version ENDF/B tapes. These programs will assist in the Phase-II ENDF/B data evaluation. Using the second program, File-3 overlay plots of the Version 1 and the preliminary Version-2 ENDF/B data for U^{235} , U^{238} , and Pu^{239} were generated; in addition, overlay plots of the Version-1 and final Version-2 ENDF/B data for Pu^{240} were generated. The data differences are being related to the Phase-II data testing calculated results. Figures 22 through 29 illustrate the differences between the Versions 1 and 2 ENDF/B data for U^{238} , Pu^{239} , and Pu^{240} . In all cases the Version-1 data are represented by the open circles; the asterisks correspond to Version-2 data. Significant differences between the two data sets are seen.

One of the new Version-2 ENDF/B tapes (Na 201) was received from BNL and converted to EBCDIC on a nine-track tape. The tape was processed by CHECKER and plots of the data were obtained from EDIT after these programs were modified to accept the final Version-2 formats. In addition program DAMMET was modified to accept the new formats. Major modifications to ETOE and MC^2 are required to process the final form of Version-2 ENDF/B data. These data cannot be used in MC^2 until the modifications are received from ANL.

Program ENDFAI was modified to handle the final Version-2 ENDF/B formats. In addition this modified code, ENDFAI-B, is able to handle overlapping inelastic-level and continuum data. The punched-card output contains the energy-dependent temperature for the Maxwellian distribution for the continuum as well as the usual type of card output. Also the minimum energy of 1.0×10^4 ev for inelastic scattering was reduced to 1.0×10^3 ev. ENDFAI-B was checked out, resulting in modifications to TOAD which must read the ENDFAI-B output and write the data set on a disk for use by the PRISM segment of GRISM. This modified code, TOAD-B, was checked out, requiring, in turn, modification of

Figure 22. U^{238} ENDF/B Comparison, Radiative-Capture Cross-Section

U-238 ENDF/B COMPARISON. MATS. 1047 AND 1103

729507
0005 0000

Figure 23. U²³⁸ ENDF/B Comparison, Fission Cross-Section

U-238 ENDF/B COMPARISON. MATS. 1047 AND 1103

729507
0003 0000

Figure 24. U^{238} ENDF/B Comparison, Inelastic-Scatter Cross-Section

PU-239 ENDF/B COMPARISON. MATS. 1051 AND 1104

729507
0011 0000

Figure 25. Pu^{239} ENDF/B Comparison, Radiative Capture Cross-Section

PU-239 ENDF/B COMPARISON. MATS. 1051 AND 1104

129507
0010 0000

Figure 26. Pu²³⁹ ENDF/B Comparison, Fission Cross-Section

Figure 27. Pu²⁴⁰ ENDF/B Comparison, Radiative Capture Cross-Section

PU-240 ENDF/B COMPARISON. MATS 1053 AND 1105

729537
060970 0005

Figure 28. Pu²⁴⁰ ENDF/B Comparison, Fission Cross-Section

PU-240 ENDF/B COMPARISON. MATS 1053 AND 1105

729537
060970 0003

Figure 29. Pu²⁴⁰ ENDF/B Comparison, Inelastic-Scatter Cross-Section

the PRISM segment of GRISM. The modified segment, PRISM-B, was checked out using ENDF/B Version-2 data for U^{233} as processed by ENDFAI-B, TOAD-B, and MOMUS. Further checkout is planned. A computer program, TOADCON, was written to convert the TOAD input data to the formats required by TOAD-B. The program was checked out.

E. NUCLEAR MODEL CALCULATIONS

A survey of methods used to calculate compound-nucleus reaction cross-sections was completed. A unified model of compound-nucleus reactions has evolved using some methods obtained in the survey. Other methods including a fission model were developed to help fill gaps in calculational techniques. The work is summarized in AI-AEC-12931 (to be published). A computer program called COMNUC which encompasses the proposed unified model of compound nucleus was written and tested. The output data from this code are those reaction cross-sections required for an ENDF/B evaluation.

Methods for analyzing intranuclear gamma-ray cascades are also described in AI-AEC-12931. The use of a cascade calculation permits more accurate calculation of fast-neutron capture cross-sections. In addition, branching ratios for particle emission can be obtained for use in multiparticle cascade reactions, i. e. $(n, 2n)$ and $(n, n'x)$.

A three-coupled channel optical-model code has been prepared. This code will provide the ability to calculate direct-reaction cross-sections for even nuclei and supply the required compound-nucleus formation cross-sections for the subsequent compound-nucleus calculation.

F. DOCUMENTATION

The following reports were written and published during GFY 1970:

- "The Evaluation of Several ENDF/B Nuclide Cross-Sections by a Monte Carlo Technique, " AI-AEC-MEMO-12915
- "An Evaluation of Uranium-235 Neutron Cross-Section Data for Energies Above 15 kev, " AI-AEC-MEMO-12916
- "Effect of Fast-Breeder Reactor Calculations of Using Region-Dependent Multigroup Cross-Sections, " AI-AEC-12843
- "Comparisons of GRISM and MC² Results for Heavy Isotope Resonance Absorption Cross-Sections, " AI-AEC-MEMO-12933

The following papers were presented during this fiscal year:

- "Comparison of Self-Shielded Resonance-Capture Cross-Sections for U²³⁸ Calculated by the GRISM and MC² Codes," ANS (June 1970)
- "The Application of Interactive Computer Graphics to Nuclear Data Evaluation Problems," Invited Paper, Second International Conference on Nuclear Data for Reactors, Helsinki, Finland (June 1970)

III. EVALUATION OF EFFORT DURING FISCAL YEAR 1970

As a result of the rapid and successful re-evaluation of the uranium-235 cross-section data the delay in continuing the ENDF/B Phase-II data testing is expected to be minimized. The concept of a task force in which a limited number of experts in the area of neutron cross-section evaluation and measurements are brought together for an intimate exchange has been shown to be highly successful. It is strongly recommended that this concept be made a basis for further ENDF/B data evaluation by the CSEWG (Cross-Section Evaluation Working Group).

Experience gained over the last year with the FORTRAN graphics system used in SCORE has resulted in the generation of an improved FORTRAN graphics package. The system is designed to allow either minimal knowledge of the operation of a 2250 on the part of a user or the most sophisticated applications by users with a detailed knowledge of a 2250. Extensive testing of this package has been completed and SCORE is being modified to use the new subroutines. This new compact version of the interactive computer graphics system SCORE will now permit installations, constrained to minimal computer configurations, to use this system in an efficient and economic manner.

Analysis of fast-neutron cross-section data of interest to the LMFBR program has in the past been hampered by lack of a unified calculational model. The recently completed unified model of compound-nucleus reactions will now permit consistent calculation of compound-nucleus reactions of interest of cross-section evaluators. The remaining direct-reaction cross-sections may be calculated by an optical-model code which also provides the necessary input compound-nucleus formation probabilities for the reaction cross-section calculations. The results are useful for understanding the behavior of fast-neutron cross-sections and as an aid to the production of evaluated data in regions where no experimental data exist.

An evaluation of tantalum and tungsten isotopic cross-sections was begun. The effort began by compiling all the data on Ta^{181} and Ta^{182} into workable form: a SCISRS-type tape. This included obtaining appreciable data directly from authors and adding it to the tapes received from the National Neutron Cross-Section Center. Similar operations for the tungsten isotopes were also begun.

In the first look at the data, details such as energy resolution, impurities, sample thicknesses, and normalizations were gleaned from the literature references. Extensive evaluations of a few reactions were accomplished during this period.

Of critical importance to the handling of large amounts of data is a means for visual data display. To supplement the SCORE system which is currently limited to small displays and no hard copy, steps were taken to develop a capability for large (6 ft) colored hard-copy plots.

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