IDO-17009
September 1964

MASTER

325
11-12-64

A TRANSPORT STUDY OF THE NEUTRON FLUX,
ADJOINT, AND IMPORTANCE FOR
THE ADVANCED REACTIVITY MEASUREMENT FACILITY-II

N. C. Kaufman

PHILLIPS
PETROLEUM
COMPANY

ATOMIC ENERGY DIVISION

NATIONAL REACTOR TESTING STATION
US ATOMIC ENERGY COMMISSION

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

2.00
PRICE ~~\$.50~~

AVAILABLE FROM THE
OFFICE OF TECHNICAL SERVICES
U. S. DEPARTMENT OF COMMERCE
WASHINGTON 25, D. C.

LEGAL NOTICE

This report was prepared as an account of Government sponsored work. Neither the United States, nor the Commission, nor any person acting on behalf of the Commission:

A. Makes any warranty or representation, express or implied, with respect to the accuracy, completeness, or usefulness of the information contained in this report, or that the use of any information, apparatus, method, or process disclosed in this report may not infringe privately owned rights; or

B. Assumes any liabilities with respect to the use of, or for damages resulting from the use of any information, apparatus, method, or process disclosed in this report.

As used in the above, "person acting on behalf of the Commission" includes any employee or contractor of the Commission, or employee of such contractor, to the extent that such employee or contractor of the Commission, or employee of such contractor prepares, disseminates, or provides access to, any information pursuant to his employment or contract with the Commission, or his employment with such contractor.

PRINTED IN USA

IDO-17009
AEC RESEARCH & DEVELOPMENT REPORT
Reactor Technology
TID-4500 (32th Ed.)
Issued: September 1964

A TRANSPORT STUDY OF THE NEUTRON FLUX, ADJOINT, AND IMPORTANCE
FOR THE ADVANCED REACTIVITY MEASUREMENT FACILITY-II

by

N. C. Kaufman

PHILLIPS
PETROLEUM
COMPANY

Atomic Energy Division

Contract AT(10-1)-205

Idaho Operations Office

U. S. ATOMIC ENERGY COMMISSION

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

ABSTRACT

The ARMF-II reactor was studied using the S-XI neutron transport code. Core flux, adjoint, and importance distributions and neutron energy spectra were obtained with samples of PbO_2 , $\text{U}(238)\text{O}_2$, or ThO_2 in the sample position. The results of these calculations at selected energies and positions are presented in graphical form.

TABLE OF CONTENTS

	<u>Page</u>
Abstract	iii
Table of Contents.	iv
Index of Figures	v
Introduction	1
General Problem Formulation	1
S-XI Output Interpretation	6
Results and Discussion	7
APPENDICES	
Appendix A - Problems with S-XI Use	17
Appendix B - S-XI Input Parameters	20
References	21

TABLES

<u>Table Number</u>	<u>Description of Table</u>	
I	Size and Composition of ARMF-II Regions	2
II	Group Structure in Lethargy Space	4
III	Mesh Spacing ΔR in Mean Free Paths as Given in MIST(7)	18

INDEX OF FIGURES

<u>Figure No.</u>	<u>Description of Figure</u>	<u>Page</u>
1	ARMF-II reactor core diagram	3
2	ARMF-II reactor core divided into regions for representation in a cylindrical mockup	3
3	Vector directions used in an S_2 calculation	8
4	Real flux spatial distribution for entire reactor: groups 18 and 17	8
5	Detail of real flux spatial distribution in cadmium tube: groups 18 and 17	8
6	Adjoint spatial distribution for entire reactor: group 18	8
7	Detail of adjoint spatial distribution in cadmium tube: group 18	9
8	Detail of adjoint spatial distribution in cadmium tube: group 17	9
9	Real flux spatial distribution for entire reactor: group 15	9
10	Adjoint spatial distribution for entire reactor: group 15	9
11	Real flux and adjoint spatial distribution for entire reactor: group 10	10
12	Real flux and adjoint spatial distribution for entire reactor: group 2	10
13	Real flux spectrum in cadmium tube with PbO_2 sample.	10
14	Real flux spectrum in cadmium tube with ThO_2 sample.	10
15	Real flux spectrum in cadmium tube with $U(238)O_2$ sample	11
16	Adjoint spectrum in cadmium tube with PbO_2 sample.	11
17	Adjoint spectrum in cadmium tube with ThO_2 sample.	11
18	Adjoint spectrum in cadmium tube with $U(238)O_2$ sample	11

Index of Figures(Cont'd)

<u>Figure No.</u>	<u>Description of Figure</u>	<u>Page</u>
19	Importance spectrum in cadmium tube with PbO_2 sample	12
20	Importance spectrum in cadmium tube with ThO_2 sample	12
21	Importance spectrum in cadmium tube with $U(238)O_2$ sample	12
22	Real flux spectrum at 11.8 cm radius	12
23	Adjoint spectrum at 11.8 cm radius	13
24	Importance spectrum at 11.8 cm radius	13
25	Mesh point spacing distribution	19

ACKNOWLEDGEMENTS

The author wishes to express his appreciation to W. K. Foell for his help and advice throughout the course of this work. Special thanks are also due R. W. Goin (now with Argonne National Laboratory) for his help with the use of S-XI and to D. J. Aller for assistance in preparing the many graphs presented.

INTRODUCTION

The ARMF-II is a water moderated, U-235 fueled reactor.⁽¹⁾ Its active core consists of plate type uranium-aluminum assemblies arranged as shown in Figure 1. In the center of the reactor is a cadmium tube, 20 mils thick, into which various experimental samples may be inserted. The overall reactor system is designed to provide precision reactivity measurements on these samples.

To interpret activation and reactivity measurements on samples containing resonance absorbers in terms of the resonance integral of the various sample materials,⁽²⁾ it is necessary to know the relative values of the importance* in the cadmium tube for various neutron energies. Since these values cannot at present be determined experimentally, the use of computer calculations of the relative importance spectrum in the tube is required to make the necessary corrections. Furthermore, the required computer mockup can be used to provide data on the overall core flux and adjoint distributions.

Initially, a diffusion code, AIM-6,⁽³⁾ was considered for this work. But, because the gradient of the particle current must change very rapidly across the cadmium interfaces, it was felt that the results obtained would not be sufficiently accurate to correct precision data. Therefore, a transport code was needed, since it would consider in sufficient detail the transmission through the tube.

The particular transport code chosen was the one-dimensional S-XI⁽⁴⁾ code written by B. Duane. This code solves the Boltzman Transport Equation using the discrete S_n approximation.⁽⁵⁾ It is written for use on the IBM 7090 computer, which has a total memory of 32,000 words. Apart from the limitation of computer size, it can handle any number of energy groups and mesh points and provides great versatility with its many options.

General Problem Formulation

The particular geometrical arrangement of fuel used in the ARMF-II suggested that for use with a one-dimensional code the reactor core could

The importance will be defined as the product of the real flux and the adjoint at each energy and position: $\phi(r,u) \phi^(r,u)$.

be best represented by a collection of concentric annular regions. The criterion applied in the choice of region size was that each annular region contain the same area as the region in the reactor that it is to represent. Figure 2 shows the reactor divided into the regions to be considered as uniform composition. A six inch thick water region surrounding the reactor was used to describe the reflector. Table I presents the size, composition, and atom densities for each region in the S-XI code. The atom densities were the results of regional homogenizations.

TABLE I
Size and Composition of ARMF-II Regions

Region	Inner and Outer Radii in cm	Region Composition	Atom Densities atoms/cm ³
1	0 - 1.4732	(a) PbO ₂	N _{Pb} = .01 N _O = .02
		(b) ThO ₂	N _{Th} = .01 N _O = .02
		(c) U(238)O ₂	N _{Th} = .01 N _O = .02
2	1.4732 - 1.5240	Cd	N _{Cd} = .0464
3	1.5240 - 4.7244	131-gram fuel elements in water	N _{Al} = .022593 N _U = .0000794 N _O = .020857 N _H = .041714
4	4.7244 - 14.1224	179-gram fuel elements in water	N _{Al} = .022593 N _U = .0001085 N _O = .020857 N _H = .041714
5	14.1224 - 22.5552	57.14% 179- and 25-gram fuel elements in water plus 42.86% water	N _{Al} = .012910 N _U = .000115 N _O = .026259 N _H = .052518
6	22.5552 - 37.7952	All water	N _O = .033160 N _H = .066922

Figure 1

ARMF-II Reactor Core Diagram at Midplane

PPCo.-B-5957

Figure 2

ARMF-II Reactor Core as it was Divided into Regions for Use in the S-XI Computer Mockup

Eighteen energy groups were deemed to be sufficient to describe the reactor spectrum. Because it was anticipated that most problems in obtaining computer solutions would be experienced at the cadmium absorption energies and because the corrections for importance were to be made at the epi-thermal resonances of the sample materials, the group spacing was primarily designed to provide the most detailed data at the near-thermal energies. The uppermost energy was arbitrarily selected as 10 MeV, and the spacing of the higher energy groups was selected such that it might adequately describe the fission spectrum. The details of the group structure used are presented in Table II.

TABLE II
Group Structure in Lethargy Space

Group	Upper Limit (ev)	Lower Limit (Lethargy)	Group Width (Lethargy)
1	1.0×10^7	0.0	1.25
2	2.87×10^6	1.25	1.75
3	4.98×10^5	3.00	4.25
4	7.10×10^3	7.25	1.75
5	1.20×10^3	9.00	1.25
6	3.54×10^2	10.25	1.25
7	1.01×10^2	11.50	.75
8	47.9	12.25	.50
9	29.0	12.75	.75
10	13.7	13.50	.75
11	6.48	14.25	.75
12	3.06	15.00	.50
13	1.86	15.50	.50
14	1.125	16.00	.25
15	0.876	16.25	.25
16	0.683	16.50	.25
17	0.532	16.75	.25
18	0.414	17.00	

Since atom densities may be entered at each mesh point, one of the advantages of S-XI is that only microscopic cross sections for the core materials are needed. Provision has been made to include in these entries first moment, second moment, up, and down scattering cross sections.* To provide the necessary microscopic cross section, two other computer codes were used: GAM-I⁽⁶⁾ and SOFOCATE.⁽⁷⁾

GAM-I is a P_1 multigroup code for the calculation of fast neutron spectra and was used to calculate the first 17 group cross sections. This code integrates the P_1 equations over quarter lethargy units from 10 MeV to 0.414 eV to obtain 68 "fine" groups. The desired 17 group cross sections are then obtained by averaging over the 68 group spectrum. SOFOCATE was used to obtain thermal, or 18th group, cross sections. These were calculated by averaging over a Wigner-Wilkins thermal spectrum with a temperature of 293° K.

Unfortunately, neither code calculates up scattering or second moment cross sections, and SOFOCATE does not provide first moment in-group cross sections. In the S-XI input, these missing cross sections were assumed to be zero.

In order to convert the cross section output of GAM-I into terms useful to S-XI, it was necessary to use the following relationships for each energy group:

$$\sigma_{TR}(S-XI) = \sigma_{Removal}(GAM) + \sigma_{In-group\ scatter}(GAM)$$

$$\sigma_{first\ moment}(S-XI) = \sigma_{P(1)}(GAM)/3.$$

Otherwise, the GAM-I output was directly usable. The SOFOCATE cross sections were directly usable after noting that

$$\sigma_{TR}(S-XI) = \sigma_{scatter}(SOF) + \sigma_{absorption}(SOF)$$

* Up scatter refers to scattering collision which causes the neutron to increase in energy such that it moves into a higher energy group. Down scatter causes the neutron to move into a lower energy group. In-group scatter causes the neutron to remain in the same group as the incident neutron.

The axial neutron losses were described by entering a fictitious cross section equal in magnitude to DB^2 , where D is a diffusion coefficient, and B is the geometric vertical buckling. It was assumed that the greatest leakage occurred from the water in the core. Therefore, DB^2 was calculated for water, divided by the hydrogen atom density for water, and added as an additional microscopic hydrogen cross section. Thus, the leakage was included in all regions containing water in proportion to the amount of water present.

S-XI Output Interpretation

The detail of the input used in S-XI is presented in Appendix B, and some remarks regarding program use and problems encountered are presented in Appendix A. For the output interpretation, it is sufficient to say that the S_2 approximation was used, that space-energy scalar fluxes, adjoints, and importances were requested, and that fission eigenvalue convergence was required.

Ideally, the output quantities are calculated on the following bases:

$$\text{Flux:} \quad \phi(r,u)\Delta u = \int_{\Omega} \phi(r,u,\Omega) \Delta u d\Omega$$

$$\text{Adjoint:} \quad \phi^*(r,u) = \int_{\Omega} \phi^*(r,u,\Omega) d\Omega$$

$$\text{Importance:} \quad \phi(r,u) \phi^*(r,u) \Delta u = \int_{\Omega} \phi(r,u,\Omega) \phi^*(r,u,\Omega) \Delta u d\Omega$$

However, the code actually considers this solid angle integration by taking a weighted average of the integrand values in each of the discrete directions used. Referring to Figure 3, in the S_2 calculation these directions would be those of the vectors A and B, where Q is a mesh point in the reactor.

It is important to note that when comparing output values of one group with those of another, a correction must be made for the Δu term in the flux and importance outputs.

RESULTS AND DISCUSSION

Studies were made to determine the relative changes in the neutron spectrum within the sample region resulting from the replacement of a PbO_2 sample by a ThO_2 and a U^{238}O_2 sample. The PbO_2 was used as a reference since it is essentially a pure scattering material relative to ThO_2 or UO_2 . In addition, the spatial distributions of the flux and adjoint were studied for the entire reactor mockup. The results of these studies are presented in graphical form in Figures 4-24 for representative lethargy groups.

It was found that a change in the sample region produced a change in the spatial distributions only in the first 3 cm of reactor radius. Consequently, spatial distributions are presented only for the reactor containing a PbO_2 sample. To show the effect of the cadmium tube and the effect of down scatter in providing thermal neutrons to the sample region, details of the distributions in the first 3 cm are shown for the PbO_2 sample at the lowest energy groups.

The graphs of the spectra at the center of the sample region are presented in Figures 13-21. These spectra were compared with one another to determine whether a spectrum change had occurred at any but the resonance energies. A further comparison was made between the spectra within the cadmium tube to those in the fuel region (Figures 22-24) to determine the effect of the cadmium tube at the sample resonance energies. None of the spectra include the contribution of group 18 because it was not possible to determine a suitable lethargy "width" for this group.

Corrections based on this work brought experimental results into good agreement with theoretical resonance integral calculations. While to date only corrections to ThO_2 and U^{238}O_2 data have been made, the further use of transport code calculations is anticipated in conjunction with experiments involving other sample materials.

Figure 3

One half of a Unit Hemisphere
Showing the Vector Directions A
and B along Which an S_2 Calculation
Considers Neutron Current Flow

Figure 4

Real Scalar Flux for the ARMF-II
Groups 17 and 18

Figure 5

Real Scalar Flux for ARMF-II
Groups 17 and 18

Figure 6

Adjoint Distribution for ARMF-II
Group 18

Figure 7
Adjoint Distribution for ARMF-II
Group 18

Figure 8
Adjoint Distribution for ARMF-II
Group 17

Figure 9
Real Scalar Flux for the ARMF-II
Group 15

Figure 10
Adjoint Distribution for the
ARMF-II: Group 15

Figure 11

Real Scalar Flux and Adjoint
Distribution for the ARMF-II

Figure 12

Real Scalar Flux and Adjoint
Distribution for the ARMF-II
Group 2

Figure 13

Real Flux Spectrum at the Center
of the Cadmium Tube PbO_2 Sample

Figure 14

Real Scalar Flux Spectrum in Center
of Cadmium Tube ThO_2 Sample

Figure 15

Real Scalar Flux Spectrum in Center of Cadmium Tube $U(238)O_2$ Sample

Figure 16

Adjoint Spectrum at the Center of the Cadmium Tube PbO_2 Sample

Figure 17

Adjoint Spectrum at Center of the Cadmium Tube ThO_2 Sample

Figure 18

Adjoint Spectrum at Center of the Cadmium Tube $U(238)O_2$ Sample

Figure 19

Importance Spectrum at the Center of the Cadmium Tube PbO_2 Sample

Figure 20

Importance Spectrum at Center of Cadmium Tube ThO_2 Sample

Figure 21

Importance Spectrum at Center of the Cadmium Tube $\text{U}(238)\text{O}_2$ Sample

Figure 22

Real Flux Spectrum at 11.8 cm Radius

Figure 23
Adjoint Spectrum at 11.8 cm Radius

Figure 24
Importance Spectrum at
11.8 cm Radius

PAGES 14 to 16
WERE INTENTIONALLY
LEFT BLANK

APPENDIX A

Problems With S-XI Use

Several comments pertaining to the use of S-XI will be presented here for the benefit of others who wish to use this code, for, because of its great versatility, the S-XI input becomes lengthy and contains subtle difficulties for the unfamiliar.

Because the input for this problem was long and because four group cross sections were available, the ARMF-II problem was run first with four groups. The mistakes discovered with this faster running four group case made this approach worthwhile. When the code was running well, 18 group cross sections were added, and new troubles were traced directly to the cross section entry.

Originally, it was planned to use a punched binary output of the flux, adjoint flux, current, and adjoint current from the S_2 calculation as an input for an S_4 calculation to replace the "flat" guess the computer ordinarily assumes. However, the size of the problem posed with S_2 was so large that the increase to S_4 would cause a core storage overload. The binary output was used, however, to make runs in which only the contents of the sample region were changed, since these changes produced a small perturbation to the reactor as a whole.

Unfortunately, because S-XI was primarily intended for use on reactors with non-thermal spectra, the rate of convergence in a thermal system is slow. This aspect should definitely enter into considerations of S-XI use. For the ARMF-II, convergence of the eigenvalue to $\pm 10^{-3}$ was obtained after 175 free flights (36 minutes).

The greatest number of problems were encountered in the selection of a proper mesh spacing. Within a region this spacing is determined by the material cross sections. At and near an interface, a gradual transition in this spacing must occur from that of one region to that of the other, or else eigenvalue oscillation or negative flux values may occur. The spacing, particularly in the reflector region, appears to influence the rate of convergence.

The criteria for the selection of mesh spacing for the ARMF-II were those suggested by MIST⁽⁸⁾ and presented in Table III. Because group one was the source group, group one cross sections were used in conjunction with these criteria in all but the cadmium tube region.

In this region, because a strong thermal absorber is present, group 18 cross sections were used. A gradual transition was employed in the spacing from that within the tube to that in regions on either side. A maximum rate of transition was found only by trial and error.

TABLE III

Mesh Spacing ΔR in Mean Free Paths
as given in MIST⁽⁸⁾

$$\Sigma_{0c}/\Sigma_t$$

<u>N</u>	<u>.1</u>	<u>.8</u>	<u>.1</u>	<u>.5</u>	<u>0</u>
2	2/3	5/9	4/9	20/57	1/3
4	2/9	5/24	4/21	20/117	1/6
6	2/15	5/39	4/33	20/177	1/9
8	2/21	5/54	4/45	20/237	1/12
10	2/27	5/69	4/57	20/297	1/15

N = order of S_n approximation

The original problem posed had 120 mesh points, but even with S_2 and after the convergence acceleration routine had been removed, an overload occurred. Rather than use a cell calculation, a process of mesh point removal was begun until, with 87 points, the overload was eliminated. The rate of transition was held constant during this removal.

It is estimated that any more than 90 points would cause overload for the problem. Furthermore, since the final spacing is slightly greater than that suggested by MIST for the cross sections used, the approach employed was conservative. The final mesh spacing used in each region is presented in a graphical form in Figure 25. Any deviations from smooth transitions are due to the trial and error removal ultimately required.

Figure 25
 Mesh Spacing Distribution

APPENDIX B S-XI Input Parameters

The material presented here is intended for those who are familiar with the input required for S-XI. For a thorough discussion of the following parameters, see reference 2.

In the ARMF-II calculations, the following values were used as control parameter input (800 series):

Case	+	Eigenvalue acceleration	+72
Eigenvalue estimate	1.1	All formats	38, 37, 36, 36, 18, 18, 0, 0
Alterations	0	All perturbations	0
Eigenvalue error limit	10^{-3}	Sensors	0
Action balance error limit	10^{-3}	All homogenization routines	0
Geometry	1 (cylindrical)	Accelerations	0
Angular sensors	0	Output control	516
Free flights	variable	Number of theory words	4012
Number of radii plus 1	87	Adjoint normalization	10^{10}
Energy groups	18	Flux normalization	10^{10}
Axial angles	1	Minimum inverse period	.00125
Relative angles	.3	Maximum inverse period	10^{20}
Eigenvalue definition	2 (fission)	Minimum eigenvalue	0.5
Number of delay groups	0	Maximum eigenvalue	2.5
Number of mixtures + ingredients	23		

REFERENCES

1. E. E. Burdick, E. Fast, and D. W. Knight, The Advanced Reactivity Measurement Facilities - A Description and Performance Evaluation, IDO-17005 (1964).
2. W. K. Foell, Resonance Absorption of Neutrons in Mixtures of Thorium-232 and Uranium-238: An Investigation of Interference Between Absorbers, Stanford University Thesis, (April 1964).
3. H. P. Flatt and D. C. Baller, "The AIM-G Code," NAA Program Description, (January 1961).
4. B. Duane, "Neutron and Photon Transport," GE-ANPD XDC 59-9-118 (1959).
5. C. E. Lee, The Discrete S_n Approximation to Transport Theory, LA 2595 (June 1961).
6. G. D. Joanou and J. S. Dudek, GAM-I: A Consistent P_1 Multigroup Code for the Calculation of Fast Neutron Spectra and Multigroup Constant, GA-1850 (June 1961).
7. R. J. Wagner, 650 SOFOGATE - A Code to Determine Thermal Constants on IBM-650, IDO-16758 (March 1962).
8. G. E. Putnam and D. M. Shapiro, MIST, IDO-16856 (May 1963).

**PHILLIPS
PETROLEUM
COMPANY**

ATOMIC ENERGY DIVISION