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Atomics International
North American Rockwell

P.O. Box 309
Canoga Park, California 91304

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CONTENTS

<u>AEC Task No.</u>	<u>Project Title</u>	<u>Page</u>
5-B	Reactor Physics, Fast-Reactor Physics Experiments. . . .	5
5-E	Theory and Computation for Reactor Analysis and Design	16
26-A	Cross-Section Analysis	20

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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 1970		
General Order:	7701	Subaccount:	14610
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Principal Investigators: T. H. Springer, R. J. Tuttle, L. A. Mountford,
H. N. Royden

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 REPORTING PERIOD

A. EXPERIMENTAL STUDIES

No experimental investigations were conducted during this quarterly reporting period because disassembly of Core 17 and the square matrix system was carried out in preparation for the installation of the hexagonal matrix for Core 20 which has a hexagonal pin-type fuel element in the test region.

B. DATA ANALYSIS

The central reactivity worths of a wide variety of samples placed in Core 18, the Na-voided version of Core 17, were analyzed and are compiled in Table 1. As would be expected, the specific worth of Pu increased in the Na-voided core relative to the Na-filled core. The increase in reactivity worth was about 11%. The worth of Ta, on the other hand, became somewhat less negative, the change being of the order of 14%. A 184-gm sample of ^{238}U exhibited a similar change. Its worth in Core 18 was 13% less negative than it was in Core 17.

TABLE 1
SPECIFIC WORTHS OF SOME MATERIALS IN CORE 18

Sample	Mass of Isotope (gm)	Specific Worth (¢/gm)	
Carbon	17.0468	-4.66×10^{-4}	$\pm 0.21 \times 10^{-4}$
Aluminum	26.3816	-4.822×10^{-4}	$\pm 0.13 \times 10^{-4}$
Oxygen*	15.6503	-6.997×10^{-4}	$\pm 0.23 \times 10^{-4}$
Inconel-750	81.5572	-4.669×10^{-4}	$\pm 0.043 \times 10^{-4}$
Stainless Steel	77.8543	-3.577×10^{-4}	$\pm 0.044 \times 10^{-4}$
Tantalum	163.7868	-3.1076×10^{-3}	$\pm 0.0021 \times 10^{-3}$
^{235}U	59.0070 (0.250-in. diam by 4.00-in. long)	$+0.98576 \times 10^{-2}$	$\pm 0.00061 \times 10^{-2}$
^{235}U	183.3142 (0.438-in. diam by 4.00-in. long)	$+0.99554 \times 10^{-2}$	$\pm 0.000221 \times 10^{-2}$
$^{235}\text{U}^\dagger$	89.2407 (0.436-in. diam by 4.003-in. long)	$+0.97778 \times 10^{-2}$	$\pm 0.00050 \times 10^{-2}$
$^{239}\text{Pu}^\S$	58.3744 (0.358-in. diam by 3.64-in. long)	$+1.4403 \times 10^{-2}$	$\pm 0.0010 \times 10^{-2}$
$^{239}\text{Pu}^\S$	58.3744 (0.375-in. diam by 3.79-in. long)	$+1.4450 \times 10^{-2}$	$\pm 0.0011 \times 10^{-2}$
^{238}U	184.7329 (0.438-in. diam by 4.00-in. long)	-7.007×10^{-4}	$\pm 0.018 \times 10^{-4}$

*In the form of Al_2O_3 .

†In the form of $^{235}\text{UO}_2$ and corrected for oxygen.

§In the form of $^{239}\text{PuO}_2$ and corrected for oxygen. Not corrected for higher Pu isotopes. Sample is 91.4% ^{239}Pu , 7.9% ^{240}Pu , 0.66% ^{241}Pu , and 0.04% ^{242}Pu .

A paper dealing with the measurements of the change in the specific worth of Ta as a function of S/M, was prepared and was accepted by the ANS for presentation at the Winter Meeting. The paper discusses the measurements of the reactivity worth of Ta over a range of variation of surface-to-mass of about 5000. The results of these studies have been reported in previous Quarterly Reports as well as in the Annual Report for GFY 1970.⁽¹⁾ Computational comparisons and studies relative to these experiments were continued during this reporting period and are described in the next section.

A correction factor of 9.2% was calculated to account for the contribution made by fast neutrons to the energy deposited in the Li^7F TLD detectors used to measure the heating rate in the Ta control rod mockup.⁽¹⁾

C. ANALYTICAL STUDIES

Calculations of the reactivity worth of several ^{235}U , ^{238}U , and PuO_2 samples in Cores 14, 15, 16, and 17 were completed using the modified cross sections obtained from the ESCAPE code. These calculations take into account self-shielding and self-multiplication of the smoothly varying portion of the cross section and were performed for the purpose of comparing the results with those obtained from the TRIX code cross sections.

Work was initiated to modify the ESCAPE code in such a way that it will treat samples containing more than one isotope.

The calculation of Core 17 flux-weighted cross sections for several $N\ell$ values of Eu_2O_3 were completed. These cross sections will be used in the calculation of the reactivity worth of Eu_2O_3 over a range of $N\ell$ values where experiments were recently conducted.⁽¹⁾

First-order perturbation calculations of the worth of tantalum, using unperturbed real and adjoint fluxes and self-shielded cross sections, show excellent agreement with the experiments for samples with $N\ell$ values of 0.033×10^{-24} atoms/cm² or less (i.e., for cylindrical samples less than 0.250-in. diam). Above this diameter, while the measured specific reactivity continues to decrease logarithmically with thickness, the calculation decreases less rapidly. For the largest single sample (1.775 in. diam by 4.0 in. long) the first-order perturbation value is 23% higher (more negative) than the experimental value.

7701-46178

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

The self-shielded cross sections were produced by GRISM, which uses TRIxie for resonance self-shielding and then produces group-averaged cross sections with fine-group spectrum weighting. Cross sections above and below the resonance energy range (that is, above 67 kev and below 3 ev) were self-shielded by means of ESCAPE, a collision-probability code. Variations on these methods have shown the calculated worth of the thick samples to be insensitive to the resonance treatment.

In order to obtain better agreement with the experiments, calculations were carried out during this reporting period using the exact perturbation method. This method differs from first-order perturbation calculations in that either the unperturbed real or adjoint flux is replaced by its perturbed values. The perturbed real flux was used for these calculations, being calculated by CAESAR, as before, except that the central void contained a tantalum region simulating each sample in atomic thickness and mass. The correctly-self-shielded tantalum cross sections were used for these calculations. The volume-averaged real flux for each sample was then combined with the unperturbed adjoint flux and self-shielded cross sections in a perturbation calculation.

The exact perturbation calculations produced considerably better agreement, not only in magnitude, but also in curvature, as can be seen in Figure 1. The discrepancy for the largest single sample was reduced from 23 to 9%.

Some preliminary and approximate calculations have shown that further improvement could result from properly self-shielding the inelastic scattering cross section. Use of the infinitely dilute cross section leads to an excessively softened spectrum in the calculations for large samples, which in turn leads to an overestimate of the worth.

Studies were made on the application of the Monte Carlo code VIM to the analysis of ECEL experiments. A procedure for incorporating the thermal scattering capability of the HWOCR-SAFE code into VIM, enabling VIM to be used in the analysis of fast systems with a thermal driver (such as ECEL Core 17 and Core 20) was outlined. Implementation of this procedure has been initiated. Work was also initiated on the incorporation into VIM of the thermal cross section data used in the HWOCR-SAFE code. This involves modification of the VIM cross section library tape generation procedures to include the HWOCR-SAFE generation procedures for the thermal range.

A three-dimensional version of the CCP Monte Carlo code for the calculation of the escape probability for a cluster of fuel rods has been written and is in checkout.

Calculations concerning the sensitivity of experimental measurements such as fission rates and reactivity worths to progressive sodium voiding in the ECEL pin-type core are being continued in preparation for the series of experiments scheduled to be undertaken in GFY 1972. Changes in k_{eff} were previously calculated to be very small as a function of progressive Na voiding in one half of the central pin-type fuel element of ECEL Core 20. The recent calculations show that the worth of ^{238}U will change by about 14% as a result of a 6-in.-high voided region. The worths of B and ^{235}U are relatively insensitive to the Na voiding.

A new version of RABBLE has been received from P. Kier of ANL. The version incorporates an improved regional slowing down source calculation which is more accurate and faster. Negative fluxes should not occur using the new version.

The flux-weighting version of TRIx has been run to completion successfully. The majority of checkout has been completed.

D. DOPPLER REVIEW

The GE-440 timesharing-computer version of DOPFIT has been combined with portions of the previous IBM-360 version to obtain a new IBM-360 code for processing large quantities of Doppler experimental data. This was done for two reasons. First, it is easier to prepare input for the 360-65 computer when the quantity of data is large; immediate turnaround is not required for large production runs. Second, graphical output is essential in evaluating the quality of calculated fits to the experimental points. (Chi-squared tests are not sufficient.) The CI-120 plotter associated with the 360-65 computer provides this capability. The combined version of the code, called DOPFIT-II, has been debugged and checked out. Minor bugs are still uncovered from time to time, as use of the code in production entails a great variety of input data and options. These are corrected as they arise.

A comparison of Doppler experiments done in sodium-present and sodium-voided spectra at two different critical facilities has been carried out with DOPFIT-II. These are ZPR-3-48 and -49 at ANL-Idaho and ECEL-17 and -18 at AI;

all have spectra representative of large, ceramic-fueled LMFBR's. Results are presented in Table 2.

TABLE 2
COMPARISON OF DOPPLER MEASUREMENTS ON
NATURAL UO_2 SAMPLES IN ECEL-17, -18,
ZPR-3-48, AND -49

Assembly	Doppler Coefficient, $C^*(\gamma = 0.9)$ ($10^{-4}/^\circ\text{K}$)	Temperature Nonlinearity Exponent, γ^*
ECEL-17 (sodium present)	2.19 ± 0.19	1.5 ± 0.6
ZPR-3-48 (sodium present)	2.37 ± 0.11	0.95 ± 0.16
ECEL-18 (sodium voided)	2.24 ± 0.32	1.8 ± 1.1
ZPR-3-49 [†] (sodium voided)	2.22 ± 0.09	0.84 ± 0.13

*C and γ are determined from least-squares data fits to the integral form of the following expression: $(1/\rho_0)(d\rho/dT) = C(T_0/T)^\gamma$.

[†]Based on data of J. M. Gasidlo et al, private communication.

The quantity C represents the best-fit Doppler coefficient at absolute temperature T_0 normalized to ρ_0 , the total worth of the Doppler sample at T_0 . The data do not determine the exponent γ , representing nonlinearity of reactivity with temperature, as accurately as the coefficient C. This result is expected; the exponent γ is analogous to a higher order coefficient in a polynomial fit. The inaccuracy in γ masks any possible small change due to the harder spectrum with sodium removed.

ECEL results for UO_2 have larger uncertainties than the ZPR-3 results because of the use of a smaller sample, which gives a smaller reactivity signal. The results for the coefficients C from the two facilities are in reasonably good agreement, as can be seen from the table. AI data were not accurate enough to give a good measurement of γ ; even so, the AI results for γ are consistent with the ANL results considering the uncertainties in the former.

The ZPR-3-48 result for C is about 7% higher than was reported in the previous quarterly. This change was due to a more careful determination of ρ_0 , the sample worth, by interpolation in a plot of specific worth vs effective sample

size. (ρ_0 was not measured.) The larger uncertainty in this C value results from uncertainties in this interpolation.

The results for C should not be taken to mean that the Doppler coefficient is independent of sodium voiding, because of the normalization to sample reactivity; the UO_2 samples were worth less in the sodium-voided assemblies.

A summary of the above work has been accepted for presentation at the 1970 ANS Winter Meeting in Washington, D. C.⁽²⁾

Corrections to critical-assembly Doppler measurements in UO_2 samples near room temperature due to crystalline-lattice effects have been investigated. A simple algebraic approximation for the effective temperature in a crystalline lattice has been derived. It is based on conclusions drawn by Schenter⁽³⁾ and many previous workers regarding the validity of a simple Debye approximation to the Dolling UO_2 phonon spectrum. The Debye temperature used has usually been derived from specific-heat measurements. In a very recent paper by Borgonovi, et al,⁽⁴⁾ it has been pointed out that this procedure leads to a serious overestimate of crystalline effects on the Doppler coefficient. The reason is that the higher frequencies in the phonon spectrum are associated primarily with motion of the oxygen atoms; these frequencies make important contributions to the specific heat, but obviously not to the Doppler effect, which is concerned only with motion of the uranium atom. For UO_2 , the Debye temperature for the Doppler effect turns out to be 300°K rather than the values 600 to 650°K derived from specific heat. The resulting room-temperature correction for crystalline binding in UO_2 is about a factor of five smaller than the correction (roughly 20%) based on the higher Debye temperature. The validity of the Debye approximation itself was confirmed by Borgonovi, et al.

The DOPFIT-II code has been used to analyze Doppler measurements in the following critical assemblies: ZPR-3-51, -53, and -59 (ANL-Idaho); ECEL-10, -12, -14, -15, and -16 (AI); FCA-3-1 (JAERI). Further analysis is needed before detailed results can be presented. Some preliminary remarks can be made about the ZPR-3-51 results, however. Measurements were made at the core center, halfway out to the reflector, and at the core-reflector interface. The Doppler coefficient decreased with increasing radius, as expected, dropping at the interface to about half its value at the center. The nonlinearity exponent γ

increased from 0.65 at the center to 0.81 at the interface; a higher value would be expected near the reflector because of the harder spectrum there. Very little change was found for either C or γ when the buffer surrounding the sample at the center was changed from nickel to stainless steel.

E. PREPARATION FOR FORTHCOMING EXPERIMENTS

All of the 2-in. by 2-in. square-matrix tubes in the central 9 by 9 array of both halves of the ECEL reactor system were removed and the hexagonal matrix system was installed in place. The matrix system was carefully realigned and then reclamped into place. This task completes the modification of the matrix system itself. Readjustment of safety rod mounting brackets must still be made along with minor relocations of other reactor components.

A partial shipment of UO_2 pellets (62 kg out of a total of 360 kg) was received during this reporting period. Columns of pellets were formed and successfully inserted into a pin-type fuel elements. Superficial examination of the pellets was conducted and indicated that the pellets are acceptable.

Fuel drawer loading diagrams for Core 20 were prepared and loading methods for transition region drawers, safety rods, and fuse blocks were tested.

Contact was made with the AEC Division of Reactor Licensing regarding our license amendment for Core 20 operation. No technical problems have been encountered, but some rewriting of the Technical Specifications will be required to get it into the presently accepted format.

Cladding of about 3 kg of PuO_2/UO_2 pellets has been initiated.* The pellets are being loaded into 8-in.-long by 0.250-in.-OD, Type 304 stainless-steel tubes that are insertable in the ECEL Core 20 pin-type fuel elements.

III. EVALUATION OF EFFORT TO DATE

The results of the Doppler Review task have thus far shown that Doppler measurements performed at ANL and AI are reasonably consistent for similar spectra. The systematically analyzed data from both of these laboratories, and possibly others, appear therefore to be useful in the generation of a consistent set of Doppler data for use by the reactor designer.

*Fabrication costs were funded by North American Rockwell Corporation.

Calculations concerning the experiments on Ta control rod worths continue to show that, as far as the critical experiment is concerned, exact perturbation and eigenvalue difference techniques are required to correctly predict the measured results. The reasonably good agreement obtained by these techniques may be construed as an indication that the Ta cross section set and the techniques are acceptable in reactor design work involving complex control arrangements such as 18-rod clusters.

The experimental results obtained with Eu_2O_3 have indicated that this compound may be superior to Ta as a control material, but the calculational comparison has not yet been completed. The validity of the existing cross-section data that would be required for the physics design of a Eu_2O_3 control system for a full-scale reactor has therefore not been established.

The uncertainties in heating rates in Ta control rods, as determined by TLD techniques in critical assemblies, remain fairly high ($\pm 20\%$), although it now appears that the fast neutron contribution to the dose is not large and that corrections for this factor can be made reliably.

Replacement of the 9 by 9 array of 2-in. by 2-in. matrix tubes at the core center with the hexagonal matrix system proceeded smoothly with no major problems. The investigation of the spectrum in the pin-type test region of Core 20 is therefore expected to be undertaken on schedule.

IV. NEXT REPORT PERIOD ACTIVITIES

The assembly, checkout, and operation of the pin-type Core 20 will be accomplished and spectrum measurements will be completed. Studies of full-size Ta control rods in the center of the pin-type test region will be initiated.

A final report covering the Doppler Review Task will be prepared and issued.

Calculations of the reactivity worth of the Eu_2O_3 samples in Core 17 will be completed and used for comparison with the experiment, and a report on the Ta calculation and experiment will be prepared.

Work on the application of the VIM code to the analysis of ECEL Core 17 experiments will be continued.

REFERENCES FOR TASK 5-B

1. "Annual Technical Progress Report, LMFBR Physics Programs, GFY1970," AI-AEC-12969, August 15, 1970
2. R. J. Tuttle and T. H. Springer, "The Reactivity Worth of Ta in a Fast Reactor Spectrum," to be presented at the American Nuclear Society Winter Meeting, Washington, D. C., November 16-19, 1970
3. R. E. Schenter, "Effects of UO₂ Crystalline Binding on Doppler Coefficients Calculations for Fast Reactor Systems," BNWL-442
4. G. M. Borgonovi, D. H. Houston, J. U. Coppel, and E. L. Slaggie, "Crystal Binding Effects on Doppler Broadening of Neutron Absorption Resonances," Phys. Rev. C1 (1970), pp 2054-2059

Program:	Reactor Physics		
AEC Task:	5-E — Theory and Computation for Reactor Analysis and Design		
Project Manager:	H. A. Morewitz		
Reporting Period:	July-September 1970		
General Order:	7701	Subaccount: 14320	AEC Category: 04-01-61-02.1

Principal Scientists: 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 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. PROGRESS DURING REPORT PERIOD

Arrangements were made to run the VIM code on the Lawrence Radiation Laboratory CDC 6600 at Berkeley. Certain modifications to VIM were found to be necessary due to operating system differences between the LRL computer installation and the Los Angeles Data Center or Kirtland Air Force Base installations. Initialization loops were inserted to allow the proper use of VIM-1 since provision has not been made at the LRL installation for setting the computer core to zero before execution of the code. All versions of the VIM code are now operational on the LRL CDC 6600.

A paper titled, "Monte Carlo Eigenvalue Calculations of Fast Critical Assemblies Using VIM-1," was presented at the ANS annual meeting on July 1, 1970.

Work continued on a topical report discussing benchmark critical assembly studies using VIM-1. Additional ZPR-3-48 runs were made at Kirtland Air Force Base and at Lawrence Radiation Laboratory as a part of this study.

A cylindrical benchmark calculation of ZPR-3-48 has been run at LRL and a detailed comparison of the results of it, a heterogeneous cylinder calculation (ANL ZPR-TM-4, Figure 10), and previously reported heterogeneous and homogeneous versions, is now being made. One result that appears to be emerging is that the use of an "average" blanket composition, as opposed to separate axial and radial blanket compositions, permits more leakage and is only slightly more reactive, though it contains 9% more Pu^{239} .

The effect of cylindricizing core and blanket outlines has been examined and found to be small on k_{eff} but differences were observed in all core vs blanket effects, including absorption, reactivity, and total flux. Cylindricizing core and blanket outlines increased core and decreased blanket contributions, with a small net increase in k_{eff} .

The modifications for monitoring group averaged total and absorption cross sections have been made and checked out in VIM-1. In typical 35000-50000 history runs it has been observed that group fluxes integrated over large regions (such as core and blanket) have converged remarkably well in all important groups. These fluxes show probable statistical errors of only 1 to 2% for these runs, and due to natural physical correlation from one group to another, excellent spectral plots have been obtained. At the same time, $\nu\bar{\Sigma}_f$'s for core and reflector were obtained with a statistical uncertainty of about 5% or less in all but the very lowest energy groups. $\bar{\Sigma}_a$ and $\bar{\Sigma}_t$ behaved even better. These results were obtained without the aid of the most appropriate estimation procedures for obtaining group constants. Considerable improvement could be obtained with a small increase in running time per history by using such estimation procedures and the necessary coding procedures are now being outlined. It seems clear, therefore, that VIM can be used to obtain group cross sections simultaneously with other reactor parameters, providing a viable alternative to present analytic methods as well as a valuable check of these methods since the statistical quality of the group cross sections obtained by VIM can be improved considerably by the optimization of the appropriate estimators without unduly compromising the efficiency of the code in performing criticality studies.

Consultations were held with F. L. Fillmore regarding the use of VIM-1 in the analysis of fast critical assemblies at ANL-Idaho. A VIM-1 neutron cross section tape based on ENDF/B (Version I) data for U^{238} , U^{235} , Pu^{239} , Pu^{240} , Pu^{241} , C, Na, Fe, Cr, Ni, Mo, and Al was generated on the PSD IBM 360/65 and sent to ANL-Idaho for use on their IBM 360/75. A VIMB run was made for the generation of cross sections for oxygen based on ENDF/B version I data. Oxygen will be added to the VIM-1 cross section tape in preparation for ZPPR-2 runs to be made in the near future at ANL-Idaho. VIM-1 is now operational at ANL-Idaho.

The version of the VIM-1 code which allows one to calculate homogenized critical assemblies while preserving the irregular outline between core and blanket has been combined with the heterogeneous version of the code. The COMMON and DIMENSION statements of the VIM-1 code have been rewritten to allow more efficient usage of the code on both the IBM 360 and the CDC 6600. This was done in order to hold to a minimum the differences between the codes for the two computers. The input requirements for the spherical and cylindrical geometry versions of VIM-1 were simplified and made to conform as closely as possible to the heterogeneous version of the code.

All quantities tallied in VIM-1 were listed and are now calculated in double precision on those computers whose single precision word size is not adequate (i.e., IBM System 360).

Work continued on the method for treating cross sections in the unresolved resonance region. A subroutine was written and checked out which generates a ladder of pseudo-resolved resonances in a narrow energy range of the unresolved resonance region. The interface between this subroutine and the UNIDOP program (which generates Doppler broadened point cross sections) was checked out. The subroutine for generating cross section probability tables for the unresolved region based on the UNIDOP output has been written and checked out.

Reports on FTR assemblies were studied in preparation for running a VIM-1 calculation of the FTR-4 critical assembly when the "as-built" composition and loading diagrams become available.

III. EVALUATION OF EFFORT TO DATE

The recent addition of group cross section monitoring into VIM-1 and the encouraging results (re: convergence) indicates that VIM can be used as a source of multigroup data. Thus the decision to use point cross section data rather than multigroup data in the data library for the VIM series of codes is well justified. Furthermore, since computer high speed memories are getting larger as well as faster, the strain on computer resources to produce point cross section libraries will diminish rather than increase and the decision to go this route will pay off in steadily improving descriptive and computational capacity resulting from updated versions of the VIM library. The one obstacle to the use of point cross section data, the unresolved resonance region, is being handled by applying a probability table approach, in the development of which steady progress is being made.

The statistical quality and reasonability of the results obtained with VIM thus far, along with its successful operation on both IBM 360 and CDC 6600 computers indicates that it is now ready to be used for the implementation of perturbation, adjoint, and optimized estimation procedures needed for the solution of difficult fixed source problems and others in which small changes in k_{eff} must be accurately calculated.

IV. NEXT REPORT PERIOD ACTIVITIES

A revised VIM-1 users manual and source deck will be sent to the Argonne National Laboratory code center. The probability table treatment of unresolved resonances will be completed and inserted into the VIM library while the necessary code modifications will be made in the VIM-1 program to utilize this procedure. Work will begin on the use of optimized estimators in VIM for reducing the variance in computed group cross sections. The implementation of perturbation Monte Carlo by a fixed source version of VIM will be initiated.

A topical report on benchmark critical assembly studies using VIM-1 will be published.

Leo B. Levitt and Jerome Spanier will participate in a panel discussion entitled, "A Random Sampling of Ideas," at a Monte Carlo Seminar at ORNL, October 5-7, 1970.

Program: General Reactor Physics
AEC Task: 26A, Cross Section Analysis

Project Manager: H. A. Morewitz

Reporting Period: July-September 1970

General Order: 07762

Subaccount: 13130

AEC Category: AT(04-3)-701

Principal Scientists: H. Alter, C. L. Dunford, P. F. Rose

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 multi-group 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. MAJOR ACCOMPLISHMENTS IN FISCAL YEAR 1970

Not applicable.

III. PROGRESS DURING REPORT PERIOD

Resonance region (below 100 kev) neutron cross section data for Ta^{181} , Ta^{182} , W^{182} , W^{183} , W^{184} , and W^{186} have been evaluated for the ENDF/B data files. Sections of the reports documenting these new ENDF/B evaluations have been drafted.

The evaluated 2200 m/s cross sections are given in Table 3. Negative energy resonances were devised so that the thermal range cross sections can be generated from resonance parameters. Good agreement with measured data was obtained in all instances (Figures 2 through 7). For W^{186} the neutron width of the 18.81 ev resonance was adjusted from 0.30 to 0.28 ev to obtain agreement, since values calculated from positive energy resonances alone were otherwise too large.

TABLE 3
EVALUATED 2200 m/s CROSS SECTIONS FOR TANTALUM
AND TUNGSTEN ISOTOPES (BARNs)

Isotope	Cross Section			
	σ_c		σ_s	σ_t
	Positive Energy Resonances	All Resonances		
Ta^{181}	16.3	21.1 ± 3.0	6.3 ± 1.0	27.4 ± 3.0
Ta^{182}	8215.	8250 ± 600	32 ± 25	8282 ± 600
W^{182}	14.4	20.5 ± 0.5	11.6 ± 1.0	32.1 ± 2.0
W^{183}	8.6	10.0 ± 0.3	3.4 ± 1.0	13.4 ± 1.0
W^{184}	0.8	1.8 ± 0.2	3.9 ± 1.0	5.7 ± 1.0
W^{186}	40.2	37.5 ± 2.0	$0.4^{+2.0}_{-0.2}$	37.9 ± 3.0

The evaluated potential scattering cross section of the tantalum isotopes, 8.5 ± 1.0 barns, is based on measurements made on natural tantalum. The value of 8.0 ± 20 b for tungsten isotopes is based on optical model theory and comparison of calculated and measured total cross sections at 100 kev. The current ENDF/B value of 5.0 b is apparently due to an erroneous use of the thermal scattering cross section for the potential scattering cross section.

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Figure 2. Calculated and Measured Neutron Cross Sections of Ta^{181} Between 0.002 and 1.0 eV

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Figure 3. Calculated and Measured Neutron Capture and Total Cross Sections of Ta^{182} Between 0.01 and 3.0 eV

Figure 4. Comparison of Calculated to Measured
Neutron Cross Sections of Tungsten-182
Between 0.01 and 1 ev

Figure 5. Comparison of Calculated and Measured
Neutron Cross Sections of Tungsten-183
Between 0.01 and 3 ev

Figure 6. Comparison of Calculated and Measured Neutron Cross Sections of Tungsten-184 Between 0.01 and 3 eV

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Figure 7. Comparison of Calculated and Measured Neutron Cross Sections for Tungsten-186 Between 0.01 and 10 eV

Average values of Γ_γ , D , and the strength function $s = \langle \Gamma_n^0 \rangle / \langle D \rangle$ were derived from the resolved resonance data. Results are summarized in Table 4. The upper limits of the resolved resonance range are increased appreciably from the version 1 ENDF/B files for tungsten. The new limits are about 4500, 760, 3000, and 3500 ev for W^{182} , W^{183} , W^{184} , and W^{186} , respectively, compared to current limits of 281, 287, 2100, and 334 ev.

TABLE 4
AVERAGE PARAMETERS FROM RESOLVED RESONANCES

Isotope	$\langle D \rangle$ (ev)	$\langle \Gamma_\gamma \rangle$ (mv)	$\langle \Gamma_n^0 \rangle / \langle D \rangle$ (ev) ^{1/2} · 10 ⁴
Ta ¹⁸¹	4.4 ± 0.5	56 ± 2	1.8 ± 0.3
Ta ¹⁸²	3.5 ± 1.2	67 ± 20	1.0 ± 0.7
W ¹⁸²	62 ± 12	63 ± 7	2.4 ± 0.6
W ¹⁸³	15.5 ^{+1.5} ₋₃	66 ± 10	2.44 ± 0.86
W ¹⁸⁴	69 ⁺¹⁰ ₋₅	68 ± 4	2.6 ± 0.7
W ¹⁸⁶	80 ⁺²⁰ ₋₄	65 ± 7	2.4 ± 0.6

Resolved levels were analyzed using plots of the number of resonances below a prescribed energy vs energy. These 'level density' plots typically have a steep section at low energies, a nearly linear section over a large energy range at higher energies, and a section of gradually decreasing slope at still higher energies, Figure 8. The plots were interpreted to mean that at low energies some p-wave resonances are resolved, at higher energies almost no p-wave but nearly all s-wave resonances are resolved, and above the linear section some s-wave resonances are unresolved. The reciprocal of the slope of the linear section was taken to be the average s-wave level spacing and the $E = 0$ intercept to be the number of resolved p-wave resonances. The resonances having the smallest scattering widths were assumed to be the p-wave resonances and were deleted. The high energy limits of the resolved range were taken where 80% of the scattering level widths are resolved. The smaller 20% does not contribute appreciably to the cross sections, and can thus be neglected.

Figure 8. Number of Experimentally Identified W^{182} Resonances Below a Given Energy vs Energy

Measured cross sections in the unresolved resonance range have also been evaluated. Cross sections calculated from unresolved resonance parameters were fitted to the measured data by varying $\langle \Gamma_\gamma \rangle$, $\langle D \rangle$, s_0 , s_1 , and s_2 . Fits within the range of measured values were obtained with energy independent strength functions. The results are shown in Figures 9 through 13.

The inelastic scattering levels at 6.3 kev in Ta¹⁸¹ and 16 kev in Ta¹⁸² were ignored. These levels involve a change of parity and are thought to have low excitation. No measured cross sections for these levels were found. This omission allows the upper end of the unresolved resonance range to be extended to ~ 100 kev for all isotopes except W¹⁸³ (46.5 kev) without inelastic scattering interference. This is convenient because the ENDF/B format does not permit unresolved resonance parameters for inelastic scattering. The current upper limits are 10 kev.

Resonance integrals above 0.5 ev were calculated from evaluated parameters and compared to an evaluation of several measured values. The results are given in Table 5. Agreement within experimental error was obtained for all except W¹⁸⁴.

TABLE 5
COMPARISON OF CALCULATED AND MEASURED
RESONANCE INTEGRALS
(barns)

	Isotope				
	Ta ¹⁸¹	W ¹⁸²	W ¹⁸³	W ¹⁸⁴	W ¹⁸⁶
Negative Energy Resolved	1	2	0	0.3	0
Positive Energy Resolved	709	593	345	14.9	521
Unresolved	13	2	20	1.5	1
Calculated Total	723	597	365	16.7	522
Measured	740 $\pm$ 40	590 $\pm$ 10	380 $\pm$ 15	13 $\pm$ 2	490 $\pm$ 50

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Figure 9. Comparison of Measured Capture Cross Sections of W^{182} with Values Calculated Using Evaluated Unresolved Resonance Parameters

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Figure 10. Comparison of Measured Capture Cross Sections of W^{183} with Values Calculated from Evaluated Unresolved Resonance Parameters

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Figure 11. Comparison of Measured Capture Cross Sections of W^{184} with Values Calculated from Evaluated Unresolved Resonance Parameters

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Figure 12. Comparison of Measured Capture Cross Sections of W^{186} with Values Calculated from Unresolved Resonance Parameters

*Below 3 kev points plotted are averages of 20 measured points.

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Figure 13. Comparison of Measured Capture Cross Sections of Ta^{181} with Values Calculated from Evaluated Unresolved Resonance Parameters

To aid in the current ENDF/B evaluation for the isotopes of tantalum and tungsten and in order to apply the results to future ENDF/B cross section evaluations, a number of approaches to provide tools needed for the visual evaluation of measured and calculated data have been assessed. These include check-out and evaluation of the CDC 6600 computer programs SCIREF, SCIBIN, and SCIDAT, evaluation of an ORTHOMAT mechanical plotting program, and modification of an existing CRT program to plot data directly from a SCISRS tape. This last approach has been successfully completed.

Features of this program include an initial reading of all pertinent SCISRS data into core, extensive searching of data is thus done with rapid core access as opposed to data accessed by tape or disk; variation of the computer core region size required as related to the amount of data to be evaluated at any given time; linear averaging of data, 1, 2---5---10---30 increments of the data are averaged to remove much of the structure; and overlay of plots. The latter is very important for the performance of evaluations in reasonable time spans. The program was further modified to read cross section data calculated from the COMNUC code, read miscellaneous input data, plot and cross plot combinations of the above, sum discrete inelastic excitation functions, and process and manipulate differential elastic scattering data as such or generated from Legendre coefficients. Several normalizations for the Legendre expansions are permitted.

The program has been used to complete the plotting and evaluating of the available high energy tantalum data and is currently being used to plot the high energy data for the tungsten isotopes. The plots form the basis for the high energy data evaluation and will be used for documentation purposes.

Deformed optical model calculations for Ta^{181} were completed. The 4 PLUS code was used in place of JUPITOR, which proved to be difficult to work with and required excessively long running time per calculation. 4 PLUS does the required calculations faster and provides the necessary input data for compound nucleus theory calculations.

Energy-dependent optical model parameters for a two-level deformed model of Ta^{181} were determined. These parameters gave a good representation of the total cross section at energies above 500 kev. Deformed nucleus optical model calculations for two coupled channels were used to obtain total elastic and

compound-nucleus formation cross sections along with the associated transmission coefficients for energies ranging from 100 kev to 17 Mev. Statistical compound nucleus theory as described in AI-AEC-12931⁽¹⁾ was used to separate the compound nucleus cross section into its component parts from 100 kev to 3 Mev. Legendre coefficients from compound-nucleus and direct calculations agree well with the data of A. B. Smith at low energies. Inelastic and capture cross sections obtained from the compound-nucleus calculation also agreed well with available measurements.

Merging of recent tantalum cross section data into one SCISRS file was completed. Small errors in the Ta¹⁸¹ SCISRS data tape continue to be bothersome. The latest was a factor-of-ten error in the elastic cross sections compared to those given in ANL-7363.⁽²⁾ Similar efforts for the tungsten files are also underway. Cross section uncertainties were converted to a consistent readable format and data for all tungsten isotopes were merged to facilitate comparisons with the natural tungsten cross sections.

A short computer program was written to tabulate the experiments and corresponding data on a SCISRS tape.

Detailed analysis of the Ta¹⁸¹ cross section was completed. Cross checks of the different reactions with the total cross section were made. Due to the scarcity of data, deduction of the reaction cross sections is a formidable task which has been aided by theoretical calculations. Extensive comparisons of Ta¹⁸¹ theoretical cross sections to the evaluated error bands of the experimental data have indicated areas of disagreement. Results of additional theoretical calculations were used to resolve the anomalies.

Telephone discussions with C. W. Reich of Idaho Nuclear have confirmed their recommended Ta¹⁸² level scheme (IN-1317).⁽³⁾ Some questions arose about the failure of their rotational bands to give I(I+1) proportionality. Dr. Reich pointed out that this is due to "coriolis-mixing" and that by accounting for this mechanism he was able to calculate the energy levels very closely. A level diagram for the Ta¹⁸² nucleus was needed as input to calculate Ta¹⁸² inelastic scattering cross sections.

Surveys of tungsten cross section data show a paucity of information. This increases the importance of the relatively abundant elemental tungsten cross

section measurements. Therefore elemental tungsten data for many neutron energies and reaction types are being evaluated. This approach will help to fill in gaps in isotopic data as well as produce agreement with the elemental data.

Theoretical calculations to aid in the evaluation of the tungsten isotopic cross section data are progressing. Additional hand-transcription of results onto computer cards was completed for subsequent evaluation and use.

A short study of the "direct interaction" mechanism was completed. The goal was to provide a theoretical basis for filling in the capture data gap between 5 and 14 Mev. Investigation shows it is reasonable to choose an average 14 Mev value from among neighboring nuclei. This cross section is assumed to be predominantly due to direct interaction. One then assumes the direct interaction cross section to be virtually constant with energy until about 5 Mev where the compound nucleus mechanism competes. For the latter mechanism both data and theoretical calculations are available. This approach is largely due to Lane.

ENDF/B Version 2, tapes 202, 203, and 204 were received from BNL and converted to EBCDIC, 9 track tapes. Each tape was processed by CHECKER. Plots of the data on tape 203 were obtained from EDIT.

A version of MC² which will accept the Version 2 ENDF/B formats was received from ANL. The code was not suitable for our requirements. The areas of the code which reflect a change in programming due to the Version 2 ENDF/B formats were investigated and have been incorporated into the RPI version of MC² which is currently in use at Atomics International.

An updated version of SCORE has been created which utilizes the new Fortran Graphics Subroutine Package previously described. Checkout of this version of SCORE was carried out during the month of July at the AEC computing facilities in Idaho Falls. Most of the program errors were detected at that time and corrected. In order to complete the checkout of this version of SCORE, the system was made operable at North American Rockwell's Space Division. It is planned that SCORE, Version 1, be released along with adequate documentation during the next quarter. Meanwhile, in addition to the checkout of the inclusion of the new graphics package, several minor improvements involving retrieval and display of angular data, insertion of nodes for curve fitting, and print-out of Legendre fits to angular data will be completed.

An improved version of the Idaho Nuclear computer program, used to adjust parameters for the Reich-Moore and Breit-Wigner resonance models, has been included and tested in an older version of SCORE. This option has been successfully tested. Minor modifications will be required to include this updated package in SCORE III. It is planned that the release version of SCORE will contain this version of SAP.

During this reporting period, a two-day conference was held at Aldermaston Weapons Research Establishment to discuss their experiences using SCORE as an aid in the evaluation of neutron data. They considered SCORE to be an extremely useful tool but improvements were needed in certain areas such as data output which previously has been given a very low priority. They demonstrated the hard copy feature which they have included in SCORE using an SC 4060 and stressed this feature as crucial to practical evaluation activities. A package for the SC 4020 and the CI 120 is now ready for inclusion as previously reported. A list of other suggested improvements was discussed and responsibility for incorporating the necessary changes assigned to either AI or AWRE depending on the special competence of each. Aldermaston will continue to report experiences and suggestions as their uses of SCORE increase.

A conference was also held at Kernforschungszentrum, Karlsruhe, concerning the use of SCORE for neutron data evaluation at that laboratory. We have recently sent a program tape to Karlsruhe but SCORE has not yet become operational because of difficulties in gaining access to the necessary hardware at Karlsruhe. Some of the difficulties were surmounted as a result of discussions with persons in the computing area. Within six months we should begin to receive some reports on their experiences with SCORE.

A plan for the inclusion in SCORE of parameter fitting of resonance data with the Adler model was outlined in discussions with Drs. Felix and Donatella Adler. Work has started on this plan and should be completed during this fiscal year.

A deficiency has been detected in the numerical method used by 4 PLUS to solve the set of coupled Schrodinger equations describing the neutron interaction with a deformed nucleus. This difficulty may arise when the incident neutron energy lies below the energy of one or more of the strongly coupled levels

(virtual excitation) because the "shooting method" for solving the differential equations is not stable in this case.

In order to resolve this problem, the equations have been recast as a two-point boundary value problem to be solved with a system of second-order difference equations. A block relaxation algorithm has been chosen to solve these difference equations to ensure stability. Necessary programming for inclusion in 4 PLUS has been completed and testing begun.

IV. EVALUATION OF EFFORT TO DATE

The completion of the cross section data evaluation for the tantalum isotopes will provide users of the ENDF/B data file an improved set of information. The most significant improvement, in addition to the updating of the Ta¹⁸¹ data file, was the production of a complete data file for Ta¹⁸². No such file was previously available. The information contained in these files is currently required by reactor designers to evaluate possible control rod worth configurations for LMFBR systems. The currently ongoing evaluation for the tungsten isotopes is well along and it is expected to be completed as scheduled.

A significant problem encountered in the work of the above evaluations was the aborted attempt to use the JUPITOR computer code (written and distributed by ORNL), as a theoretical aid. This unsuccessful attempt involved an unfortunate loss in both program-directed manpower and applicable computer costs. While success in operating the program on our local computer was finally attained, the cost per unit calculation was so great as to place normal use of this program beyond the scope of our current budget. Having once determined that this code could not practically be used as an evaluation aid, several 'in-house' computer codes were successfully combined to provide a simpler and less complete model than that available in JUPITOR for calculating the required data. The net result was that while the needed calculations were performed, the cost involved has produced a major budgetary perturbation.

A version of SCORE has been completed which will allow meaningful testing in practical neutron cross section evaluation situations. This version is now in the final testing stage. It contains many improved interactive mechanisms and a Fortran Graphics Subroutine Package. This package results from nearly a

year's experience with a more primitive system and will allow greater flexibility in programming new features for later versions of SCORE. New emphasis will be placed on providing useful output in card, printed or data set form. Work in areas of current responsibility including automated Adler resonance parameter fitting and the EXFOR experimental data format will continue.

V. NEXT REPORT PERIOD ACTIVITIES

The data evaluations for the isotopes of tantalum and tungsten will have been completed, the data sets sent to the NNCSC at Brookhaven and documentation published and distributed.

The evaluation of the Version 2 ENDF/B data files by intercomparison and correlation with the CSEWG specified benchmark fast critical assemblies will be near completion.

The tasks of interfacing the computer graphics code SCORE with both the CSISRS experimental data files at BNL and with the Adler-Adler resonance theory modules will continue. Documentation of Version 3 of SCORE will be completed.

REFERENCES FOR TASK 26A

1. C. L. Dunford, "A Unified Model for Analysis of Compound Nucleus Reactions," AI-AEC-12931, July 15, 1970
2. A. B. Smith, P. T. Guenther, R. Hayes, and J. F. Whalen, "Fast Neutron Scattering from Tantalum, Rhenium, and Platinum," ANL-7363, August 1967
3. R. G. Helmer, R. C. Greenwood, and C. W. Reich, "Ta¹⁸² Level Scheme," in "Nuclear Technology Branch Annual Progress Report, Period Ending June 30, 1969," Ed. R. M. Brugger and R. L. Heath, IN-1317, January 1970, pp 102-105