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QUARTERLY TECHNICAL PROGRESS REPORT
LMFBR PHYSICS PROGRAMS
JULY-SEPTEMBER 1971

AEC Research and Development Report

Atoms International
North American Rockwell

P.O. Box 309
Canoga Park, California 91304

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LMFBR PHYSICS PROGRAMS
JULY-SEPTEMBER 1971

**The preceding Progress Report (Annual) was
AI-AEC-13005**

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CONTRACT: AT(04-3)-701 (Task 5)
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Program:	General Reactor Physics		
AEC Task:	4 - Cross-Section Analysis		
Project Manager:	H. A. Morewitz		
Reporting Period:	July-September 1971	189A:	13493
General Order:	6524	Subaccount:	13130
		Category:	04-40-01-03.1

Principal Investigators: H. Alter, P. F. Rose, R. S. Hubner

I. PROJECT OBJECTIVES

The objectives of this project include the evaluation 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 microscopic 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 and evaluate the compiled data, and nuclear model calculations will be developed and used to help fill gaps in measured 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 utilized 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. PROGRESS DURING REPORT PERIOD

A. ENDF/B DATA

A partial re-evaluation of U^{235} for the ENDF/B-3 file was completed. This re-evaluation includes new resolved resonance parameter data, as well as smooth total, capture, fission, and elastic scattering background cross-section data

Figure 1. Spline Fit to Glasgow and Foster U^{235} Total Cross Section Measurements

generated by J. R. Smith of Aerojet Nuclear Corporation. Smith extended the resolved energy region up to 82.0 ev.

Unresolved resonance parameter data were received from T. A. Pitterle, of WARD. Pitterle's information extended the unresolved resonance from 15 to 25 kev, which was required for the ENDF/B-3 U^{235} file.

The final modification to the U^{235} data file was made at AI. The experimental Glasgow and Foster data for the U^{235} total cross section was received from the National Neutron Cross Section Center, and processed as follows. A spline fit to the measured values between 2 and 15 Mev was obtained. This fit to the experimental data is shown in Figure 1. Data from this curve were interpolated to the ENDF/B energy grid for the U^{235} total cross section. The new U^{235} total cross section (represented by asterisks) is compared with the old values (represented by the open circles) in Figure 2. The new elastic scattering cross section in this energy range was then obtained by subtracting from the new total cross section the sum of the remaining partial cross sections. The old and new elastic scattering cross section for U^{235} are compared in Figure 3.

The modified data file was processed with the CHECKER code, and several minor errors corrected. The corrected data were then again processed with CHECKER, found free of the type errors that CHECKER catches, and forwarded to the NNCSC at Brookhaven, for incorporation into ENDF/B-3.

The detailed reevaluation of the neutron cross-section data for the tungsten isotopes continued during this report period. The scarcity of measured data for the capture cross section for these isotopes emphasized the importance of evaluating available measurements of the capture cross section in natural tungsten. Use of this data has helped resolved much anomalous information; however, the 1967 Karlsruhe measurements are still higher than all other reported data. One particularly good experiment was that performed at Obninsk in 1965. This was a measurement of the absolute cross section, using Sb-Be neutrons. There are no normalization problems, and the experimental errors are small in both cross section and energy resolution.

A topical report, AI-AEC-12990 (ENDF-150), which reports in detail on the re-evaluation of the Ta^{181} and Ta^{182} isotopes was written and published. This report is in the process of being distributed.

6524-4623

Figure 2. Comparison of ENDF/B-2 and ENDF/B-3 U^{235} Total Cross Sections ($2.5 \text{ Mev} \leq E \leq 15.0 \text{ Mev}$)

6524-4624

Figure 3. Comparison of ENDF/B-2 and ENDF/B-3 U^{235} Elastic Scattering Cross Sections ($2.5 \text{ Mev} \leq E \leq 15.0 \text{ Mev}$)

B. ANALYSIS OF BENCHMARK CRITICAL ASSEMBLIES

Revised specifications for several GEDANKEN-type calculations were distributed to the Cross Section Evaluation Working Group Data Testing Subcommittee. The revisions were necessary, because of excessively long computing times encountered by the users of MC² in attempting to meet the original specifications. These calculations are designed to shed some light on the discrepancies among the multigroup constants calculated by the several data-testing participants.

The Atomics International version of the MC² code has been successfully compiled and executed on the UC-Berkeley CDC 7600. The test problem ran five times faster on the CDC 7600 than on the CDC 6600. Since 7600 time is a factor of three more costly, the overall savings achieved by running MC² on the 7600 is significant.

C. SCORE - INTERACTIVE COMPUTER GRAPHICS

During this report period, the interactive computer graphics program, SCORE III, was used for actual data fitting of the Pu²³⁹ fission, capture, and total cross sections in the 0.1 to 50 ev range, using the single-level and multi-level options of Program CODILLI-2 (CODILLI with SCORE).^{*} SCORE III, Experimental Version A, provides a versatile tool having many advantages over normal batch-mode data-processing schemes. The program has been used in the mode incorporating CODILLI-2 to excellent advantage for preliminary least-squares fitting of the individual cross sections.

Operation of SCORE III-A requires, first of all, the preparation of suitable data tapes (experimental cross sections, experimental errors) and of a preliminary library of assumed resonance energies and line widths for the nuclide being investigated, as well as for the nuclides which appear as impurities in the experimental targets; a subroutine dealing with the resolution function needed in Program CODILLI-2 must also be provided. At present, a subroutine suitable for the analysis of Linac measurements is built into CODILLI-2.

^{*}Collaboration of P. F. Rose (AI), D. B. Adler (UI), F. T. Adler (UI), N. H. Marshall (ANC-Idaho).

The performance of the program can best be illustrated by considering sequences of scope pictures generated during the data analysis. The figures were obtained as hard copy from the content of the IBM 2250 CRT scope. They illustrate some of the various data displays and interactive choices. Figure 4 shows one of the three main option lists, along with a plot of the experimental data within the selected energy range. After an expanded-data display, the resonance module is entered, and another set of options appear. Among these is the selection of isotopes that make up the target. Atom fraction, potential scattering, and mass data are interactively entered into the calculation at that point, as shown in Figure 5.

An important step in the resonance analysis is the classification of resonances. Choices are made, as shown in Figure 6, whether to: (1) include the resonance in the calculation, (2) fit the resonance, and/or (3) apply a multi-level or a single-level analysis to the fitting.

After the least-squares fitting calculation performed by CODILLI-2 is completed, decisions are made by considering the "residuals" (i. e., the χ values over the region of an individual resonance, displayed as shown in Figure 7). By light pen, one can then choose one resonance for an expanded display from the panel shown in Figure 7; Figure 8 shows the expanded view of a single resonance, where changes in resonance energy and half widths can be introduced either in the numerical values by means of the keyboard, or by changing with the light pen the vertical lines defining the position of the resonance energy and the half width of the resonance line. This picture can also be expanded in energy scale, to show several resonances around the resonance being investigated. The use of the visual data, together with the practically simultaneously computed χ values, is a distinct advantage for interactive fitting with SCORE III-A. After completion of the fitting procedure, the data and the theoretical curve are displayed, as shown in Figure 9.

A current limitation of the SCORE program is the restriction that only 500 data points can be used in display and/or data analysis. This does not allow the fitting of more than one or two resonances at a time, if good data (many close-spaced data points) are used. Another restriction deals with the subroutine ADLISP. This subroutine, which accesses the calculated data points, is currently restricted to 150 calculated points, which is insufficient.

6524-4625

Figure 4. Option List and Plot

SELECT DESIRED ISOTOPES

74	0	1.00000E 00	92	233	1.00000E 00
92	235	5.00000E-01	92	335	5.00000E-01
92	238	1.00000E 00	94	239	2.50000E-01
94	239	7.50000E-01	94	240	1.00000E 00

ATOM FRACTION: 1.00000E 00

POTENTIAL SCATTERING (BARNs): 10.0

ATOMIC WEIGHT (AMU): 239.0

DELETE

6524-4626

Figure 5. Enter Input Options

Z = 94 A = 239 G = 7.50000E-01

ENERGY	CALCULATE	FIT	MULTILEVEL
7.80103E 00	YES	YES	YES
1.09120E 01	YES	YES	YES
1.18777E 01	YES	YES	YES
1.43086E 01	YES	YES	YES
1.46583E 01	YES	YES	YES
1.76329E 01	YES	YES	YES
2.22342E 01	YES	NO	YES
2.38758E 01	YES	NO	YES
2.62228E 01	NO	NO	NO
2.72329E 01	NO	NO	NO
3.54220E 01	NO	NO	NO
4.13731E 01	NO	NO	NO
4.16230E 01	NO	NO	NO
4.44350E 01	NO	NO	NO
5.00330E 01	NO	NO	NO
5.25331E 01	NO	NO	NO
5.55822E 01	NO	NO	NO
5.91536E 01	NO	NO	NO

6524-4627

Figure 6. Resonance Option Choice

Z = 94 A = 239 G = 7.50000E-01

POLE ENERGY		CURRENT	RESIDUAL PREVIOUS
7.84816E 00	•	5.97783E 01	8.09856E 03
1.09745E 01	•	3.40491E 02	8.24918E 03
1.19350E 01	•	5.43554E 01	1.23276E 04
1.43700E 01	•	6.24807E 01	2.26548E 03
1.47245E 01	•	1.32749E 02	1.39795E 04
1.77140E 01	•	2.00620E 02	9.27237E 03

6524-4628

Figure 7. χ Values for Two Successive Cases

Z = 94 A = 239 G = .750000E-01

FISSION L R FISSION

POLE ENERGY 1.47245E 01

HALF WIDTH 4.05440E-02

FISSION G 8.32364E-03

FISSION H -1.13784E-03

6524-4629

Figure 8. Expanded Display of Single Resonance

Figure 9. Comparison of Theoretical Fit to Data

Because of the small buffer in the IBM 2250, detail is often scissored from the display when too many data points are used. This is, at times, very serious, when control information is lost.

III. EVALUATION OF EFFORT TO DATE

An effort has been initiated to determine the reasons for the discrepancies among the multigroup constants calculated by the several data-testing participants. The resolution of this problem will help dispel some of the current dissatisfaction with the CSEWG data-testing program.

The successful compilation and execution of the MC² program on the UC-Berkeley CDC 7600 will result in significant economies in all future running of the MC² code.

SCORE III-A, in its present state, has proved to be an excellent tool for interactive data fitting, if adequate care is taken in the preparation for the least-squares data fitting. The program appears most useful for preliminary fitting, and probably for final detailed adjustments of parameters. The interdependence and interaction of the use of SCORE III-A, and of simultaneous fitting routines such as TANDEM and TRIPLE, needs further investigation, following more extensive practical use of all programs. The provision of hard copy from SCORE III-A fitting represents an essential improvement over earlier versions of the program. Comparison of results of analyzing fission, capture, and total data cannot be performed on one scope; thus, the hard copy feature is needed to make the necessary judgments before completing the fitting, and, above all, before altering the permanent data file library.

The operational version of SCORE-III-A has provided several advantages for the least-squares fitting of resonance data. These are as follows: SCORE provides for a continuity of effort and thinking by the practically instant turn-around time; results can easily be compared and immediately improved by the interactive mode of operation. SCORE provides the ability to select different groups of neighboring resonances; and, by allowing for rapid changes in resonance energies (μ) and total line widths (ν), provides an intuitive insight into the sensitivity of the parameters obtained to the choices made. The interactive fitting, using changes of resonance energies and line widths, makes nonlinear

iterative fitting routines unnecessary in preliminary fits, resulting in substantial savings in use of central processor time. For adequate data, and with sufficient preliminary preparation, it appears possible to analyze narrow energy bands within a few minutes of real time scope use.

The operation of SCORE III-A on a realistic problem has pointed out several areas where improvements are desirable. These include:

- 1) The need to increase the number of acceptable data points to at least 1000, preferably 1500, with assurance that the useful options can be contained in the IBM 2250 buffer.
- 2) Cross-section and energy scales should be provided for all pictures, and without cutoff of scales.
- 3) Provisions should be made to display by option $\sqrt{E}\sigma(e)$ or $\sigma(E)$ [and not only $\sigma(E)$]; this would facilitate the visual analysis of broad resonances, and such a feature may be essential for work on fertile or low-Z elements.
- 4) Frequently, one needs to reconsider previous "display pages" on the scope. Provisions should be made to go backwards in panels, without losing information.
- 5) The routine ADSLIP needs access to more calculated points.
- 6) Space for a temporary library (including updating due to the fit in progress) would be most helpful, so that no time is lost in re-entering resonance energies and half widths by starting a new problem. This aspect is of special importance, if several data sets, corresponding to different reactions (σ_T , σ_F , σ_C), have to be fitted, or if data sets due to different authors have to be compared.
- 7) At present, only LINAC time resolution functions are provided within CODILLI-2, because of space limitations imposed by SCORE III-A; other resolution functions are needed, and space and a suitable interactive-choice panel should be provided in SCORE III-A.

IV. NEXT REPORT PERIOD ACTIVITIES

Re-evaluated data for the tungsten isotopes will be put into the ENDF/B-3 format, and forwarded to the National Neutron Cross Section Center. The re-evaluation of the Eu^{151} and Eu^{153} isotopes will continue.

Results of the GEDANKEN calculation will be analyzed, to help determine the cause of discrepancies in multigroup constants generated from the same reference set of microscopic data. Comparison of VIM-derived multigroup constants with those calculated by data-testing participants has indicated possible areas of discrepancy encountered by the other participants.

A topical report, summarizing the results of interfacing SCORE with CODILLI-2 (SCORE-III-A) and the applications of SCORE-III-A to the fitting of Pu^{239} resonance data, will be written.

ENDF/B-3 data will be processed and evaluated, prior to continuing the Phase II data program for the CSEWG benchmark critical assemblies.

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Program:	Civilian Power, LMFBR		
AEC Task:	5-B - Reactor Physics, Fast-Reactor Physics Experiments		
Project Manager:	H. A. Morewitz		
Reporting Period:	July-September 1971	189A:	13236
General Order:	7701	Subaccount:	14610
		Category:	04-01-61-02.2

Principal Investigators: T. H. Springer, R. J. Tuttle, L. A. Mountford,
H. N. Royden, J. M. Otter

I. PROJECT OBJECTIVES

The objectives of this project are to: (1) determine reactivity, temperature, and Doppler coefficients of various materials in a variety of fast-reactor spectra, (2) investigate effects due to different geometric arrangements of such materials, including the variation of the surface-to-mass ratio, (3) provide experimental results for checking theoretical predictions, and (4) develop improved experimental and theoretical methods for treatment of problems in the field of fast-reactor physics.

II. PROGRESS DURING REPORT PERIOD

A. EXPERIMENTAL STUDIES

The experimental measurements of the reactivity worths of nearly full-scale control rod mockups in the center of the pin-type, UO_2 fueled, sodium-voided test region of Core 20 were completed. The reactivity worths were obtained as a function of axial position from a point where the front of the rod was just inside the reactor (~ 1 in. inside the axial depleted UO_2 blanket) to a point where the rod was symmetrically located with regard to the core midplane. Two types of geometrical arrangements of materials were studied; one consisted of an 18-pin cluster, and the other consisted of a solid rod, 2 in. in diameter.

The 18-pin cluster (see Figure 10) was constructed of 18 stainless steel tubes, each 0.750 in. in OD with a 0.035 in. wall. The tubes were arranged in a hexagonal array (1.25 in. pitch) around a 1.0-in. diameter stainless steel rod at the center. The 18 tubes were surrounded by a 6-in. OD by 0.065-in. wall stainless steel tube that simulated the housing around a typical control rod.

Figure 10. 18-Pin Cluster

The overall length of the multipin configuration was 34.75 in. Three different materials (tantalum, boron carbide, and lead) were placed in the 18 tubes, and one set of worth measurements was made with each. A fourth worth measurement, wherein the 18 tubes were void, was also conducted, in order to evaluate the reactivity effects of the structural materials alone.

In the case of the tantalum multipin cluster, 13 tantalum rodlets, each 0.156 in. in diameter, were clustered within each of the 18 steel tubes, thus simulating a solid tantalum rod (see Figure 11). The total cross-sectional area of tantalum in all 18 pins was 4.47 in.² The tantalum had a length of 34.75 in. and a mass of 42.1 kg.

In the case of boron carbide, the material, in powder form, was vibratorily compacted into each of the 18 stainless steel tubes, thus giving a total cross-sectional area for boron carbide of 6.54 in.², a length of 35.76 in., and a mass of 4.97 kg. A 52% theoretical density (1.30 gm/cm²) was achieved within each tube.

The lead was in the form of ballast shot, which was poured directly into each stainless steel tube. The total length of the lead column was 36 in., and the total mass of lead in all 18 tubes was 25.2 kg.

The 18-pin cluster mockups, data for which are summarized in Table 1, were placed inside the central hexagonal matrix cell of the test region for all measurements.

The second type of geometrical arrangement, the 2-in. diameter rod, consisted of tantalum in three different lengths, one 3 ft, one 5 ft, and one 6 in. The reactivity worths of these rods were determined, both within the central matrix cell of the test region and within the hexagonal through-tube of the central hexagonal test fuel element.

B. DATA ANALYSIS

Analyses of the data obtained during the various control rod mockup measurements were carried out during this quarterly period, and are summarized in Figures 12 and 13. The reactivity effects of the multipin control rod systems (Figure 12) are positive as the leading edge of the rod enters the core.

7701-46193
Figure 11. Pin-Type Test Region With Central Full-Scale 18-Pin Control Rod

TABLE 1
CONTROL ROD MOCKUP SPECIFICATIONS

Material in 3/4 in. Tubes	Mass of Material in Tubes (kg)	Length of Material in Tubes (in.)	Distance From Front of Mockup to Front of Material (in.)	Material Cross Section of Material in Tubes (in. ²)	Effective Density in 3/4 in. Tube Area	
					gm/cm ³	% TD
Ta	42.1	34.75	1.75	4.47	11.30	68
B ₄ C	4.97	35.76	0.68	6.54	1.30	52
Pb	25.2	36.00	0.56	6.54	6.53	58
"Void"	19.3*	-	-	-	-	-

*Mass of structural material (stainless steel) into which Ta, B₄C, and Pb materials are placed

7701-46205

Figure 12. Multipin Control Rod Mockup Worths, Core 20 (Sodium-voided)

7701-46206

Figure 13. Worths of 2-in. Diameter Tantalum Rods, Core 20 (Sodium-voided)

This trend seems to indicate that, at least in the sodium-voided situation (the central hexagonal channel is empty), neutron scattering predominates over absorption as the rod enters the blanket. The absorption effect in the tantalum and boron carbide rods begins to predominate as the leading edge of the rod enters the core, and the integral worth becomes negative, reaching values of -23.7 and -31.7¢ for tantalum and boron carbide, respectively, at the location in which the rods are situated symmetrically with respect to the core midplane. For the rod that consists only of the steel structural material, and for the rod that contains lead, the integral worths remain positive throughout the traverses, reaching values of +3.0 and +4.5¢, respectively, at the location of symmetry. By correcting for the effect of the structural material alone, one obtains net integral worths of -26.7 and -34.7¢ for the tantalum and boron carbide alone.

The reactivity worths of the multipin control rod systems are arbitrarily set equal to zero at the -24 in. position, since this is the position of the leading edge of the rod at the beginning of the experiment. Since the rods have some additional reactivity effects, relative to the condition in which they are fully withdrawn, some account must also be taken of the latter effect. This effect has been evaluated in a separate series of analyses that are based upon control rod position information. Reactivity worths of 1.53, 1.68, 1.71, and 1.68¢ for the voided, lead, boron carbide, and tantalum rods, respectively, were derived.

The reactivity effects of solid, cylindrically shaped, tantalum rods (Figure 13) show similar trends to those of the multipin systems. Initially, a positive reactivity is observed as the 2-in. diameter by 3-ft long rod is driven into the blanket from a point where the leading edge of the rod is at -24 in. At about -18 in., the peak positive effect is reached; and, from that point, the integral worth becomes more negative. At the position of symmetry, relative to the core midplane, the integral worth of the 3-ft long tantalum rod was determined to be $-16.58 \pm 0.14\text{¢}$, after correction ($+0.38 \pm 0.14\text{¢}$) for the rod in a totally withdrawn position.

Since the 5 ft rod is mounted on the same drive mechanism as is the 3 ft rod, its starting point for the traverse is the core midplane, where its integral worth is adjusted to correspond to that of the 3 ft rod at the same position. At the location of symmetry, the worth of the 5-ft long rod is $-15.65 \pm 0.14\text{¢}$. The longer rod has a somewhat less negative integral worth, since it extends through both blanket regions, where the reactivity effects are positive.

The worth of the 3-ft long rod, at its point of symmetry, can be compared directly with that of the slightly shorter multipin rod at the same position. The ratio of the integral worth of the former to that of the latter is ~ 0.70 . This ratio is essentially identical to the ratios of the cross-sectional areas, thus implying that both rods have nearly the same degree of self-shielding.

During an earlier reporting period, measurements were made of the axial fission neutron importance distribution. These measurements were made by means of a small Cf^{252} spontaneous fission source, moved along the axis in the test channel of the central fuel element. The source was moved in 1 in. increments over a distance of 55 in., from 18 in. into the movable half to 1 in. out of the fuel element in the stationary half. This distance covers the region from 2 in. in the lower axial blanket, through the core and upper axial blanket, to 9 in. above the upper axial blanket.

The inverse kinetics method was used to analyze reactor power data, and the importance was derived from the difference in apparent reactivity observed at two different power levels. Two separate runs were made at each power — one, in which the source was initially in the reactor and then driven out and back in, and another, reversing this procedure, starting with the source out, driving in, and then back out. All results were in agreement, and thus were averaged to give the importance as a function of position.

These results are shown in Figure 14, along with calculated values for comparison. To eliminate the random scatter of the experimental points, a smooth curve was generated by repetitively smoothing the measured values. (This smoothing uses a third-order polynomial, and so does not distort the shape of the distribution.)

The calculated values, normalized to the experiment at the core midplane, were produced by the diffusion code, CAESAR (using group constants derived from AI-ENDF), in slab geometry, with only the core and blanket regions represented. The increasing degree of disagreement that is observed in the blanket region is probably attributable to apparently erroneous U^{238} cross sections in the region below 4 kev, to the use of a U^{235} fission spectrum rather than the Cf^{252} fission spectrum, to the less-than-ideal theoretical treatment of neutron scattering inherent in a diffusion calculation for that region, and to neglecting,

7701-46207

Figure 14. Fission Importance
in ECEL-20

AI-AEC-13013

in the calculation that was performed, the other materials that are located outside of the blanket.

Preliminary analysis of TLD exposure data from the full-size, 18-pin, tantalum control rod cluster in ECEL-20 was completed. Based on the dispersion observed for groups of four TLD rods irradiated at the same locations, the standard deviation of the average is about $\pm 1\%$. The observed dose is quite flat across the cluster, being, relative to a pin in the inner ring, 4% higher in a pin at the corner of the outer hex ring, and 2% lower in a pin between corners of the outer hex ring.

In order to relate the recorded TLD dose to the dose absorbed in the surrounding material, a factor, developed by T. E. Burlin,^{*} has been used. Burlin's derivation was reviewed, and has been generalized to include the photoelectric and pair production energy absorption. Burlin's factor, as originally derived, implies that only the Compton effect is significant; this situation is not correct for tantalum. A computer program is being formulated to calculate the generalized factor.

C. ANALYTICAL STUDIES

Initial measurements of the Doppler effect in SEFOR (GEAP 13702) indicate a value of -0.0081 ± 0.0014 for the value of $T(dK/dT)$, assumed by GE to be a constant. A preliminary fit to the SEFOR data has been made, using the form $T^{0.82}(dK/dT) = \text{constant}$; this fit appears to be better. The value 0.82 for the temperature exponent resulted from a recent survey[†] of fast Doppler measurements.

ZPPR-2 Doppler measurements have been analyzed with DOPFIT-II, with the results shown in Table 2. As in previous experiments, no significant increase of the Doppler temperature exponent (γ) with sodium voiding was noticed. The value 2.14×10^{-4} for the sample-normalized Doppler coefficient at $\gamma = 0.8$ is consistent with previous experiments in LMFBR spectra. As can be seen from Table 2, sodium voiding reduced the Doppler coefficient by 35%. The signal-to-noise ratio in the axial blanket was too small to permit determination of γ .

^{*}T. E. Burlin, "A General Theory of Cavity Ionization," Brit. J. Radiol., 39 (1966) p 727

[†]"Annual Technical Progress Report, LMFBR Physics Programs, GFY 1971," AI-AEC-13005 (August 15, 1971)

TABLE 2
ANALYSIS OF ZPPR-2 DOPPLER MEASUREMENTS
WITH DOPFIT-II

Core Condition	Sample Location (R = 0 for all)	Doppler Temperature Exponent γ	Doppler Coefficient ($d\rho/dT$) at 300°K for $\gamma = 0.8$ (per 10,000°K)
Normal	Z = 0	0.82 ± 0.07	$2.14 \pm 0.03^*$
Sodium-voided	Z = 0	0.78 ± 0.11	$1.40 \pm 0.03^\dagger$
Normal	Z = 12 in.	0.71 ± 0.18	$1.47 \pm 0.05^\dagger$
Normal	Z = 24 in. [§]	1.7 ± 1.6	$0.19 \pm 0.05^\dagger$

*Normalized to sample worth

†Normalized to sample worth at center of normal core (first case)

§In axial blanket

D. FAST REACTOR EXPERIMENTS COMPILATION

Volumes I and II of the Fast Reactor Experiments Compilation were received from BNL, and work on incorporating the recently completed Doppler review in Section 7 of the Compilation was begun.

III. EVALUATION OF EFFORT TO DATE

The series of experiments dealing with the reactivity worths of nearly full-size control rod mockups, as a function of axial position in the pin-type, UO_2 -fueled, sodium-voided test region of Core 20, was the first of this type in an LMFBR-type spectrum, and the technique appears to be very useful in evaluating various control rod materials and designs, particularly on a relative basis. The worths of the rods are sufficiently small that measurements can be done by continuous-drive techniques; consequently, time-consuming fuel manipulations, and problems concerning more difficult data interpretations, are avoided. One of the major tasks remaining in this area is that of inter-relating the results with other critical assemblies, and normalizing the measurements to full-scale LMFBR control rod designs. By the use of normalization integrals, comparisons will be made with previous, smaller-scale, experiments in Core 17, and with the larger-scale static measurements in ZPPR.

Efforts are continuing in the area of the measurement of heating rates in tantalum by means of TLD detector techniques. Reasonably good correlations have been found between the measured dose rates in the ECEL reactor and ZPR-6; consequently, the method still holds promise as an effective means for determining heating rates in zero-power critical assemblies. The primary difficulties appear to be in the correlation of TLD dose rates and sensible heat. A method, whereby the TLD detector can be calibrated directly in terms of heat energy deposited, has been devised. The technique consists in placing the tantalum sample, with TLD imbedded in it, in a sufficiently high γ field (Co^{60} and/or the STIR reactor in the shutdown condition) that a temperature rise can be detected by standard calorimetric techniques. Thus, a direct correlation between TLD dose and temperature is obtained. Once this correlation is established, a TLD measurement in a zero-power critical assembly will yield the heating rate by means of the correlation factor.

Another possible method for determining the heating rate in tantalum in a critical assembly was also briefly investigated. This method consists of a direct calorimetric measurement of the temperature rise in a slug of tantalum, using a platinum resistance thermometer and a specially designed vacuum-vessel calorimeter that will fit into the 2 x 2 matrix structure. Temperature changes of the order of 10^{-4}°C can potentially be measured. An evaluation of this technique is currently underway.

IV. NEXT REPORT PERIOD ACTIVITIES

During the October-December reporting period, the pin-type fuel elements will be unloaded, the space between the 271 fuel tubes in each element will be filled with sodium, fuel will be re-loaded into the elements, and a new critical condition will be achieved. A new series of multipin control rod measurements will be initiated, and the results will be used to compare with the sodium-voided case. Two-dimensional diffusion theory calculations (2DB) will be carried out, to provide a set of analytical values for comparison with the recently completed experiments in the voided core, and to provide a pre-analysis for the experiments to be conducted in the sodium-filled case. Intercomparison of the results with ECEL Core 17 results will be made.

The recently completed paper, concerning the review and evaluation of Doppler experiments, will be condensed and incorporated in Section 7 of the Fast Reactor Experiments Compilation. The delayed neutron parameter and neutron spectrum evaluations will be continued.

Program: Reactor Physics		
AEC Task: 5-E — Theory and Computation for Reactor Analysis and Design		
Project Manager: H. A. Morewitz		
Reporting Period: July-September 1971	189A: 13239	
General Order: 7701	Subaccount: 14320	Category: 04-01-61-0201

Principal Investigators: L. B. Levitt, R. C. Lewis, J. Spanier

I. PROJECT OBJECTIVES

The basic objective of this project is to advance the state-of-the-art 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. PROGRESS DURING REPORT PERIOD

All codes connected with Task 5-E, including VIM, U3R, and RABBLE (for testing of the probability table method), were converted to the CDC 7600. While no major problems were encountered, multi-file tape generation was much more complicated, and we were also forced to abandon, for the time being, the extended FORTRAN compiler in favor of the slower standard FORTRAN compiler. In spite of this, VIM runs 4.3 times faster on the 7600 than it did on the 6600.

Information was obtained which permitted us to regenerate our probability tables to conform to the ENDF/B Version II smooth averages. This was done, and the spherical benchmark ZPR 3-48 problem was rerun, now on the CDC 7600, using the new tables. A detailed analysis of the multigroup cross sections,

k_{eff} , and central fission ratios with respect to U^{235} was performed, and the results compared with multigroup transport results reported in AI-AEC-12999 (ENDF-147). A comparison of a few key results is shown in Table 3.

These results clearly show that VIM is producing numerical values of key parameters in the range of those produced by multigroup transport calculations for homogenized models in which this comparison is possible.

Particular attention was given to microscopic multigroup cross sections in the unresolved resonance region, since the VIM code used probability tables in this energy range. The analysis shows that the probability tables are indeed computing microscopic effective group cross sections for resonance isotopes correctly. The VIM results have also clarified some of the rather large disparities in multigroup transport results reported in AI-AEC-12999 in this energy region. VIM can therefore be used to resolve discrepancies between other multigroup sets, serving as a reference standard. This analysis can also be used to detect any data errors or differences which may still remain in the VIM library.

The analysis of the ZPR-3-48 spherical VIM calculation has also shown that the variance of the track length estimate of k_{eff} is one-fourth that of the absorption estimator, even though the same source was used for both methods.

TABLE 3
COMPARISON OF MONTE CARLO AND MULTIGROUP CALCULATIONS
OF k_{eff} AND SPECTRAL INDICES

	S4 AI	Diffusion ANL	S4 GE	S4 GGA	Diffusion INC	S4 LASL	S4 ORNL	S4 WADCO	S4 WARD	VIM
k_{eff}	0.9681	0.9668	0.9688	0.9725	0.9880	0.9654	0.9600	0.9649	0.9650	0.9664
$\frac{\sigma_{f238}}{\sigma_{f235}}$	0.0301	0.02980	0.0297	0.0293	0.0293	0.0298	0.0283	0.0297	0.0300	0.02948
$\frac{\sigma_{f239}}{\sigma_{f235}}$	0.916	0.916	0.907	0.920	0.915	0.915	0.926	0.921	0.921	0.922
$\frac{\sigma_{f240}}{\sigma_{f235}}$	0.229	0.229	0.226	0.225	0.226	0.228	0.226	0.226	0.227	0.229

Apparent source settling difficulties encountered when ZPPR-2 was run at ANL-Idaho have been traced to the method of estimating k_{eff} (analog), rather than to actual source convergence problems. The track length estimate of k_{eff} experienced much greater stability with respect to initial fluctuations resulting from the starting source guess, as well as the reduced variance mentioned previously. This was done with the same analog random walks, thereby indicating that such analog random walks are quite adequate models from which to extract information, as long as efficient estimators are used. Further improvement, utilizing the collision estimator from these same analog random walks to determine the next generation source locations, has been outlined, and is now being incorporated into VIM.

Procedures have been outlined for the development of an unbiased fixed source for use in VIM to perform Doppler and perturbation calculations. The previously mentioned improvements in source estimation will have their major effect here. A brief outline of our present thinking on fixed source generation follows.

Proposed Procedure to Obtain Unbiased Fixed Source

Use Cumulative Production Method, as follows:

- 1) Start with guess, as we do now
- 2) Set up source regions in simple geometry (sphere or cylinder), restricted to one or two dimensions, if possible, to reduce storage
- 3) Store production from first generation into regions (preserving $\bar{r}$ and $\bar{z}$, if desirable), only upon completion of the generation
- 4) Start second generation by selecting from first generation distribution; and, upon completion of generation, add neutrons produced in this generation to those of first generation
- 5) Start succeeding generations from cumulative source distribution.

Potential Problems

Some of the source is from unsettled generations. There is no automatic way to remove this bias. A possible solution is as follows:

- 1) Use track length or collision estimation to obtain source as previously, without combining generations
- 2) Compute variance and σ_{mean} for first generation (on k_{eff}) (using single history estimates)
- 3) Do same for second generation; see if results of two generations agree statistically (i. e., within $1\sigma_m$)
- 4) When four or five successive generations agree statistically, assume source is settled, and accumulate successive generations.

In heterogeneous problems, source regions will not line up with zones containing fissionable material. This may not matter, on a statistical basis; but is wrong, on a single collision. This difficulty can be circumvented by selecting coordinates only in zones containing fissionable isotopes, rejecting coordinate sets which do not meet this constraint. While this is less efficient, it will not noticeably increase running time, since it occurs only once per history. This method permits collision or track length estimation of source, whether or not it is accumulated.

Modifications were made to the editing routines of VIM, extending the number of regions in which multigroup constants may be calculated to eight. The cylindrical version of VIM was converted for use on the CDC 7600, and was modified so that it can now be used for analyzing homogeneous benchmark representations of assemblies such as ZPPR-2. As a checkout run, the 2-dimensional cylindrical benchmark model of ZPPR-2 was prepared, and submitted for execution on the CDC 7600.

Procedures have been outlined for the development of an infinite medium version of VIM for several purposes:

- 1) To produce multigroup constants comparable to MC² type calculation. VIM can then be run from 0 to 3 dimensions, to see the effect on cross sections.
- 2) These VIM results will serve as a means of isolating data handling differences from geometric effects.
- 3) It will prepare spectra in infinite media of pure scatterers for various plate types used in fast criticals. This is what our adjoint technique requires to produce unit weights.

An abstract, "The Probability Table Method for Treating Unresolved Resonances in Monte Carlo Criticality Calculations," has been accepted for presentation at the American Nuclear Society Winter Meeting, in Miami. An abstract, "The Application of the Cross-Section Probability Table Method to Describe Unresolved Resonance Data for Use in Monte Carlo Calculations," was written, and submitted to the AEC for the IAEA meeting to be held in Vienna in January of 1972.

An extension of the probability table method for unresolved resonances has been developed which permits fission, scattering, and capture cross sections to be selected from Gaussian distributions centered about the table entry. It has not been shown that such a procedure is required, but was developed as a more feasible alternative to multidimensional tables which have been proposed.

A meeting was held with the ANL Monte Carlo Committee, on the subjects of applicability of the Probability Table Method to Doppler coefficient calculation, and present and future capability of VIM to compute heterogeneity effects in fast critical assemblies. Presentations at the meeting included the results of computations of variances and covariances of reaction cross sections obtained from unresolved resonance ladders and their corresponding probability tables, as well as construction of two possible methods of more closely approximating the fluctuations of fission cross sections in the tables.

At the meeting, ANL Monte Carlo Committee received a clearer picture of the details of both the probability table method and the multigroup edit version of VIM than they previously had. Agreement was reached on which areas required further testing, which areas required further development, and the need for applying VIM to analysis of ANL Fast Critical Experiments.

III. EVALUATION OF EFFORT TO DATE

Conversion of VIM to the CDC 7600, followed by its successful analysis of ZPR3-48 and ZPPR-2, places us in the position of having the VIM-1 code operational on several large present-generation computers. The new detailed edits, made possible by increased computer storage capability, have clearly shown VIM to be capable of providing design information with high precision. This information is usually obtained only in an approximate manner for greatly simplified models of critical experiments.

We are now using VIM as a structural base, developing methods to handle central rod worth and Doppler experiments. This will lead to a VIM code system with a common library and modular construction, which will permit more accurate design information to be obtained in a routine manner.

IV. NEXT REPORT PERIOD ACTIVITIES

Implementation of the fixed source generation procedures outlined here will proceed. An infinite medium VIM code will be extracted out of the present spherical version, and used initially as a data testing vehicle. It will later form a base for development of our adjoint procedures and adjoint weighting functions. A journal article on the cross-section probability table method will be prepared, and submitted for publication.

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