Westinghouse
Astronuclear
Laboratory

SNPO-C

master Records

WANL-TME-2704
FEBRUARY 1971

ANNUAL REPORT FOR
CONTRACT YEAR 1969,
SUPPORTING RESEARCH AND
TECHNOLOGY, PROJECT 493

MASTER

DISTRIBUTION OF THIS DOCUMENT UNLIMITED

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.

Westinghouse Astronuclear Laboratory

Subcontract NP-1
CODE IDENT NO. 14683

WANL-TME-2704
FEBRUARY 1971

NOTICE

This report contains information of a preliminary nature and was prepared primarily for internal use at the originating installation. It is subject to revision or correction and therefore does not represent a final report. It is passed to the recipient in confidence and should not be abstracted or further disclosed without the approval of the originating installation or USAEC Technical Information Center, Oak Ridge, TN 37830

ANNUAL REPORT FOR CONTRACT YEAR 1969, ²⁴⁶ SUPPORTING RESEARCH AND TECHNOLOGY, ²PROJECT 493

APPROVED BY:

F. D. Retallick

F. D. Retallick, Manager
NERVA Engineering

INFORMATION CATEGORY

UNCLASSIFIED

R. G. Jones 4-7-71
AUTHORIZED CLASSIFIER DATE

WANL-TME-2704

ANNUAL REPORT FOR CONTRACT YEAR 1969,
SUPPORTING RESEARCH AND TECHNOLOGY,
PROJECT 493

R. K. Disney
J. Jedruch
R. G. Soltesz
R. S. Kaiser
S. L. Zeigler

ABSTRACT

Advances in the methods for neutronic and radiation design of NERVA are described. The transport code DOT-IIW was improved in the acceleration of convergence, handling of boundary conditions and tape operations, and extensively tested for flux and eigenvalue convergence at different orders of quadrature and in r, θ geometry. Satellite codes for preparation of cross sections, and geometry were developed. Reduction of ray effects through Lagrangian interpolation in discrete ordinate fluxes was achieved. Improvements in two-dimensional perturbation code were made.

PAGE BLANK

TABLE OF CONTENTS

<u>Section</u>	<u>Page</u>
Abstract	iii
Table of Contents	v
List of Figures	viii
List of Tables	x
1.0 Introduction	1-1
2.0 Summary and Conclusions	2-1
3.0 Recommendations for Future Studies	3-1
4.0 Code Improvement and Development	4-1
4.1 DOT Code Improvements	4-7
4.1.1 Inner Iteration Convergence Acceleration Techniques	4-9
4.1.2 DOT-IIW Boundary Conditions	4-23
4.1.3 DOT-IIW Convergence Logic	4-25
4.1.4 Upscatter Scaling Technique	4-27
4.1.5 Improved Tape Operations	4-33
4.2 Satellite Code Development	4-39
4.2.1 Cross Section Data Preparation	4-39
4.2.2 Mesh Evaluation Code in r, θ Geometry - MERTH	4-40
4.3 Two-Dimensional Perturbation Theory Code Improvement	4-44
4.3.1 Form of Forward and Adjoint Equations	4-44
4.3.2 Expansion of Scattering Cross Section	4-45
4.3.3 Perturbation Equations in Operator Form	4-47
4.3.4 Treatment of Transverse Leakage Correction	4-51
4.3.5 Equations for Forward and Adjoint Flux	4-52
4.3.6 Calculation of Prompt Neutron Lifetime	4-55

TABLE OF CONTENTS (Continued)

<u>Section</u>	<u>Page</u>
4.4 Angular Flux Interpolation Techniques	4-56
4.4.1 Geometric Considerations	4-57
4.4.2 Two-Dimensional Discrete Ordinate Flux Representation	4-62
4.4.3 Lagrangian Interpolation Technique in the Cosine of the Polar Angle	4-64
4.4.4 Direction Integrals and Quadrature Weights	4-68
4.4.5 Evaluation of Lagrangian Interpolation Coefficients	4-70
4.4.6 Results from Application of Lagrangian Interpolation Technique	4-71
4.4.7 Importance of Exact Gaussian Quadrature Directions	4-80
4.4.8 Future Developments of the Technique	4-83
5.0 Geometric and Inventory Model Development	5-1
5.1 PAX-E1 Reactor Configuration	5-1
5.2 Explicit Definition of Control Vane	5-5
6.0 Applications of DOT-IIW Code	6-1
6.1 Quadrature Data in r, θ Geometry	6-1
6.2 Comparison of Results from ANISN and DOT-IIW	6-5
6.3 Convergence Patterns in DOT-IIW	6-8
6.3.1 Acceleration Techniques	6-8
6.3.2 Quadrature Data	6-14
6.3.3 Boundary Conditions	6-16
6.3.4 Upscatter	6-16

TABLE OF CONTENTS (Continued)

<u>Section</u>	<u>Page</u>
6.3.5 Convergence Criteria	6-17
6.3.5.1 Flux Convergence	6-17
6.3.5.2 Eigenvalue Convergence	6-17
6.3.5.3 Upscatter Convergence	6-17
6.3.6 Zones of Convergence	6-19
6.4 R,0 DOT-IIW Eigenvalue Calculations	6-21
6.4.1 Quadrature Order	6-21
6.4.2 Acceleration Techniques	6-21
6.4.3 Eigenvalue	6-27
6.4.4 Fission Distribution	6-30
 7.0 References	 7-1
Appendix A: Detailed PAX-EI Model	A-1
Appendix B: Angular Quadrature Data	B-1

LIST OF FIGURES

<u>Figure Number</u>	<u>Title</u>	<u>Page Number</u>
4-1	Discrete Ordinate Transport Method for Neutronics Analysis	4-5
4-2	Discrete Ordinate Transport Method for Radiation and Shielding Analysis	4-6
4-3	Upscatter Scaling in Three Group, C-Value ($C = 1.2$) DOT-IIW Calculation	4-33
4-4	Schematic of MERTH Numerical Technique	4-41
4-5	Schematic of MERTH Numerical Technique (Section A of Figure 4-4)	4-42
4-6	Geometry Used in MAP Calculations	4-57
4-7	Discrete Ordinate, and Interpolated Flux, Mesh Point 1 at Top of Reactor	4-69
4-8	Discrete Ordinate and Interpolated Flux, Mesh Point 8 at Top of Reactor	4-70
4-9	Discrete Ordinate and Interpolated Flux, Mesh Point 12 at Top of Reactor	4-71
4-10	Discrete Ordinate and Interpolated Flux, Mesh Point 10 Side of Reactor	4-72
4-11	Discrete Ordinate and Interpolated Flux, Mesh Point 6, Side of Reactor	4-74
4-12	Interpolation with Non-Gaussian Collation Points	4-76
4-13	Surface Defining the Function $V_{nm}(\eta, \mu)$ and Locus of its Zeros ($n-m-4$)	4-77
5-1	One-Dimensional (Radial) Model of PAX-E1 Reactor Configuration with Ring Vane 105 Degrees	5-2
5-2	Two-Dimensional Mockup of PAX-E1 Reflector for (r, θ) Calculations	5-3
5-3	(r, θ) Mesh Mockup of PAX-E1 Reactor Configuration for 100 Mil Vane at 105 Degrees	5-6

LIST OF FIGURES (Continued)

<u>Figure Number</u>	<u>Title</u>	<u>Page Number</u>
6-1	Discrete Ordinate Transport Method for Evaluation of DOT-IIW	6-2
6-2	r, θ Discrete Directions Quadrature Order = 6	6-3
6-3	r, z Discrete Directions Quadrature Order = 6	6-4
6-4	r, z Discrete Directions Quadrature Order = 2	6-6
6-5	Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculation First Outer Iteration - Group One	6-11
6-6	Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculation First Outer Iteration - Group Seven	6-12
6-7	Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculations First Outer Iteration - Group Fifteen	6-13
6-8	Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation First Outer Iteration - Group One	6-24
6-9	Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation	6-25
6-10	Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation First Outer Iteration - Group Fifteen	6-26
6-11	Comparison of Calculated (DOT-IIW and EXTERMINATOR-2) and Experimentally Measured Fissions per Gram in the PAX-E1 Reactor, Radial Traverse Between Drums	6-28
6-12	Detailed Comparison between 35 and 43.8 cm of Calculated (DOT-IIW and EXTERMINATOR-2) and Experimentally Measured Fissions per Gram in the PAX-E1 Reactor, Radial Traverse between Drums	6-29
6-13	Calculated Fissions Per Gram in PAX-E1 Reactor Azimuthal Traverse at Edge of Cylindricized Core (43.8 cm)	6-32
6-14	Comparison of Group 16 Thermal Flux in DOT-IIW and EXTERMINATOR-2 Calculations, Azimuthal Traverse at Edge of Cylindricized Core (43.8 cm)	6-33

LIST OF TABLES

<u>Table Number</u>	<u>Title</u>	<u>Page Number</u>
4-1	Space Dependent Scaling Cycle as a Function of Maximum Dominance Ratio	4-16
4-2	DOT-IIW Cross Section Table	4-28
4-3	Upscatter Scaling Test Problem Cross Sections	4-31
4-4	Tape Versus Disk I/O Evaluation for DOT-IIW	4-36
4-5	Cross Section Table Illustrating the Diagonal Transport Corrections	4-47
4-6	Ranges of Variation of Angular Parameters	4-58
4-7	Zeros of the First Few Legendre Polynomials, plus Their Derivatives, and Christoffel Numbers	4-62
4-8	Comparison of Integrals of Directed Flux from Discrete Ordinate Solution and the Lagrangian Interpolation, Top of Reactor	4-67
4-9	Comparison of Integrals of Directed Flux from Discrete Ordinate Solution and the Lagrangian Interpolation, Side of Reactor	4-68
4-10	Discrete Ordinate and Interpolated Flux, Mesh Point 10 at Side of Reactor	4-73
5-1	PAX-E1 Control Vane Data	5-4
6-1	Comparison of Results from ANISN and Azimuthally Symmetric DOT-IIW Calculations	6-7
6-2	Comparison of Acceleration Techniques in r,z DOT-IIW Calculation	6-9
6-3	Comparison of Acceleration Techniques in Azimuthally Symmetric DOT-IIW Calculations	6-10
6-4	Convergence Patterns in Azimuthally Symmetric DOT-IIW Calculations	6-15

LIST OF TABLES
(Continued)

<u>Table Number</u>	<u>Title</u>	<u>Page Number</u>
6-5	Effect of Convergence Criteria in Zero Upscatter, Azimuthally Symmetric DOT-IIW Calculations	6-18
6-6	Effect of Zones of Convergence Option in Azimuthally Symmetric DOT-IIW Calculations	6-20
6-7	Summary Table of r, θ DOT-IIW Eigenvalue Calculations	6-23
A-1	PAX-E1 One-Dimensional Model with Ring Vane Prescription at 105°	A-2
B-1	Completely Symmetric Angular Quadratures in (r, θ) Cylindrical Geometry for Quadrature Order of 2	B-2
B-2	Completely Symmetric Angular Quadratures in (r, θ) Cylindrical Geometry for Quadrature Order of 4	B-3
B-3	Completely Symmetric Angular Quadratures in (r, θ) Cylindrical Geometry for Quadrature Order of 6	B-4
B-4	Completely Symmetric Angular Quadratures in (r, θ) Cylindrical Geometry for Quadrature Order of 2	B-5
B-5	Completely Symmetric Angular Quadratures (r, z) Cylindrical Geometry Quadrature Order of 2	B-6
B-6	Completely Symmetric Angular Quadratures in (r, z) Cylindrical Geometry for Quadrature Order of 4	B-7
B-7	Completely Symmetric Angular Quadratures in (r, z) Cylindrical Geometry for Quadrature Order of 6	B-8
B-8	Completely Symmetric Angular Quadratures in (r, z) Cylindrical Geometry for Quadrature Order of 8	B-9

1.0 INTRODUCTION

Analyses of the reactor design configurations of the NERVA reactor have become more complex as performance requirements for specific mission applications have become more stringent. The requirement for specified reliabilities and the reduction of analytical uncertainties in reactor core neutronic design, reflector design, and radiation shield design has placed an increasing burden on the required analytical techniques. Further requirements of analytically predicting reactor performance for various missions without experimental verification using an exact experimental assembly has made necessary improved methods of analysis. Improvements in discrete ordinate transport methods and studies of the application of discrete ordinates transport techniques in two dimensions have been carried out in the Contract Year 1969 study effort. These studies were conducted to increase the utilization of the inherent accuracy of discrete ordinate transport techniques in the NERVA program. Four specific areas of study were conducted during the Contract Year 1969 effort. These areas are:

- o Improvements in the convergence logic, method of solution, and data input/data output of a two-dimensional discrete ordinates transport code,
- o Application of r - θ geometry discrete ordinates transport techniques to prediction of neutronic performance of peripherally controlled reactors and development of r - θ modeling technique for the reflector control drum vanes,
- o Improvement of two-dimensional linear first order perturbation techniques for use with the discrete ordinates transport techniques,
- o Development of analytical techniques for interpolation of low order discrete ordinate ($<S_{12}$) angular flux data from discrete ordinates transport codes for use in calculations of the spatial attenuation of the leakage fluxes from an r,z geometry model of a radiation source.

Application of the discrete ordinates techniques at WANL prior to this work has been limited to exploratory studies in r - θ geometry and design studies relating to radiation heating, radiation environment, and shielding analyses in one and two dimensions. (1) In recent years the increased use of discrete ordinate transport techniques^(2,3,4) has led to an extended capability in the techniques. The integration of these new techniques

into existing codes has been performed so that the neutronic, radiation and shielding analyses of the NERVA reactor may be performed in consistent fashion.

Studies conducted in this contract year have used the recent code advances made in discrete ordinate transport techniques and have provided an increased capability which is more efficient than previous techniques. Results from the work in CY '69 have suggested a study plan for CY '70 which will provide for an increased utilization of discrete ordinate transport techniques in the NERVA program.

The code development or improvement work performed in CY '69 is described in Section 4.0. Section 4.1 describes the improvement in DOT-IIW two-dimensional discrete ordinate transport code. Section 4.2 describes the satellite code development for the DOT-IIW code conducted in this study program. The development or improvement of a two-dimensional discrete ordinate perturbation code, PERT-2DW, is described in Section 4.3. Section 4.4 describes the techniques developed for the interpolation of angular flux data from the DOT-IIW code solutions. Sections 5.0 and 5.0 present the details of the application of the DOT-IIW code to the r - θ geometry solutions required for NERVA neutronics design analysis.

2.0 SUMMARY AND CONCLUSIONS

Improvements and studies in discrete ordinate transport techniques for use in NERVA neutronics and radiation and shielding calculations were carried out in the CY '69 work program. The study program which has been conducted in this time period has resulted in an increased capability of the discrete ordinate transport code, DOT-IIW, which will be integrated into the standard design techniques used by the NERVA design groups. The improvements and study results are summarized as follows:

2.1 IMPROVEMENTS IN CODING THE DOT CODE

- 1) A number of coding errors and improper logic were found in the DOT code and corrected. In addition, coding improvements were incorporated to increase the applicability of the DOT code to design calculations. The corrections are discussed in Section 4.1.
- 2) Successive overrelaxation (SOR), Chebyshev (CA), and space point scaling (SPS) acceleration techniques on inner iterations, available in the latest DOT version, DOT-II were incorporated in the WANL CDC-6600 version of DOT. The SOR and CA techniques in DOT-II were corrected to perform acceleration consistent with the SPS technique. The revised WANL DOT was checked out and a simple sample problem with no upscatter and a single outer iteration, showed that the space point scaling technique results in about a 65 percent decrease in computer running time when compared to the previously used Gaussian (Normal) acceleration technique. Further discussion of the application to more complex problems is in Section 5.0.

- 3) The albedo boundary condition capability in the DOT-II code was incorporated into the WANL version. This boundary condition can be applied to top, bottom, or right boundaries and provides for a specified fraction of neutrons to return isotropically from the top, right, and/or bottom boundary as a function of energy group and mesh interval along the boundary.
- 4) The DOT code was revised and corrected to provide the capability to accept cross section data from magnetic tape in a similar fashion as the one-dimensional discrete ordinate transport code, ANISN.⁽⁵⁾ This cross section tape can be obtained from either the GAMB1T,⁽⁶⁾ SATURN,⁽⁷⁾ or APPROPOS⁽⁹⁾ codes.
- 5) The DOT code was revised to provide the output converged scalar flux data on the same logical tape unit (tape unit 1) for all types of calculations.
- 6) The technique of reading input data in subroutine FIDO was revised to include the DOT-II capability of reading sequences of numbers.
- 7) The number of options specifying the zone of convergence in the WANL version of DOT was extended. The zone of convergence logic in the DOT-II code provided only a single zone of convergence test on the average flux error in the specified zone. This was extended by allowing the user to specify as input the zones of convergence (i.e., all fissionable regions) and including the logic to test the average flux error only in the specified zones or the average flux error and the pointwise flux error in the specified zones. This capability has improved the convergence on integral quantities in zones of interest and has resulted in a substantial saving of computer time. Sample eigenvalue DOT problems indicate a 20 to 33 percent saving in computer time.

- 8) Improvement in the DOT code handling of angular flux data for top boundary source problems has been incorporated in the DOT-IIW code. Previous version of the DOT code has the capability to produce an angular flux output tape containing all angular fluxes for all groups. In the CDC-6600 version of the DOT-IIW code, the ability to read this magnetic tape selectively provided an automatic top boundary source coupling of DOT problems. A modification was made in the DOT-IIW code to provide a selective angular flux tape containing only three intervals of angular flux data. This capability provides for analysis of deep penetration problems as sequential DOT problems with top boundary source input between successive problems.
- 9) Improvements in the SPS, CA, and SOR acceleration techniques were made by recoding the CA and SOR method so as to obtain a capability consistent with the SPS method, thus providing the correct scaling of all flux quantities for use in periodic or reflective boundary condition problems. Additional improvement in the SPS acceleration technique was to use the maximum dominance ratio in the group to define the frequency of applying the SPS technique for each group. The use of a scaling cycle dependent on the dominance ratio has improved the capability of the SPS technique and helps to eliminate the problem of overambitious scaling of group solutions with high dominance ratios (ratios greater than 0.9).
- 10) Improvements in the upscatter scaling techniques in DOT were: a) removal of a mixed mode multiplication (fixed point by floating point) operation in the upscatter scaling technique of subroutine CNNP of DOT, b) the relocation of the upscatter scaling convergence test in subroutine CNNP so that scaling occurs on all outer iterations until upscatter and eigenvalue convergence tests are satisfied, and c) the inclusion of a new convergence parameter on upscatter scaling. The third change was made when the studies indicated that an interaction between acceleration techniques and

upscatter scaling produced a slow convergence in an oscillatory pattern. A separate, but less stringent, upscatter scaling convergence parameter provides for the same eigenvalue convergence in less computer time.

The above described version of the WANL DOT-II code has been produced in two variants. Variant 1 is an all FORTRAN code and variant 2 is the FORTRAN code with the GRIND subroutine coded in the COMPASS machine language of the CDC-6600 computer. This machine language work was performed by the Reactor Physics and Mathematics Department at WANL. The present version of DOT has the capability equivalent to the DOT-II, as received from RSIC, with the exception of polynomial source output/input and scalar fluxes in fast memory (not considered feasible on WANL's CDC-6600 computer) which are not included.

2.2 USE AND APPLICATION OF r - θ DISCRETE ORDINATE TRANSPORT TECHNIQUES

A NERVA critical assembly configuration was selected for (r, θ) analyses using the DOT-IIW experimentally measured fission distribution data available for this reactor system. Sixteen group transport corrected neutron cross sections were assembled for the selected reactor configuration. Using these neutron cross sections, an S_4 , one-dimensional radial transport calculation (ANISN) was performed with a 105-degree ring vane prescription to obtain a neutron cross section set with upscatter removed and a one-dimensional flux guess for use in the two-dimensional transport code (DOT-IIW) studies.

Completely symmetric angular quadratures were defined in r, θ cylindrical geometry using the DOQ⁽¹⁰⁾ (Discrete Ordinate Quadrature) computer code.

A series of r, θ eigenvalue calculations using the DOT discrete ordinate transport code were performed in which there was no azimuthal variation (i.e., one-dimensional DOT calculations), and in which a 105 degree vane ring prescription was used. The purpose of these problems was to evaluate the effect of quadrature sets on r, θ solutions and to define convergence patterns (periodic versus reflective boundary conditions; upscatter scaling versus no upscatter; convergence criteria on eigenvalue, flux and upscatter; and quadrature order) on r, θ DOT problems. The major results of these calculations were as follows:

- 1) An eigenvalue convergence of 10^{-4} and flux convergence of 2×10^{-5} is required in order to obtain results from one-dimensional DOT calculations that are substantially the same as results obtained from ANISN.
- 2) Azimuthally uniform DOT calculations indicate that an upscatter convergence of 5×10^{-4} is sufficient to converge eigenvalue DOT problems.
- 3) One-dimensional DOT eigenvalue problems of quadrature order S_2 and S_4 yield different results (eigenvalue, fission distribution, scalar flux), while higher order problems (S_6 and S_8) substantially agree with S_4 problems while requiring considerably more computer time.
- 4) The reflective boundary condition in DOT is operational and gives consistent results when compared to an equivalent problem in which the boundary conditions are periodic.
- 5) For one-dimensional DOT problems, r, θ and r, z quadrature data gives substantially the same results, and the problem using r, z quadrature data requires less computer time.
- 6) The DOT eigenvalue problems showed different results when cross sections containing upscatter were used when compared to problems in which the cross sections used had had upscatter collapsed in a previous ANISN calculation.

Test problems were run using the Gaussian (Normal), Successive Overrelaxation, Chebyshev and Space Point Scaling acceleration techniques in the previously described WANL DOT-II. A single outer iteration, zero upscatter, problem indicated that the Space Point Scaling Technique required the fewest inner iterations for convergence. (The computer time required for a design DOT problem is proportional to the total number of inner iterations). Eigenvalue DOT problems showed that cases having a higher dominance ratio (i.e., the ratio of the in-group scatter cross section to the total cross section) had difficulty converging when the space point scaling acceleration technique was used.

2.3 TWO-DIMENSIONAL PERTURBATION TECHNIQUES

A major revision of the two-dimensional perturbation code, PERT 2D,⁽¹¹⁾ was undertaken to provide an increased perturbation capability for use with the DOT-IIW code forward and adjoint flux data. The new code was named PERT-2DW. Coding revisions made to the code were principally in the area of increasing the input data capability of the code and the scope of calculations performed by the code. Revisions to the code included the capability to read cross section data in the DOT-IIW format, to read cross sections from an input tape in a similar fashion as from the DOT-IIW tape, and to provide the capability to perform mixture operations in order to do perturbations on a macroscopic material basis. The card and tape input, as well as the mixture table input are compatible with the DOT-IIW input capability and the PERT 2DW user can use the same data cards for input to the PERT 2DW code as were used in the DOT-IIW code.

The calculation of β_{eff} is performed for as many fissionable isotopes as are in the fissionable regions. The user can specify the number of isotopes for which the β_{eff} calculation is to be performed, and required input data includes the delayed fission spectrum as well as β for each of the fissionable isotopes.

The geometry capability of the PERT 2D code was originally limited to r,z geometries and the present version has been expanded so that x,y or $r-\theta$ geometries will be properly calculated. In addition to the x,y and $r-\theta$ geometry capability, the inclusion of transverse leakage effects in the calculation of material perturbations is included for both the x,y and $r-\theta$ geometries.

In addition to the capability to perform x,y , r,z , or $r-\theta$ calculations in the PERT 2DW code, the capability to provide one-dimensional calculated results for specific regions has been included in order to provide a spatial distribution of reactivity coefficients. This calculation option provides for the user to specify the calculation of the average coefficients in one dimension and the code will provide data as a function of that dimension (for example, $f(x)$ versus x for an x,y geometry calculation).

The capability of the PERT 2D code has been extended in PERT-2DW such that the user may specify the perturbation calculation in a particular zone or can specify a region defined by a left radial mesh interval, a right mesh interval, a lower mesh interval and an upper mesh interval within the overall x,y , r,z , or $r-\theta$ problem. Within either the zone to be perturbed or the region to be perturbed, the user can specify the material cross section which will be the perturbing material.

The output data from the PERT 2DW code has been expanded to provide not only the overall perturbation of the zone or region of perturbation in the DOT-IIW problem, but also to provide the data as a function of neutron group and for r,z , $r-\theta$, or x,y regions as a function of one of the spatial coordinates.

The input of data to the PERT 2DW code is now done with the FIDO subroutine from the DOT code, and the variable dimension capability of the DOT code has been carried into the PERT 2DW code such that a generalized capability results.

The principal coding effort on the PERT 2DW code has been completed and checkout of the coding of the overall code capability is continuing in order to provide an operational technique for use with the DOT-II code by the design groups.

2.4 DEVELOPMENT OF ANALYTICAL MODEL FOR $R-\theta$ DISCRETE ORDINATE TRANSPORT TECHNIQUES

In order to provide a technique by which the models of the control vanes in the NERVA reactor could be developed to represent the actual design configuration, a new method has been coded in the MERTH¹² Code (Mesh Evaluation in R, THETA). The MERTH code has been coded to assist the designer in the layout of an $r-\theta$ mesh to represent off-axis cylindrical annuli (e.g., the control vane in the reflector). At the present time the logic of the MERTH code is quite simple and the engineer can use the code to assist in the development of an analytical model which closely approximates the model. The code accepts either a regular or irregular r and θ mesh for the reflector sector being analyzed and requires an exact definition of the off-axis cylindrical annulus. Computation of the fraction of the off-axis information is provided to assist the user in choosing those mesh cells which describe the annulus in the optimum manner. This technique is operational in a simplified version and is

being used in the evaluation of the DOT code and the control vane analytical model required for the NERVA reactor designs.

2.5 ANALYTICAL MODEL OF ANGULAR FLUX IN MAP CODE

An effort was initiated to develop techniques of interpolating low order quadrature angular flux data from the DOT code in the MAP⁽¹³⁾ code. The model development has been limited to the use of Lagrangian interpolation techniques to compute the directed flux in a specified direction. The presently considered interpolation of the angular flux is only in the polar angle η with respect to the "z" axis of the unit sphere, describing the angular flux. Coding of this technique into a subroutine for inclusion in MAP has been initiated and analysis of the validity of the technique is underway.

3.0 RECOMMENDATIONS FOR FUTURE STUDIES

A number of future study efforts can be identified from the CY '69 work program. The principal areas for recommended study are the continued improvement of DOT-IIW, the improvement of the MAP code to include the techniques developed in the CY '69 study program, and a new study effort to implement the use adjoint kernel techniques in radiation transport. These areas of recommended study are summarized as follows:

DOT-IIW Improvements

- Incorporate weighted diamond difference techniques into the two-dimensional discrete ordinate transport code, DOT-IIW. Study effects of weighted diamond difference techniques on convergence patterns for NERVA type r, z geometry fixed distributed source problems, and r, θ geometry eigenvalue problems.
- Incorporate energy dependent upscatter scaling techniques into the DOT-IIW code. Study the effects of energy dependent upscatter scaling techniques on NERVA-type $r-\theta$ geometry eigenvalue problems.
- Incorporate coding techniques into DOT-IIW code to provide zonal balance tables by energy group.
- Incorporate improved Chebyshev and Successive Overrelaxation acceleration techniques in the flux solution in highly scattering and highly absorbing media problems.

MAP Code Improvements

- Study improved analytical techniques of angular flux interpolation for lower order quadrature ($< S_8$) surface angular fluxes from the DOT-IIW code.

Adjoint Kernel Investigation

- Investigate the feasibility of using adjoint kernel techniques with low order quadrature discrete ordinate calculations (forward or adjoint) to perform discrete ordinate transport coupling calculations and predict external environment of the nuclear subsystem (NSS).

An additional recommended effort is the continuation of the two-dimensional perturbation theory code development.

4.0 CODE DEVELOPMENT AND IMPROVEMENT

Code development and improvement accomplished in the CY '69 study program consisted primarily of coding efforts to increase the capability of the DOT code used in the NERVA program and code development to increase the efficiency of preparation of input data for the DOT code or use output data from it. Completed study program efforts have provided an increased discrete ordinate transport code capability which is compatible with portions of the current NERVA design techniques and is easily integrated into the complete design method used at WANL.

The code development or improvement accomplished in CY '69 is summarized as follows:

- DOT-IIW - An adaptation of the two-dimensional discrete ordinate transport code incorporating the DOT-II capabilities (as published by F. R. Mynatt of Union Carbide Nuclear Corporation, Computer Technology Center) into a CDC-6600 version of the DOT code. The original DOT code on the CDC-6600 at WANL was adapted from the earlier version of the DOT code for the IBM 7094 computer system as released by F. R. Mynatt. The DOT-IIW code contains upscatter scaling techniques, acceleration techniques on group flux (inner iteration) convergence, extended input/output options, extended boundary condition options, and is coded completely in FORTRAN IV, with versions containing CDC-6600 ASCENT or COMPASS machine assembly versions of the GRIND Subroutine for use on the CDC-6600.
- SATURN - A cross section data processing code to provide punched card to magnetic tape operations, processing of magnetic tape data to a different magnetic tape, and magnetic tape to punched card options. Additional capability is to include transverse leakage corrections to cross section data for use in x,y or r,θ analyses. Capabilities also exist to label, or relabel cross section sets to be placed on magnetic tape. In addition, the code will prepare a group dependent or group independent cross section tape for use in the WANL versions of the ANISN or DOT-IIW codes.

- MERTH - An r,θ meshing code to provide r,θ mesh models of off axis cylindrical annuli for evaluation by the user. This tool is an aid to the user and was developed for use in meshing of the NERVA control vanes in the reflector. The data from MERTH is used in defining the mesh model mockup for the DOT-IIW code.
- PERT-2DW - An adaptation and extension of the two-dimensional linear perturbation code PERT-2D, as obtained from F. R. Mynatt of Union Carbide Nuclear Corporation, Computer Technology Center. Extended capabilities include zone, material, and multiple zone perturbations with energy and spatial dependence. Prompt neutron lifetime and effective delayed neutron fraction calculation with multizoned cores is an additional capability.
- LAG - A simple code to test angular flux interpolation techniques intended for use in calculating external radiation environments from the surface angular fluxes of a DOT-IIW solution in r,z geometry. These evaluated techniques are intended to be incorporated into the MAP code for direct use in predicting external radiation environments.

The discrete ordinate transport methods for use in neutronics analysis and/or radiation shielding analysis at WANL are illustrated schematically in Figures 4-1 and 4-2. The DOT-IIW code development as well as the satellite code development in this study program are noted by asterisks in these figures. As shown in Figure 4-1, the neutron cross section data for use in either the one-dimensional discrete ordinate transport code, ANISN, or the two-dimensional transport code, DOT-IIW, are obtained from either the GAMB1T code or the LINK¹⁴ computer code system, or are data processed by the SATURN code. The SATURN code is described in detail in Section 4.2.1; the MERTH code, which is used to develop r,θ mesh models to be analyzed in DOT-IIW is described in detail in Section 4.2.2.

The data prepared on the mesh model by MERTH, the cross section data from SATURN, GAMB1T, or LINK and other required input data are input into the DOT-IIW code as shown. For certain types of analyses a one-dimensional model of the reactor assembly may be run in ANISN and the punched card data for scalar fluxes can be used as a flux guess in DOT-IIW.

The combination of these data constitute a complete data set for input to DOT-IIW. The DOT-IIW code is then used to solve for the eigenvalue, fission distribution, and scalar flux distribution in the r - θ model of the reactor.

Output data from the DOT-IIW code consists of either the multigroup angular flux data for each mesh cell for use in the PERT-2DW code or the scalar flux data by mesh cell for use in the analysis of detailed fission distribution and power factor analysis in the PFENCER¹⁵ code system. Coupling of the angular flux data from DOT-IIW into the PERT-2DW code was accomplished in the CY '69 effort along with the complete compatibility of cross section data in the PERT-2DW code with that capability in DOT-IIW. Modification of the PFENCER code package to accept DOT format fluxes on magnetic tape is to be accomplished in CY '70 under the normal NERVA work effort. This developed code capability will automate the analysis of r , θ models in the design methods at WANL and will provide for the capability to utilize the inherent accuracy of discrete transport methods in the analysis of the complex r , θ geometry models.

A similar schematic diagram of the discrete ordinate transport method for radiation and shielding analysis is illustrated in Figure 4-2. From the model description of the r , z or r , θ model of the NERVA reactor system, the neutron and photon cross section data is obtained from the GAMBIT and GAMLEG-W⁸ code. Either of these codes generate microscopic data for direct use in any of the cross section data processing codes or for direct use in DOT-IIW or ANISN.

As shown in the schematic, the APPROPOS code, which is a cross section data processing code, can prepare either neutron cross section data for direct use in DOT-IIW or ANISN, or optionally to the SATURN code, or APPROPOS can prepare a coupled set of neutron-photon cross section data based upon input library data. The GAMLEG code can be used with the APPROPOS code directly, or if desired, the user can obtain macroscopic photon cross sections for direct use in DOT-IIW or ANISN from APPROPOS.

The SATURN code functions in the overall method in a similar fashion to that described in the neutron cross section preparation with the most general use to prepare group independent cross section sets for input into the DOT-IIW code. As shown, the DOT-IIW or

ANISN codes can be used to perform coupled neutron-photon transport, neutron transport, or photon transport calculations using the cross section data from GAMBIT, APPROPOS, GAMLEG, or optionally from SATURN.

The ANISN code can provide upscatter-removed cross sections for use into DOT-IIW by magnetic data tape. The complete data set input into DOT-IIW and ANISN includes the model description data provided by the user, the cross section data obtained from one of the above described methods, and other required data. Output data from the DOT-IIW (or ANISN) code is used in the NAGS code to perform neutron or photon source calculations as well as performing total heating calculations.

In certain types of analysis, the calculation of neutron transport and photon transport can be done sequentially (with the intermediate calculation of the photon source by mesh cell performed by the NAGS¹⁶ code). The APPROPOS code provides a data deck for direct use in NAGS for use in either neutron or photon source calculations or the total heating calculation. The coupling between the DOT-IIW and NAGS is the multigroup, scalar flux data on magnetic data tape.

An additional capability provided with the DOT-IIW code is the use of the surface angular fluxes (which are on the scalar flux tape) as the input data to the MAP code. The MAP code, which performs a numerical integration over the visible surface of an r,z DOT problem surface, uses the surface angular fluxes as the source data in a point-kernel technique. Some work has been performed in the CY '70 contract work to provide angular flux interpolation techniques in the MAP code. However, the coupling between DOT-IIW and MAP was available for the CY '69 work and no coupling work was performed in this contract work.

One additional capability shown in Figure 4-2 is the use of the separable distributed source data obtained from the NAGS code as direct input into the KAP-V¹⁷ point kernel code. The entire integrated technique, as shown in Figure 4-2, is available for the NERVA design method and has been utilized for NERVA design analyses in CY '69.

Figure 4.1. Discrete Ordinate Transport Method for Neutronics Analysis

Figure 4.2. Discrete Ordinate Transport Method for Radiation and Shielding Analysis

*Project 493 Code Development

4.1 DOT CODE IMPROVEMENTS

The current version of the DOT code at WANL, DOT-IIW, was completed as a portion of the CY '69 study program. This version was derived from two earlier versions of the DOT code obtained from F. R. Mynatt. Original DOT work at WANL, which was initiated in early 1967, was the conversion of the original IBM 7094 version of the code to the CDC-6600 computer. This modified IBM 7094 version incorporated a number of revisions to provide a code compatible with WANL's needs and computer system. In early 1968, an effort to convert the principal calculation subroutine GRIND into CDC-6600 assembly language (ASCENT or COMPASS) under the CDC-6600 SCOPE 2.0 Monitor System was completed. This version of the code has been used in radiation and shielding analysis of the NERVA nuclear rocket system until the completion of the CY '69 work effort. During the time period from mid-1968, further developments in the DOT code at WANL have included the development of a capability to run asymmetric quadrature sets for analysis of radiation transport in low density or void regions.

In the study program for CY '69, the incorporation of a majority of the DOT-II code development reported by F. R. Mynatt was incorporated into the WANL DOT code. Maximum use of the FORTRAN coding performed by Mynatt provided a code of similar capabilities and coding as that in his DOT-II code. The coding improvements or developments incorporated into the DOT-IIW code have included the coding and checkout of the following capabilities:

- Incorporation of three inner iteration convergence acceleration techniques,
- Zones of convergence logic on inner iteration convergence tests,
- Incorporation of an upscatter scaling technique,
- Separate convergence test on upscatter scaling,
- Albedo boundary conditions for three boundaries,
- Cross section input by magnetic tape consistent with the ANISN code,
- Output scalar fluxes on logical tape unit 1 for all types of calculation,
- Optional selective angular flux output on magnetic tape for three axial mesh rows only,

- Top boundary source data from magnetic tape obtained from a previous DOT-IIW problem or MAP problem,
- Recoding of subroutine GRIND in CDC-6600 assembly language to include acceleration and albedo boundary condition logic.

In performing the recoding of the DOT code to include the above improvements, a number of improvements in the handling of core storage of data and a correction of certain coding errors were made to the DOT code. A number of coding improvements were incorporated to increase the applicability of the DOT code to design calculations. A number of coding errors and/or use of improper logic in the DOT code, which were present in the versions of the code obtained from ORNL or coded at WANL, were corrected in this work program. The principal areas of error encountered in the application of the DOT code to NERVA design calculations were associated with the incorporation of the upscatter scaling techniques into the DOT code as performed at WANL. In addition, corrections to the DOT code were made to provide a technique which made consistent use of core memory storage allocation for all types of calculations and, therefore, minimized core storage to run a particular type of problem with or without acceleration. The use of consistent coding techniques with the corrected DOT code as well as the consistent use of core memory storage allocation provides a code with maximum flexibility and also maximum capability.

4.1.1 Inner Iteration Convergence Acceleration Techniques

The DOT code improvement described here involved the incorporation and checkout of group flux solution acceleration techniques developed by Mynatt⁽²⁾ (and available in a released version of the DOT-II code⁽³⁾) into a CDC-6600 version of the DOT code.

The latest version of the DOT code, DOT-II, was obtained as an IBM 360/75 computer code from the Radiation and Shielding Information Center (RSIC) at ORNL. Successive over-relaxation (SOR), Chebyshev (CA), and space point scaling (SPS) acceleration techniques available in this latest version were incorporated in the WANL CDC-6600 version of DOT. SPS, SOR, and CA techniques in DOT-II were partially recoded to: a) be compatible with

the CDC-6600 version of the code, b) be consistent in the use of core memory storage for data, and c) provide consistent application of the various acceleration techniques to all flux related data in the group flux solution. A brief description of the inner iteration technique in DOT and of the four acceleration techniques will be described here. The reader is referred to Reference 2 for a more detailed description of the mathematical basis of the acceleration techniques employed in DOT-II and adapted here.

Inner Iteration Technique

The DOT code numerical procedure used in solving the discrete ordinates difference equations in a multigroup approximation involves a two-loop iterative process. The outer (power or major) iteration loop is the solution of the energy dependence in a multigroup approximation including group-to-group energy coupling. In the DOT code, this energy coupling includes the fission neutron source and the group-to-group scatter-transfer (as a Legendre polynomial of arbitrary order to approximate the particle energy-angle scattering relationship). The general anisotropic scattering approximation results in an anisotropic scattering source (either down scatter or upscatter) in a specific group from all other groups in the multigroup set.

This source of particles in a group (along with the option of including a fixed isotropic distributed source of particles in a group) provides the total fixed source of particles in a group.

The inner (or minor) iteration loop in DOT involves the solution of specific energy group flux quantities using the fixed total source (i.e., fission, inscatter, fixed) in the solution. The inner iteration loop in DOT is provided to converge the group scattering source due to scattering within a group. The inner iteration loop involves an ordered sweep of the angular and spatial mesh difference equations using recursion relations to obtain a solution of the angular and spatial dependent flux data. An evaluation of the flux convergence in the DOT code is performed on the scalar flux data at the completion of each inner iteration and this loop is terminated only after satisfying the input convergence criteria or until a specified limit of inner iterations is completed.

The inner iteration convergence logic in DOT-IIW was slightly modified from the DOT-II capability to better suit the analysis of multizoned reactor cores. The zones of convergence logic was added to improve the convergence of the types of problems encountered in design analysis of NERVA reactors. The convergence logic on an inner iteration flux solution involves the use of either a pointwise flux error after each inner iteration or the use of the average flux error after each inner iteration. This logic is described in Section 4.1.4.

In order to accelerate the group flux solution, three new convergence acceleration techniques were provided in the DOT-II code. These techniques complement the regular inner iteration convergence acceleration technique of normalized power iteration.

The DOT-IIW code incorporates a choice of four inner iteration convergence acceleration techniques by which the scalar flux solution may be obtained. These choices are defined by the DOT-IIW input parameter, A09, as follows:

Normalized Power Iteration Method (A09=0) - A spatially independent method based on an integral source ratio in a group (fission, fixed distributed, inscatter, and within group scattering). Method is applied on all inner iterations. Independent of user selection of convergence acceleration technique.

Space Point Scaling Method (A09=1) - A spatially dependent method based on particle balance equations in each mesh cell and adjacent mesh cells. Method is applied on cycle (every 2nd to 15th inner iteration) determined internal to DOT-IIW code.

Successive Overrelaxation Method (A09=2) - A spatially dependent method based on the differences in successive inner iteration flux solutions (residuals) for each mesh cell. Method is applied on every 4th inner iteration.

Chebyshev Semi-Iterative Method (A09=3) - A spatially independent method based on Chebyshev polynomials. Method is applied on every inner iteration past 3rd with use of convergence logic on the extrapolation constant.

The selection of any of these techniques requires that all groups in the multigroup set are solved using the same technique. The choice of technique to be used in accelerating inner iteration convergence is dependent upon the type of application, the

computer memory core capability, and the type of convergence desired. The user of the code must develop an individual understanding of these techniques in order to achieve the desired results in a minimum of computer time or expenditure.

A brief description of each type of convergence acceleration technique in DOT-IIW is presented in following sections and the reader is referred to Reference 2 for a more detailed description.

Normalized Power Iteration

The standard procedure of inner iteration convergence acceleration technique employed in the DOT-IIW code is an integral normalization technique (i.e., normalized power iteration). This technique has historically been used in all discrete ordinates transport codes and was available in all previous versions of the DOT code. A brief description of the technique will be presented here to illustrate the technique, but the reader is referred to Reference 2 for a detailed explanation of the method and its particular application to the inner iteration solution of the DOT code.

Normalized power iteration is a spatially independent technique which uses the ratio of the volume integral of the particle source on two succeeding inner iterations to obtain a scale factor to be applied to the flux related quantities. The scale factor to be applied to the calculated flux data of the n^{th} iterations, f_{n+1} , is obtained as follows:

$$f_{n+1} = \frac{S_g^n}{S_g^n + \Delta W_g}$$

where: f_{n+1} is the spatially independent scale factor based on the volume integral source ratio,
 S_g^n is the volume integral of the sum of the fission, fixed distributed, and inscatter source in group g,
 ΔW_g is the differential change of the volume integral of the within-group scatter source in group g between the n^{th} and $n^{\text{th}} - 1$ inner iterations.

The term, ΔW_g , is obtained from the mesh cell scalar fluxes, from the n^{th} and $n^{\text{th}} - 1$ inner iterations, ϕ_{ij}^{n+1} and ϕ_{ij}^n , the mesh cell volumes, V_{ij} , and the mesh cell within-group scatter cross section $\sum_{ij}^{gg}$, as follows:

$$\Delta W_g = \sum_{i=1}^{IM} \sum_{j=1}^{JM} V_{ij} \sum_{ij}^{gg} \left(\phi_{ij}^n - \phi_{ij}^{n-1} \right)$$

This single calculated scale factor, f_{n+1} , is applied to all mesh cell flux data (scalar flux, higher moment flux, and implicit boundary condition angular flux) at the completion of the n^{th} inner iteration to obtain the flux guess for the $n^{\text{th}} + 1$ inner iteration.

Space Point Scaling Method

Space point scaling is a spatially dependent inner iteration convergence acceleration technique using a generalization of the normalized power iteration method and applied to each mesh cell. This technique has been successfully used in ANISN and DOT-II for certain classes of problems. The application to R- θ geometry for neutronic analysis of complex design configurations such as NERVA have been limited and the use for solution of multithermal group problems necessary for NERVA design analysis is essentially non-existent. This study program involved the incorporation of the techniques (and coding) of DOT-II into the WANL version, DOT-IIW, and a study of its effect on convergence acceleration. Some minor improvements in the technique were made during this study. The description of the technique is explained in detail in Reference 2 and will be summarized here.

Space point scaling involves the application of a technique which defines a five point difference equation from the transport equation for a mesh cell, ij , and the adjacent four mesh cells. The mesh cells in this five point difference equation for mesh cell ij , are multiplied by mesh cell scale factors to equate sources and losses as follows:

$$f_{i-1,j}^{Ll_{i-1,j}+f_{i+1,j}^{Ll_{i+1,j}+f_{i,j-1}^{Ll_{i,j-1}+f_{i,j+1}^{Ll_{i,j+1}+f_{i,j}^{LO_{i,j}+}} \\ f_{i,j} \sum^R \phi_{i,j} = S_{i,j}$$

where $Ll's$ are the incoming leakage terms for the four faces of the mesh cell, ij ,

$LO_{i,j}$ is the outgoing leakage term for the four faces of mesh cell, ij ,

$\sum^R \phi_{i,j}$ is the removal term - scalar flux times volume times cross section (absorption plus outscattering) for the mesh cell.

$S_{i,j}$ is the total source - volume times source (fission, fixed, and inscatter) for mesh cell, ij , and,

f_{ij} are the scale factors associated with each mesh cell, ij

The technique used in DOT-II to solve this system of equations for the mesh cell scale factors is an iterative technique. The equation for iteration is,

$$f_{i-1,j}^{Ll_{i-1,j}+f_{i+1,j}^{Ll_{i+1,j}+f_{i,j-1}^{Ll_{i,j-1}+f_{i,j+1}^{Ll_{i,j+1}+f_{i,j}^{LO_{i,j}+}} \sum^R \phi_{i,j} = S - f_{i,j-1}^{Ll_{i,j-1}+} \\ f_{i,j+1}^{Ll_{i,j+1}+}$$

where the iteration on this equation proceeds from a guess of 1.0 for all $f_{i,j}$ and the superscript n designates the n^{th} iteration on scale factors.

The DOT-IIW convergence test on this solution of scale factors is given by:

$$\frac{1}{IJ} \sum_{i,j} \frac{f_{i,j}^n - f_{i,j}^{n-1}}{f_{i,j}^n} < 0.1 \times \epsilon$$

where IJ is the total number of mesh cells, and
 ϵ is the convergence criterion on eigenvalue (EPS)
 DOT-IIW

This convergence test on the scale factor iteration loop was arrived at from a study of the convergence behavior on r, z and r , problems of the type encountered in NERVA design. A convergence criteria associated with the overall convergence desired in the problem were selected for use in DOT-IIW and there may exist problem types which may require less stringent criteria. In addition, an upper limit of 100 iterations on the scale factor iteration loop is coded into subroutine WWESOL in DOT-IIW since, for the class of problems encountered in this study, the scale factors were obtained in less than 100 iterations. When more than 100 iterations were required the scale factor iterations normally exceeded 1000 without a converged solution.

Space point scaling as described above is applied to the inner iteration fluxes as obtained from the normal inner iteration solution in DOT-IIW. The application of space point scaling to each set of inner iteration fluxes in DOT-IIW is limited to a cyclic operation in which only the normal power iteration is used for intermediate iterations and space point scaling is applied at predetermined iterations. In DOT-IIW an estimate of the dominance ratio of the solution matrix is obtained as the maximum value of the ratio of within-group (self) scatter and the total (or transport) cross section in any mesh cell i, j :

$$R_D = \max_{i,j} \left[\frac{\sum g g}{\sum t} \right]_{i,j} \quad - \quad \text{for all } i, j$$

This estimate of dominance ratio is used to obtain the scaling cycle of the space point scaling method.

Table 4-1 illustrates the internal scale cycle logic in DOT-IIW. This data was obtained from observation of the class of problems encountered in this study. Adjustments of this scale cycle logic may be necessary for certain types of problems; but in this study, problems using the SPS method on this scale cycle were always converged in fewer iterations than the normalized power iteration. When a scale cycle of 3 was assigned for all groups (independent of the estimate of dominance ratio) certain high dominance ratio groups ($R_D > 0.9$) required more iterations than normalized power iteration. This is an indication of an overambitious scaling procedure.

A comparison of the application of the space point scaling method versus other techniques is contained in Section 6.0.

Successive Overrelaxation

The Successive Overrelaxation acceleration (SOR) technique incorporated in the DOT-IIW code is a space dependent technique which uses a mesh cell dependent scale factor based on three successive normalized power iteration solutions. The scale factor is applied to all flux related quantities. The technique internally computes the scaling factor based on the successive iterate fluxes and, therefore, requires no external input parameters. In the present application, the acceleration technique is applied at the completion of every fourth normalized power iteration. The inner iteration logic involves the computation of the normalized power iterate flux for the intermediate iterations with the required mesh cell flux residuals saved for the previous iterations.

At the completion of the third iteration in the fourth inner iteration cycle, the successive overrelaxation technique is applied to the third iterate mesh cell flux value, ϕ_{ij}^3 , to obtain an extrapolated fourth iterate flux value guess, ϕ_{ij}^4 . The technique used in DOT-IIW is as follows:

$$\phi_{ij}^4 = (1.0 - w) \phi_{ij}^2 + w \phi_{ij}^3$$

TABLE 4-1
SPACE DEPENDENT SCALING CYCLE AS A FUNCTION
OF MAXIMUM DOMINANCE RATIO

RANGE OF DOMINANCE RATIO, $\frac{\sum_{99}}{\sum_t}$	CYCLE, $\frac{\text{INNER ITERATIONS}}{\text{SCALING}}$
0.0 - 0.6	2
0.6 - 0.8	3
0.8 - 0.9	5
0.9 - 0.95	7
0.95 - 0.97	9
0.97 - 0.99	11
0.99 - 1.0	15

where the superscripts 2 and 3 are the iteration number within a four iteration cycle. The extrapolation factor, w , is calculated from the flux residuals of the previous iterations as follows:

$$w = \frac{1.0}{\left[1.0 - \frac{R_3}{R_2}\right]}$$

$$\text{Where, } R_3 = \phi_{ij}^3 - \phi_{ij}^2$$

$$R_2 = \phi_{ij}^2 - \phi_{ij}^1$$

In the current version of the DOT-IIW code the value of the denominator, $1.0 - \frac{R_3}{R_2}$, is limited to be in the range of 0.01 to 10.0 and a negative denominator results in the denominator being set to a value of 1.0

From the extrapolated flux value guess, ϕ_{ij}^4 , the scale factor for the mesh cell, ij , is computed as:

$$f_{ij} = \frac{\phi_{ij}^4}{\phi_{ij}^3}$$

and this scale factor is applied to all flux moments and implicit boundary angular fluxes.

Analysis of the effect of this acceleration technique on the solution of multigroup problems has been limited. In general, the number of inner iterations required to converge to a pointwise convergence criteria is less than the normalized power iteration number. The particular class of problems which this technique seems to be most applicable is where no deep penetration is encountered and the flux solution is one of solving the within-group scattering with little or no in or out leakage of particles from the mesh cell. A description of a limited number of test problems is presented in Section 6.0.

Chebyshev Acceleration

The Chebyshev polynomial method of improving the inner iteration convergence of within-group scattering and the group flux solutions in DOT-IIW was adapted from DOT-II coding. The technique, as described in detail in Reference 2, involves the use of the Chebyshev semi-iterative method as described by Varga.⁽¹⁸⁾ The technique results in a final driving function on the scalar flux identical to that employed in the successive over-relaxation technique described earlier. The technique in DOT-II (or DOT-IIW), however, is a spatially independent function in that the relaxation factor obtained is a single space independent quantity which is applied to all flux related quantities. As described by Mynatt in Reference 2, the technique used in DOT-II uses a physical interpretation of the normal power iteration method to obtain estimates of the parameters required in the evaluation of the Chebyshev polynomial $C_m(\rho)$ and the driving function. The driving function in DOT-II (or DOT-IIW) is given by:

$$\phi_{ij}^1 = w_{n+1} (\phi_{ij}^{n+1} - \phi_{ij}^{n-1}) + \phi_{ij}^{n-1}$$

where the expected value of the flux, ϕ_{ij}^1 , is obtained from the calculated value of the flux for the n^{th} iteration, ϕ_{ij}^{n+1} , and the calculated value of the flux from the $n^{\text{th}} - 2$ iteration, ϕ_{ij}^{n-1} . The driving function, w_{n+1} , is obtained according to the equation by Varga,

$$w_{n+1} = \frac{2 \rho_n C_m(\rho_n)}{C_{m+1}(\rho_n)}$$

and for $m = 1$, $w_1 = 1.0$. The parameter, ρ_n , which is the estimated dominance ratio of the matrix, is obtained from the within-group scattering source (S), net leakage (L), and removal (R) as follows:

$$\rho_n = \frac{S_n - L_n}{R_n}$$

The terms S, L, R for group g and for the n^{th} inner iteration are given by the volume integrals over mesh cells, ij , and discrete angles, m :

$$\begin{aligned}
 S_n &= \sum_{i=1}^{IM} \sum_{j=1}^{JM} \Sigma_{ij}^{gg} \phi_{ij}^n V_{ij} \\
 R_n &= \sum_{i=1}^{IM} \sum_{j=1}^{JM} \Sigma_{ij}^t \phi_{ij}^n V_{ij} \\
 L &= \sum_{i=1}^{IM} \sum_{m=1}^{NOA} \eta_m A_i \phi_{im}^n W_m + \sum_{j=1}^{JM} \sum_{m=1}^{NOA} \mu_m A_j \phi_{jm}^n W_m \\
 &\quad \text{for } \mu_m > 0.0
 \end{aligned}$$

where ϕ_{ij} are the mesh cell scalar flux for the n^{th} inner iteration, $\Sigma_{ij}^{gg} : \Sigma_{ij}^t$ are the within-group scatter and total (or transport) cross section for the material in mesh cell ij , $V_{ij} : A_i : A_j$ are mesh cell volumes, and surface areas, ϕ_{im}^n and ϕ_{jm}^n are the boundary surface angular fluxes, and $\mu_m : \eta_m : W_m$ are discrete ordinate quadrature data.

If a fixed boundary source is present in the problem and group then the total boundary source is added to the net leakage term, L .

The present Chebyshev technique as applied in DOT-IIW commences with the third inner iteration and is applied to each inner iteration until the change of the parameter $\frac{1}{\rho_n}$ converges to satisfy convergence logic given by:

$$\left(\frac{1}{\rho_n} - \frac{1}{\rho_{n-1}} \right) < \frac{0.001}{2} \left(\frac{1}{\rho_n} + \frac{1}{\rho_{n-1}} \right)$$

When the above condition is satisfied, the driving function, w_n , which produced the values of $\frac{1}{\rho_n}$ and $\frac{1}{\rho_{n-1}}$, is used for all subsequent iterations.

The extrapolated flux related quantities used for the $i^{\text{th}} + 1$ iteration, are obtained in DOT-IIW by scaling all scalar flux and related by the spatially-dependent factor

$$f_{ij} = \frac{\phi_{ij}^n}{\phi_{ij}^{n+1}}$$

where the fluxes ϕ_{ij} , ϕ_{ij}^{n+1} are for each mesh cell ij . This factor, f_{ij} , is then used to obtain the extrapolated values in DOT-IIW of the scalar flux, higher flux moments, and boundary surface angular fluxes.

As presently coded, the Chebyshev acceleration technique is not applicable to problems containing implicit (periodic and reflective) boundary conditions at the right, top, or bottom surfaces. This behavior was encountered in the application of the Chebyshev technique to design problems as noted in Section 6.0. No application of this technique beyond simple test problems on r,z geometry was attempted in this study program.

Selection of Convergence Acceleration Technique

One consideration in the selection of any of the acceleration techniques is the core memory requirement to store the data required for the particular acceleration method. The use of the DOT-IIW code on certain computers with limited core memory may require the user to either reduce his problem size (i.e., mesh, angular quadrature, P_ℓ scattering approximation) or to bypass using certain acceleration techniques. In the DOT-IIW code, the core memory allocation for each of the acceleration techniques is coded consistently in that the same data array is used to store data. The size of this array is adjusted to be of a size adequate to contain the required data as follows:

<u>Convergence Acceleration Method</u>	<u>Extra Core Memory Storage Requirement</u>
Normalized Power Iteration	None
Space Point Scaling	$5 \times IM \times JM$
Successive Overrelaxation	$IM \times JM$
Chebyshev	$IM \times JM$

The variables IM , JM are the number of radial and axial intervals in the problem.

A second consideration is the effectiveness of the technique for certain problems. Experience obtained in this study program indicated that the space point scaling method is the most effective for a broad class of problems with the largest time savings in the application to fixed distributed source problems such as photon transport problems. In deep penetration problems, the space point scaling method will most generally be better. The effectiveness of the space point scaling technique is strongly dependent on the mesh cell dimensions (size in centimeters and mean free paths) and the user is cautioned against requiring tight flux convergence for large mesh cell conditions. These conditions in a multigroup problem require considerable intuition by the user to define a mesh model. The successive overrelaxation method employed here was effective for the class of problems solved in this study program but additional experience must be gained in the application to other classes of problems. The Chebyshev technique is not applicable to the types of problems used in this study (i.e., r, θ) since the periodic and reflective boundary conditions (top, bottom, and right) cannot be calculated by the technique. In simple test cases of r, z geometry, the technique does work but was only slightly better than the normalized power iteration. This behavior is due to the space independent driving function of the method.

One advantage of the SOR technique is its limited use of computer core memory. The technique requires only one additional storage array of size $IM \times JM$. This array contains the residual, R_2 , which is the difference between the mesh cell flux values and the first and second iteration of the four inner iteration cycle.

4.1.2 DOT-IIW Boundary Conditions

The DOT-IIW code has provisions for specifying the boundary conditions at each of the four external surfaces of a problem. These four boundaries are labeled "left," "right," "top," and "bottom" as indicated below for the various geometries.

The user has a choice of the following six boundary conditions:

- Vacuum** - the angular flux (ϕ_{mig} or ϕ_{mijg}) leaving the specified boundary is not returned and the incoming angular flux is equal to 0.0. The code allows the particles to escape from the system.
- Reflective** - The angular flux leaving the specified boundary is returned at the same boundary with perfect, mirror-reflection, as a function of spatial position, energy, and angle; i.e., the exiting flux is returned in the mirror reflection direction of the direction in which it left the system.
- Periodic** - The angular flux leaving the specified boundary is returned at the opposite boundary as a function of spatial position, energy, and angle; i.e., the exiting flux at the right boundary (or top boundary) is returned in the exact direction in which it left the system at the left boundary (or bottom boundary).

- White - The angular flux leaving the specified boundary is integrated over the angular variable. This flux is then returned isotropically at the same boundary as a function of spatial position, energy, and angle.
- Albedo - The angular flux leaving the specified boundary is integrated over the angular variable. The flux is then returned isotropically at the same boundary as a function of spatial position, energy, and angle and proportional to the input space-and energy-dependent albedo i.e., a fraction of the particles is returned.
- Source - The angular flux leaving the specified boundary is not returned. The angular flux that is returned at the boundary is input angular flux (boundary source) data as a function of spatial position, energy, and angle.

The code allows the following choices of boundary conditions:

<u>Left</u>	<u>Right</u>	<u>Top</u>	<u>Bottom</u>
Vacuum	Vacuum	Vacuum	Vacuum
Reflective	Reflective	Reflective	Reflective
Periodic	Periodic	Periodic	Periodic
	White	White	White
	Albedo	Albedo	Albedo
	Source	Source	

By careful forethought, the use of symmetry conditions in setting up the problem geometry may reduce problem complexity by a factor of two or more. It is also evident that:

- 1) A vacuum boundary condition at the left boundary is impossible for R, Z and R, θ geometries.
- 2) A periodic boundary condition for one boundary is an impossible specification. Opposite boundaries or all four boundaries must be specified as periodic.

3) A periodic boundary condition at the left and right boundary is impossible for R, Z and R, θ geometries.

4) An input albedo boundary specification greater than 1.0 generates particles.

Under the current contractual work, all of the available boundary conditions were checked out. In addition, the albedo boundary condition was added and checked out.

The WANL DOT-IIW code also provides automated coupling between successive linked-geometry DOT calculations using the boundary source option from magnetic tape. This boundary source tape is the format of the output angular flux tape from DOT-IIW and in addition the MAP code generates a magnetic tape in this format for automated coupling of DOT and MAP solutions.

4.1.3 DOT-IIW Convergence Logic

The DOT-IIW numerical procedure used in solution of the discrete ordinates difference equations in a multigroup approximation involves a two-loop iterative process. This process is described briefly in Section 4.1.1. Convergence logic in DOT-IIW occurs on the outer (power major) iteration loop as well as the inner(minor) iteration loop. A brief description of the convergence logic as incorporated in DOT-IIW is given in following sections.

Inner Iteration Convergence Logic

An evaluation of the flux convergence in the DOT-IIW code is performed on the scalar flux data at the completion of each inner iteration. The inner iterations are continued until the scalar flux converges according to one of two criteria:

1. If pointwise scalar flux is not desired; i.e., the input quantity, $G06 = 0.0$, then an integral convergence test is used with EPS as the criterion. Integral convergence is achieved if:

$$\frac{\sum_i \sum_{ij} \left| \frac{\phi_{ijg}^n - \phi_{ijg}^{n-1}}{\phi_{ijg}^n} \right| V_{ij}}{\sum_i \sum_{ij} V_{ij}} \leq \text{EPS}$$

where the summation is over the all-mesh cells, ij , or the mesh cells ij in the zones of convergence specified by the DOT input data A10 and the 28\$ array. The superscript, n , denotes the n^{th} inner iteration.

2. If pointwise scalar flux convergence is desired ($G06 \neq 0.0$), then a pointwise scalar flux criterion is used for all mesh cells in the system or for all mesh cells in the zones of convergence specified by the DOT input data A10 and the 28\$ array and using G06 as the convergence criterion in a test of the maximum flux deviation in the mesh cells of interest as follows:

$$\text{MAX} \left| \frac{\phi_{ijg}^n - \phi_{ijg}^{n-1}}{\phi_{ijg}^n} \right| \leq G06$$

If convergence on inner iterations has not been achieved after the maximum number of inner iterations specified by input for a group, then the inner iteration logic is terminated by the DOT-IIW code.

Analysis of the convergence pattern of R- θ eigenvalue problems indicated that a substantial portion of computer time was being spent in attempting to converge scalar fluxes in regions or mesh cells which had a negligible effect on the final results. The zone of convergence logic in the ORNL DOT-II code provided only a single zone of convergence for the flux convergence tests. This logic was extended in the DOT-IIW code: a) to allow the user to specify as input the zones of convergence (e.g., all fissionable zones); b) to test the average or pointwise flux error only in the specified zones of convergence.

This capability has improved the convergence on integral quantities in zones of interest and has resulted in a substantial savings in computer time.

4.1.4 Upscatter Scaling Technique

In the DOT code, the energy dependence of the neutron (or particle) behavior is represented by a multigroup approximation which treats all neutrons (or particles) by average velocity parameters within each group of a multigroup set. The solution of the multigroup particle fluxes requires an energy coupling algorithm between groups which in the DOT code is represented by:

- A Legendre polynomial expansion of the scattering from any group to any other energy group (including scattering within a group) and,
- Fission events which produce source neutrons or particles in a number of groups.

In the majority of applications of a multigroup approximation to the solution of eigenvalue, flux distributions, or other parameters, the procedure for solving the multigroup set of equations proceeds as a cyclic procedure involving first the solution of each of the group solutions in an order of decreasing energy (increasing lethargy) from the first group to the last group. The neutron source within each group during the pass through groups is the fission source from an assumed (or previous) multigroup flux guess (or an assumed fission guess), the fixed distributed source, and the inscatter source from all other groups. As the solution proceeds through the groups the procedure uses the latest available group flux solutions to provide the scatter-transfer source from all groups to the group being calculated. In the case of scatter-transfer from a higher energy group to a lower energy group this results in the use of the "best" estimate of current outer iteration fluxes as the data for the calculation of the scatter-transfer source. In contrast, the scatter-transfer from a lower energy group (i.e., upscatter) has only the previous outer iteration fluxes available to compute the scatter-transfer source (or the initial flux guess on the first outer iteration). The upscatter source in a particular group is analagous to the fission source in that it is always based on the previous outer iteration multigroup flux data. This iteration lag in the upscatter source of one outer iteration requires multiple outer iterations to solve for the correct spatial and energy

dependence of a multigroup problem. If fissions are present, then the interrelationship of fissions and groups containing upscatter (i.e., thermal groups) can require a large number of outer iterations to completely converge the multigroup solution.

A group independent upscatter scaling technique has been incorporated in the DOT-IIW code to accelerate the convergence of upscatter. This technique is in addition to techniques of normalization of the fission source for eigenvalue convergence and group flux acceleration techniques. This group independent upscatter scaling technique is patterned after the DTF-IV technique. (19)

The group independent technique involves the use of the total upscatter cross section in each group for each material in a DOT problem. In the DOT-IIW code this total upscatter cross section σ_g^{up} (i.e., the total cross section for outscatter from group g to all groups, $g-1$, and above) is calculated in subroutine S860 as follows:

$$\sigma_g^{up} = \sum_{g'=1}^{g'-1} \sigma_{g \rightarrow g'}$$

Total upscatter cross sections are computed automatically in DOT-IIW and are stored in the cross section table for each material and group in the table position following the total (or transport corrected) cross section. This internally revised cross section table is shown in Table 4-2. As shown, the cross section table is expanded to allow the total upscatter cross section in position IHT+1, and all of the scatter-transfer data is shifted down by one table position.

The upscatter scaling technique in DOT-IIW uses the total upscatter cross section, $\sigma_{g,ij}^{up}$ for the material at each mesh cell, ij , the scalar fluxes at each mesh cell, ϕ_{ij} , and the mesh cell volume, V_{ij} , to compute the total upscatter source as follows:

TABLE 4-2

DOT-IIW CROSS SECTION TABLE

DESCRIPTION

Position No.	Description
1	$\left. \begin{array}{l} 1 \\ 2 \\ \bullet \end{array} \right\} \sigma_g^{at}, \text{ arbitrary activity cross sections}$
2	
•	
IHT-2	$\sigma_g^a, \text{ absorption cross section}$
IHT-1	$\nu \sigma_g^f, \nu \text{ times fission cross sections}$
IHT	$\sigma_g^t, \text{ total (or transport) cross section}$
IHT+1	$\sigma_g^{up}, \text{ total upscatter cross section}$
IHT+2	$\left. \begin{array}{l} \bullet \\ \bullet \\ \bullet \end{array} \right\} \sigma_{g'g}, \text{ upscatter cross section for} \\ \text{scatter-transfer into group } g \\ \text{from group } g'$
•	
•	
•	
IHS	$\sigma_{gg}, \text{ within-group scatter cross section}$
IHS+1	$\left. \begin{array}{l} \bullet \\ \bullet \\ \bullet \\ \bullet \\ \bullet \end{array} \right\} \sigma_{g'g}, \text{ downscatter cross section for} \\ \text{scatter-transfer into group } g \\ \text{from group } g'$
•	
•	
•	
•	
•	
ITL	

$$S_1^u = \sum_{g=1}^{IGM} \sum_{j=1}^{JM} \sum_{i=1}^{IM} \sigma_{g,ij}^{up} \phi_{ijg} V_{ij}$$

The convergence parameter computer to test convergence in DOT-IIW is as follows:

$$UPSSF = 1.0 - \frac{S_2^u}{S_1^u}$$

which is the ratio of total upscatter source for successive outer iterations. This quantity is tested versus the input upscatter convergence parameter, A14*, to determine convergence.

This total upscatter source, S_1^u , is computed at the completion of an outer iteration in the latter portion of subroutine OUTER using the scalar fluxes calculated in the current outer iteration.

At the completion of the subroutine OUTER operations, the DOT-IIW code transfers to subroutine CNNP for convergence tests. In this subroutine, the upscatter scaling factor is computed and scaling of the scalar fluxes and associated quantities is carried out. The initial step in the upscatter scale logic in subroutine CNNP is the switch of the present iteration total upscatter source, S_1^u , with the previous iteration total upscatter source, S_2^u . This switch is made to preserve the source, S_1^u , for the next outer iteration scaling operation. The group independent upscatter scaling factor, TEMP, is then computed as a total source ratio as follows:

$$TEMP = \frac{F + Q}{F + Q - (S_2^u - S_1^u)}$$

where: F is the total, volume integral, fission source for the present outer iteration

$$F = \sum_g \sum_i \sum_j \nu \Sigma_{ijg}^f \phi_{ijg} V_{ij}$$

* The default option in DOT-IIW is that if A14 is input as 0.0, then A14 is set equal to EPS which is the eigenvalue convergence parameter.

Q is the total, volume integrated, fixed distributed source

$$Q = \sum_g \sum_i \sum_j Q_{ijg} V_{ij}$$

The term, $S_2^U - S_1^U$, is the difference in total upscatter source between the present and previous outer iterations. ** This quantity will approach 0.0 as the upscatter converges.

The upscatter scale factor, TEMP, is then applied to the scalar fluxes, higher flux moments, (if anisotropic scattering is present), horizontal (left and right) surface boundary angular fluxes, and to the vertical (top and bottom) surface boundary angular fluxes.

One additional operation⁽²⁰⁾ in the upscatter scale technique has been added in DOT-IIW. This is patterned after a late version of the DTF-IV upscatter scaling logic which involves the scaling of the present iteration total upscatter source, S_2^U , by the quantity, TEMP, so that the source, S_2^U , is consistent with the scaled scalar fluxes. This addition has a definite damping effect on the convergence pattern of the upscatter scaling and eigenvalue of a DOT problem.

The convergence test on upscatter occurs after scaling in DOT-IIW so that all flux quantities are scaled on every outer iteration. If upscatter is not converged, the code logic requires another outer iteration. If upscatter is converged then the code logic continues the normal convergence logic.

Two problems were selected to test the upscatter scaling technique in the DOT-IIW code. A series of test problems derived from these basic two were executed with various DOT-IIW input parameters. The stability of the convergence patterns were compared. Similar problems were run in the ANISN code to provide a basis of comparison.

** Note that S_2^U and S_1^U are reversed to allow for the recomputation of S_1^U at the completion of the next outer iteration.

TABLE 4-3

UPSCATTER SCALING TEST PROBLEM CROSS SECTIONS

c - Value (Mean Number of Secondaries Per Collision) of 1.2

Table Position	Description	Group Number		
		1	2	3
1	σ_g^a	0.0	0.0	0.0
2	$\nu \sigma_g^f$	0.2	0.2	0.2
3	σ_g^t	1.0	1.0	1.0
4	$\sigma_{g+2 \rightarrow g}^s$	0.333333	0.0	0.0
5	$\sigma_{g+1 \rightarrow g}$	0.333333	0.333333	0.0
6	$\sigma_{g \rightarrow g}$	0.333333	0.333333	0.333333
7	$\sigma_{g-1 \rightarrow g}$	0.0	0.333333	0.333333
8	$\sigma_{g-2 \rightarrow g}$	0.0	0.0	0.333333

The first test problem is derived from the S_n method c-value problems used by Carlson and Bell⁽²¹⁾ to examine the accuracy of the S_n method. For the purpose of testing the upscatter scaling technique a three group critical radius problem was employed. This three group test problem had an assumed c-value of 1.2, where

$$c = \frac{\nu \sigma_g^f + \sum_{g=1}^3 \sigma_{g \rightarrow g}^s}{\sigma_g^t}$$

Cross sections employed are shown in Table 4-3. A S_2 angular quadrature critical radius of 2.3297 centimeters with 16 equal sized radial mesh intervals and 2 axial mesh intervals of 1.0 centimeter each were used. The left, top, and bottom boundary conditions were mirror reflective conditions. The convergence pattern for the upscatter source error is shown in Figure 4-3. The three test problem conditions shown are with no upscatter scaling, with the upscatter scaling but without the addition of scaling the upscatter source (S_2^u) by TEMP, and the convergence with the current DOT-IIW technique. As shown, the convergence pattern is improved with the current group independent technique and the improvement in running time could be significant for problems requiring multiple outer iterations with tight flux convergence on inner iterations.

A second test problem is a one-dimensional mockup of a NERVA critical experiment as described in Section 5.0. The results obtained with this problem are described in Section 6.0.

4.1.5 Improved Tape Operations

In the CY'69 work the DOT-IIW code was modified to efficiently use the I/O devices (tape or disk) available on WANL's CDC-6600 computer. These modifications have resulted in reduced running time and a reduced probability of positioning errors on I/O devices.

Figure 4.3. Upscatter Scaling in Three Group, C-Value ($C = 1.2$), DOT-IIW Calculation

The DOT-IIW code, in computing the scattering source in Subroutine OUTER must read the present outer iteration flux tape as well as the previous outer iteration flux tape to compute the source. This computation involves reading both tapes in sequence. These tape operations were previously accomplished by backspacing the tapes to position the flux tape at the proper group fluxes. Backspacing is an acceptable technique when using tape I/O devices but disk backspacing is inefficient on the WANL CDC-6600 devices. To backspace a disk device, the disk head must be positioned. The file is read down to the previous record minus one. This sequence is repeated for each backspace operation. As a result, when the user attempted to substitute disks for tapes in DOT calculations, the PP (Peripheral Processor) time increased from a factor of 2 to 10, depending on the size of the problem. Obviously, the two backspace operations in Subroutine OUTER had to be removed to achieve optimum I/O operations. The backspace operations were removed by reprogramming Subroutine OUTER in the DOT-IIW code to rewind and read down with FORTRAN to the proper position on the I/O device.

At WANL, the computer user is free to choose either tapes or disks for his I/O devices. The timing specifications of the devices are as follows:

<u>Device</u>	<u>Access Time</u>	<u>Transfer Rate</u>
Disk Storage (Model 6638)	50-140 milliseconds	1.68 million characters/sec
Magnetic Tape (Model 607)	7 milliseconds	120 thousand characters/sec

From the above specifications, it is clear that running time using either all disks or all tapes can vary considerably depending on the information to be read. To put these figures in more meaningful terms, the following computer times were calculated from the device specifications as a function of record length for both disk (50 milisecond average access time) and tape devices.

<u>Record (Characters)</u>	<u>Tape Read Time (Milliseconds)</u>	<u>Disk Read Time (Milliseconds)</u>	<u>Tape is _____ Times Faster than Disk</u>
100	7.8	50.06	6.42
1000	15.3	50.6	3.31
2000	23.6	51.2	2.17
3000	31.9	51.8	1.62
5000	48.5	53.0	1.09
10000	90.0	56.0	0.62
50000	422.0	79.8	0.19
100000	837.0	109.5	0.13

It is obviously clear that: (1) for short records, tape devices are much faster than disks because of the faster access time, and that (2) for longer records, disk devices are much faster than tapes because of the larger transfer rate. In practice, the "break-even" point is not as clearly defined as the hypothetical times given above. In the multiprocessing environment of the WANL CDC-6600, up to seven jobs may be processed at one time, and these jobs may be competing for the same disk device. Under these conditions, the disk access time may degrade to 250 milliseconds resulting in a shift in the "break-even" point.

To verify the theoretical performance figures and to bracket the "break-even" point, two different DOT calculations were set up. The first calculation contained a record length of 904 sixty-bit words. The second calculation contained a record length of 11,960 sixty-bit words. Each calculation was run on two versions of the DOT-IIW code. The first version contained the backspace operations; the second version contained the rewind and read modifications performed under the current contractual work. The results are shown in Table 4-4.

Subsequent calculations set the "break-even" point at approximately 4000 words per record for DOT-IIW calculations. The results of these calculations indicate that the typical design calculation is sufficiently complex (> 10,000 words per record) to effect a noticeable reduction in both PP (Peripheral Processor) and Elapsed (Increased "throughput") time on the CDC-6600 computer system.

TABLE 4-4

TAPE VERSUS DISK I/O EVALUATION FOR DOT-IIW

<u>Parameter</u>	<u>Case No. 1</u>	<u>Case No. 2</u>	<u>Case No. 3</u>	<u>Case No. 4</u>	<u>Case No. 5</u>	<u>Case No. 6</u>
CP time (seconds)	747.2	746.4	746.3	1110.3	1111.4	1107.6
PP time (seconds)	386.0	467.7	519.5	383.6	387.9	231.2
CP + PP** time (seconds)	1133.2	1214.1	1265.8	1493.8	1499.3	1338.8
Elapsed time (seconds)	1463.*	1765.	1583.*	2147.	1628.	1549.
Device	Tapes	Tapes	Disks	Tapes	Tapes	Disks
Operation	Backspace	Rewind and read	Rewind and read	Backspace	Rewind and read	Rewind and read
No. of Words per Record	904	904	904	11,960	11,960	11,960

* Rollout - Rollin Performed. Rollin minus Rollout time has been subtracted from total elapsed time.

** WANL computer users are billed on a 1) CP + PP + 10 seconds rate, or 2) total elapsed time rate, whichever is less.

Outer Iterations Convergence Logic

Outer iterations in an eigenvalue problem, search problem, or problem containing upscatter, are continued until both the source term and upscatter source term have converged. The problem is converged when the following condition is satisfied:

$$\left| 1 - \frac{S_n}{S_{n-1}} \right| \leq \text{EPS.}$$

In an eigenvalue calculation, S_n is given by:

$$S_n = \frac{1}{k_n} \sum_g \sum_i \sum_j \nu \Sigma_{gij}^f \phi_{ijg} V_{ij}$$

In a search, S is given by the above integral with a k_n of unity. In a fixed source calculation with fissions, S_n is given by:

$$S_n = \sum_g \sum_i \sum_j \left[Q_{ij} + (\nu \Sigma_{gij}^f \phi_{ijg} V_{ij}) \right]$$

where Q_{ij} is the fixed distributed source.

The upscatter source is converged when:

$$\left| 1 - \frac{S_n^u}{S_{n-1}^u} \right| < A14$$

where S_n^u is defined as:

$$S_n^u = \sum_g \sum_i \sum_j \Sigma_{gij}^{UP} \phi_{ijg}^* V_{ij}$$

where ϕ_{ijg}^* is the upscatter-scaled flux.

If the upscatter scale convergence criterion, A14, is input as 0.0, then A14 is set equal to EPS for the upscatter convergence test.

If convergence on outer iterations has not been achieved after the maximum number of outer iterations, input quantity D05, have been completed, then the outer iterations are terminated. The DOT-IIW code then proceeds as if convergence had been obtained and prints out the balance tables, scalar fluxes, activities, fission density, etc.

4.2 SATELLITE CODE DEVELOPMENT

4.2.1 Cross Section Data Preparation Code - SATURN

The use of the DOT-IIW code for neutronic analysis of the NERVA reactor requires that the neutron cross section data be modified to account for the leakage of neutrons in the transverse direction of the two-dimensional geometry. Since the principal neutronics application of the DOT-IIW code would be the r - θ geometry, then the capability to include the transverse leakage effect as a fictitious absorption was necessary. This capability could either be contained in the DOT-IIW code with input parameters supplied by the user or a separate code could be developed. The second approach was selected in this study since a multipurpose code which performs cross section data handling was also needed.

The SATURN code was developed during this study program to provide the following tape or card operations.

- Generation of a group dependent or group independent magnetic tape for DOT input from punched card input data containing multigroup cross section data.
- Generation of a group independent magnetic tape for DOT input from an existing magnetic tape.
- Generation of a punched card data deck from an existing group dependent magnetic tape.
- Label or relabel of a cross section magnetic tape

The above operations are completely compatible with the ANISN code to provide constant one- and two-dimensional code capability. The need for group independent cross section data on magnetic tape arises from the large arrays of cross section data required for complex DOT or ANISN problems. A group independent magnetic tape is ordered such that each binary record includes cross section data for all materials and one group. A group dependent magnetic tape is ordered such that two binary records include the set identification data and cross section data for one material and all groups. The group independent tape does not include any identification records and includes only the number of records equal to the number of groups. In addition to the above capabilities, the SATURN code provides an additional

option for each of the above cross section handling functions. The option available to the user is the addition of a transverse leakage correction to the cross section data.

This operation can be used to selectively add a fictitious absorption term, $D_g B^2$, to the total ($\sum_g^t$) and absorption ($\sum_g^a$) neutron cross section for each group g as follows:

$$\sum_g^t = \sum_g^t + D_g B^2$$

$$\sum_g^a = \sum_g^a + D_g B^2$$

The diffusion coefficient, D_g , is calculated as $1.0 / (3.0 * \sum_g^t)$, and the transverse buckling is calculated in the same manner as in ANISN by:

$$B_g^2 = \left[\frac{\pi}{\Delta Z + \frac{C}{\sum_g^t}} \right]^2$$

The user of SATURN specifies the transverse dimension, ΔZ , and the extrapolation constant C ($\frac{1}{0.71}$). The user at option may specify cross section sets (by identification number) to be excluded from the transverse leakage correction calculation.

4.2.2 Mesh Evaluation Code in r, θ Geometry--MERTH

In order to provide a technique by which the models of the control vanes in the NERVA reactor could be developed to represent the actual design configuration, a new method has been coded in the MERTH Code (Mesh Evaluation in R, Theta). The MERTH code was coded to assist the designer in the layout of an r - θ mesh to represent off-axis cylindrical annuli (e. g., the control vane in the reflector). At the present time the logic of the MERTH code is quite simple and the engineer can use the code to assist in the development of an analytical model which closely approximates the model. The code accepts either regular or irregular r and θ mesh for the reflector sector being analyzed and requires an exact definition of the off-axis cylindrical annulus. Computations of the fraction of the off-axis cylindrical annulus in each mesh cell of the r - θ geometry is performed by a numerical technique and data is provided to assist the user in defining those mesh cells which best describe the off-axis cylindrical annulus. This technique is operational in a simplified version.

The control vane employed in the NERVA reactor is a boron containing plate attached to a rotating beryllium control drum. The drum can rotate a full 180° and the design calculations required include the 0° , 180° , and intermediate drum positions. The control vane itself is of 50 to 100 mils in thickness. This geometry requires that the user define the control vane explicitly in the reflector in order to predict the radial and azimuthal power distribution as a function of drum position as well as the control drum worth.

The technique used in the MERTH code provides an $R-\theta$ mesh which approximates an off-axis cylindrical annulus control vane, as shown schematically in Figures 4-4 and 4-5. The technique employed in the MERTH code involves the use of a coordinate system centered at the control drum centerline. Data for the cylindrical annulus is then translated to the $r-\theta$ mesh required for DOT with the origin at the reactor core centerline. As shown schematically in Figure 4-4 the control vane is subdivided into a number of equal size annular sectors, abcd. This area is then represented as the line segment, ei, of angular width, $\Delta\theta$. Points of intersection between the $r-\theta$ mesh line and the line segment, ei, are calculated by the code and portions of the area, abcd, is assigned to each mesh cell in which the area lies, (e.g., $1/2 \Delta\theta [R_g^2 - R_f^2]$). The user of MERTH performs multiple runs to find that mesh cell description of adequate number which will provide a continuous (at least one common point for adjacent mesh cells) mesh model of the cylindrical annulus. Capabilities included in the MERTH code include the ability to input data for specific regions and overlay the mesh cell description of regions until the entire mesh cell description of regions required of a DOT problem are assembled in a MERTH problem. This data can then be punched for DOT input.

Figure 4-4. Schematic of MERTH Numerical Technique

Figure 4-5. Schematic of MERTH Numerical Technique (Section A of Figure 4-4)

4.3 IMPROVEMENT OF THE TWO-DIMENSIONAL PERTURBATION THEORY CODE PERT-2DW

Perturbation theory codes,^(22,23) developed for use in design analyses, commonly use as input the forward and adjoint scalar flux generated by one of the multigroup diffusion codes. While adequate for treating reactor configurations in the categories of geometry and composition which are amenable to a diffusion theory treatment, the application of these methods to reactors with narrow, highly enriched regions, leads to errors in predicted distribution of the forward and adjoint flux and subsequently to inaccurate predictions of material reactivity worths from calculations with the perturbation theory.

The more accurate treatment of neutron distribution in space and energy, which is inherent to transport theory, can be used to generate the forward and adjoint angular flux for input to the perturbation theory codes. This has been done for one-dimensional geometry,⁽¹⁹⁾ and attempts have been made to synthesize the two- and three-dimensional perturbation theory calculations using as input one-dimensional transport theory forward and adjoint fluxes.⁽²⁴⁾

The recent availability of a two-dimensional discrete ordinate transport theory code DOT⁽¹⁵⁾ has created a base on which two-dimensional perturbation theory methods can be developed. This section describes the work done to develop a preliminary version of a two-dimensional perturbation theory code, using as input the forward and adjoint angular flux in an x, y , r, z , or $r-\theta$ geometry. The present capability of the code is limited to the use of an isotropic scattering cross section approximation with a transport correction i. e., diagonal transport, applied to the in-group scattering terms.

To make the code capable of evaluating the changes in the group-to-group transfer, the group in- and out-scattering in both upward and downward direction in energy has been treated explicitly and detailed results have been displayed as a function neutron reaction. In addition, the calculation of the prompt neutron lifetime based on the average group velocities has been included.

4.3.1 Form of the Forward and Adjoint Flux Equations

For a given reactor geometry and composition, the calculation of the space, angle, and energy distribution of the forward and adjoint flux may be carried out in two-dimensional discrete ordinate transport code, DOT. The equation solved for the forward flux is:

$$\left[\underline{\Omega} \cdot \nabla + \Sigma_a(\underline{r}, E) + \Sigma_s(\underline{r}, E) \right] \phi(\underline{r}, E, \underline{\Omega}) = S(\underline{r}, E, \underline{\Omega}) + \int_0^\infty \int_{4\pi} dE' d\underline{\Omega}' \left[\chi(E) \rightarrow \Sigma_f(\underline{r}, E') + \Sigma_s(\underline{r}, E' \rightarrow E, \underline{\Omega}' \rightarrow \underline{\Omega}) \right] \phi(\underline{r}, E', \underline{\Omega}') \quad (1)$$

and for the adjoint flux

$$\left[-\underline{\Omega} \cdot \nabla + \Sigma_a(\underline{r}, E) + \Sigma_s(\underline{r}, E) \right] \phi^\dagger(\underline{r}, E, \underline{\Omega}) = S(\underline{r}, E, \underline{\Omega}) + \int_0^\infty \int_{4\pi} dE' d\underline{\Omega}' \left[\chi(E') \rightarrow \Sigma_f(\underline{r}, E) + \Sigma_s(\underline{r}, E \rightarrow E', \underline{\Omega} \rightarrow \underline{\Omega}') \right] \phi^\dagger(\underline{r}, E', \underline{\Omega}') \quad (2)$$

The solution of these equations in DOT proceeds from representing the flux as discrete direction angular flux and by expanding the differential scattering cross section in Legendre polynomials as follows:

$$\Sigma_s(\underline{r}, E' \rightarrow E, \mu_0) = \sum_{n=0}^{\infty} \frac{2n+1}{2} \Sigma_{sn}(\underline{r}, E' \rightarrow E) P_n(\mu_0) \dots \quad (3)$$

where $\mu_0 = \underline{\Omega} \cdot \underline{\Omega}'$ and μ is the cosine of the angle between the direction of neutron motion and the outward directed normal. Also

$$\Sigma_s(\underline{r}, E' \rightarrow E, \underline{\Omega}' \rightarrow \underline{\Omega}) = 2\pi \Sigma_s(\underline{r}, E' \rightarrow E, \mu_0) \quad (4)$$

on the basis of azimuthal symmetry of scattering about the original direction of neutron motion.

4.3.2 Coefficients in the Expansion of Differential Scattering Cross Sections

The treatment of cross sections and the assumptions regarding anisotropic scattering affect the form of equations (1) and (2), from which the perturbation equation is derived, and for this reason will be given here in detail.

The coefficients $\sum_{sn}(\underline{r}, E' \rightarrow E)$ of (4) are determined beforehand, from theoretical or experimental values of $\sum_s(\underline{r}, E' \rightarrow E, \mu_0)$, by applying to it the relations,

$$\sum_{sn}(\underline{r}, E' \rightarrow E) = \int_{-1}^{+1} \sum_s(\underline{r}, E' \rightarrow E, \mu_0) P_n(\mu_0) d\mu_0 \dots \quad (5)$$

and the normalization,

$$\sum_{sn}(\underline{r}, E') = \int_0^{\infty} \sum_{sn}(\underline{r}, E' \rightarrow E) dE = \sum_s(\underline{r}, E) \dots \quad (6)$$

From application of (5) and (6)

$$\begin{aligned} \sum_{s0}(\underline{r}, E') &= \sum_s(\underline{r}, E') \\ \sum_{s1}(\underline{r}, E') &= \bar{\mu}_0 \sum_{s0}(\underline{r}, E') \dots \dots \dots \end{aligned} \quad (7)$$

When scattering is nearly isotropic, the expansion (3) can be limited to the first two terms:

$$\sum_s(\underline{r}, E' \rightarrow E) = 1/2 \sum_{s0}(\underline{r}, E' \rightarrow E) + 3/2 \mu_0 \sum_{s1}(\underline{r}, E' \rightarrow E) \dots \dots \quad (8)$$

Which, when integrated over E and μ_0 , gives the correct $\sum_s(\underline{r}, E)$.

An alternate approach is to apply the diagonal transport correction to the scattering cross sections and treat scattering as an isotropic event in the laboratory system of coordinates. This is equivalent to assuming that changes in energy do not involve changes in neutron direction, and changes in direction do not involve a change in energy. Thus

$$\sum'_s(\underline{r}, E' \rightarrow E, \mu_0) = \sum_{s0}(\underline{r}, E' \rightarrow E) - \sum_{s1}(\underline{r}, E) \delta(E' - E) \dots \quad (9)$$

where $\sum_{s0}$ and $\sum_{s1}$ are still defined by (7).

When integrated over E and added to $\sum_a(\underline{r}, E')$, this gives the familiar transport cross section

$$\begin{aligned} \sum_{tr}(\underline{r}, E') &= \sum_a(\underline{r}, E') + \sum_{s0}(\underline{r}, E') - \sum_{s1}(\underline{r}, E') \\ &= \sum_a(\underline{r}, E') + (1 - \bar{\mu}_0) \sum_{s0}(\underline{r}, E') \dots \dots \end{aligned} \quad (10)$$

Integration in (6) is commonly carried out by dividing up the total energy range into energy intervals chosen to give a multigroup structure. The resulting coefficients for scatter-transfer

from any group to any other group constitute the elements of the cross section scattering matrix. The addition of σ_a , $\nu \sigma_f$ and σ_{tr} , averaged over the same energy intervals, completes the cross section table. An example of the arrangement of such a table, formed for each isotope is given in Table 4-5.

For purpose of illustration, Table 4-5 is given for a three-group scheme with full downscatter and full upscatter. The table entries are shown as outscatter terms and are not in the input format of DOT.

Note that the transport correction is applied only to the in-group scatter term of the total cross section, converting it into a transport cross section, and to the in-group scattering terms of the scattering matrix, which are located on its diagonal, hence the name "diagonal transport correction."

4.3.3 Perturbation Equations in Operator Form

Application of the multigroup approximation for energy and expressing cross sections in their isotropic components as in Table 4-5, plus the substitution of the transport cross section $\Sigma_{tr}(g)$ for

$\Sigma_a(g) + \sum_{g'} \Sigma_s(g \rightarrow g') - \bar{\mu} \Sigma_s(g)$ and $\Sigma_s^*(g \rightarrow g) = \Sigma_s(g \rightarrow g) - \mu \Sigma_s(g)$ for $\Sigma_s(g \rightarrow g)$ allows equations (1) and (2) to be expressed in matrix form as follows (the fixed source is omitted for clarity):

$$\begin{bmatrix} \mu \cdot \nabla + \Sigma_{tr}(1) - \Sigma_s^*(1 \rightarrow 1) & -\Sigma_s(2 \rightarrow 1) & -\Sigma_s(3 \rightarrow 1) \\ -\Sigma_s(1 \rightarrow 2) & \mu \cdot \nabla + \Sigma_{tr}(2) - \Sigma_s^*(2 \rightarrow 2) & -\Sigma_s(3 \rightarrow 2) \\ -\Sigma_s(1 \rightarrow 3) & -\Sigma_s(2 \rightarrow 3) & \mu \cdot \nabla + \Sigma_{tr}(3) - \Sigma_s^*(3 \rightarrow 3) \end{bmatrix} \times \begin{bmatrix} \phi(1) \\ \phi(2) \\ \phi(3) \end{bmatrix} =$$

TABLE 4-5 CROSS SECTION TABLE FOR THREE GROUPS
WITH DIAGONAL TRANSPORT CORRECTIONS

g'	$g=1$	$g=2$	$g=3$
	$\sigma_a(1)$	$\sigma_a(2)$	$\sigma_a(3)$
	$\nu \sigma_f(1)$	$\nu \sigma_f(2)$	$\nu \sigma_f(3)$
	$\sigma_a(1) + \sum_g \sigma_s(1 \rightarrow g) - \bar{\mu} \sigma_s(1)$	$\sigma_a(2) + \sum_g \sigma_s(2 \rightarrow g) - \bar{\mu} \sigma_s(2)$	$\sigma_a(3) + \sum_g \sigma_s(3 \rightarrow g) - \bar{\mu} \sigma_s(3)$
1	$\sigma_s(1 \rightarrow 1) - \bar{\mu} \sigma_s(1)$	$\sigma_s(2 \rightarrow 1)$	$\sigma_s(3 \rightarrow 1)$
2	$\sigma_s(1 \rightarrow 2)$	$\sigma_s(2 \rightarrow 2) - \bar{\mu} \sigma_s(2)$	$\sigma_s(3 \rightarrow 2)$
3	$\sigma_s(1 \rightarrow 3)$	$\sigma_s(2 \rightarrow 3)$	$\sigma_s(3 \rightarrow 3) - \bar{\mu} \sigma_s(3)$

$$= \lambda_0 \times \begin{bmatrix} \chi(1) \nu \Sigma_f(1) & \chi(1) \nu \Sigma_f(2) & \chi(1) \nu \Sigma_f(3) \\ \chi(2) \nu \Sigma_f(1) & \chi(2) \nu \Sigma_f(2) & \chi(2) \nu \Sigma_f(3) \\ \chi(3) \nu \Sigma_f(1) & \chi(3) \nu \Sigma_f(2) & \chi(3) \nu \Sigma_f(3) \end{bmatrix} \times \begin{bmatrix} \phi(1) \\ \phi(2) \\ \phi(3) \end{bmatrix} \dots$$

and for the adjoint,

$$\begin{bmatrix} -\mu \cdot \nabla + \Sigma_{tr}(1) - \Sigma_s^*(1 \rightarrow 1) & -\Sigma_s(1 \rightarrow 2) & -\Sigma_s(1 \rightarrow 3) \\ -\Sigma_s(2 \rightarrow 1) & -\mu \cdot \nabla + \Sigma_{tr}(2) - \Sigma_s^*(2 \rightarrow 2) & -\Sigma_s(2 \rightarrow 3) \\ -\Sigma_s(3 \rightarrow 1) & -\Sigma_s(3 \rightarrow 2) & -\mu \cdot \nabla + \Sigma_{tr}(3) - \Sigma_s^*(3 \rightarrow 3) \end{bmatrix} \times \begin{bmatrix} \phi^+(1) \\ \phi^+(2) \\ \phi^+(3) \end{bmatrix} =$$

$$= \lambda_0^+ \times \begin{bmatrix} \chi(1) \nu \Sigma_f(1) & \chi(2) \nu \Sigma_f(1) & \chi(3) \nu \Sigma_f(1) \\ \chi(1) \nu \Sigma_f(2) & \chi(2) \nu \Sigma_f(2) & \chi(3) \nu \Sigma_f(2) \\ \chi(1) \nu \Sigma_f(3) & \chi(2) \nu \Sigma_f(3) & \chi(3) \nu \Sigma_f(3) \end{bmatrix} \times \begin{bmatrix} \phi^+(1) \\ \phi^+(2) \\ \phi^+(3) \end{bmatrix} \dots \dots \dots (12)$$

The above equations are given in a three-group form as an illustration.

If the cross section matrices are written as matrix operators $\underline{H}$ and $\underline{G}$ for the forward flux and as $\underline{H}^+$ and $\underline{G}^+$ for the adjoint flux, the two equations become

$$\underline{H} \underline{\Phi} - \lambda_0 \underline{G} \underline{\Phi} = 0 \quad (13)$$

$$\underline{H} \underline{\Phi} + - \lambda_0^+ \underline{G}^+ \underline{\Phi}^+ = 0 \quad (14)$$

Observe that $\underline{H}^+ = \underline{H}^T$, $\underline{G}^+ = \underline{G}^T$ and $\lambda_0^+ = \lambda_0$, where the superscript T denotes a matrix transpose. The neutron balance implied by (13) and (14) applies at each mesh cell volume, and each energy group, as well as for the system as a whole.

Equations (13) and (14) are connected through the adjoint relation

$$\int \underline{\Phi}^+ \underline{H} \underline{\Phi} dV = \int \underline{\Phi} \underline{H}^+ \underline{\Phi}^+ dV \quad (15)$$

$$\int \Phi^+ \underline{G} \Phi dV = \int \Phi \underline{G}^+ \Phi^+ dV \quad (16)$$

Where required for conformability, the flux vectors are transposed. The integrals are carried out over the reactor volume V and require that both the forward and the adjoint flux go to zero on its outside surface.

The above equations define the forward and the adjoint flux as forming a biorthogonal set spanning the extrapolated reactor volume and whose eigenvalue, λ_0 , can be calculated from either of:

$$\int \Phi^+ \underline{H} \Phi dV - \lambda_0 \int \Phi^+ \underline{G} \Phi dV = 0 \quad (17)$$

$$\text{or} \quad \int \Phi \underline{H}^+ \Phi^+ dV - \lambda_0 \int \Phi \underline{G}^+ \Phi^+ dV = 0 \quad (18)$$

Equation (17) is conventionally subjected to the perturbation and the reactivity change calculated from it. It will be shown later, however, that the same result can be obtained by perturbing the mathematically equivalent equation (18). The interpretation of the groupwise results is not as clear, in that case, however.

Equation (17) will now be subjected to a first order perturbation, i.e., it will be assumed that the forward and adjoint flux are unchanged by the perturbation and that the response to the perturbation will be reflected only in the eigenvalue, which will assume a new value λ_p . Thus, from (17)

$$\int \Phi^+ \delta \underline{H} \Phi dV - \delta \lambda_0 \int \Phi^+ \underline{G} \Phi dV - \lambda_0 \int \Phi^+ \delta \underline{G} \Phi dV = 0 \quad (19)$$

$$-\delta \lambda_0 = \frac{-\int \Phi^+ \delta \underline{H} \Phi dV + \lambda_0 \int \Phi^+ \delta \underline{G} \Phi dV}{\int \Phi^+ \underline{G} \Phi dV} = \lambda_0 - \lambda_p \quad (20)$$

$$= \frac{1}{K_0} - \frac{1}{K_p} \text{ since } K_{\text{eff}} = \frac{1}{\lambda_0}$$

The above equation is the required perturbation equation. It will be given first in the discrete ordinate form, corresponding to the solution for the flux and adjoint, and then its numerical solution will be described.

The perturbation matrices, $\underline{\underline{H}}$ and $\underline{\underline{G}}$, required by equation (20), are formed by changing all macroscopic cross sections in the volume of the reactor to be perturbed. This change takes the form of either a uniform change of number density of an existing core constituent, or the addition of a new perturbing material at a specified density; thus $\delta \underline{\underline{H}} = \underline{\underline{\nabla}} \cdot \delta N$. Under these conditions, the volume integrals in the numerator of equation (20) will have non-zero values only in the region perturbed, and will be zero in those regions where $\delta \underline{\underline{H}} = 0$.

The perturbation matrices are as follows:

$$\delta \underline{\underline{H}} = \begin{bmatrix} 0 + \delta \Sigma_{tr}(1) - \delta \Sigma_s^*(1 \rightarrow 1) & -\delta \Sigma_s(2 \rightarrow 1) & -\delta \Sigma_s(3 \rightarrow 1) \\ -\delta \Sigma_s(1 \rightarrow 2) & 0 + \delta \Sigma_{tr}(2) - \delta \Sigma_s^*(2 \rightarrow 2) & -\delta \Sigma_s(3 \rightarrow 2) \\ -\delta \Sigma_s(1 \rightarrow 3) & -\delta \Sigma_s(2 \rightarrow 3) & 0 + \delta \Sigma_{tr}(3) - \delta \Sigma_s^*(3 \rightarrow 3) \end{bmatrix} \quad (21)$$

$$\delta \underline{\underline{G}} = \begin{bmatrix} \chi(1) \delta \nu \Sigma_f(1) & \chi(1) \delta \nu \Sigma_f(2) & \chi(1) \delta \nu \Sigma_f(3) \\ \chi(2) \delta \nu \Sigma_f(1) & \chi(2) \delta \nu \Sigma_f(2) & \chi(2) \delta \nu \Sigma_f(3) \\ \chi(3) \delta \nu \Sigma_f(1) & \chi(3) \delta \nu \Sigma_f(2) & \chi(3) \delta \nu \Sigma_f(3) \end{bmatrix} \quad (22)$$

Examination of these matrices reveals that the changes in the number densities will affect only the macroscopic cross sections, but will leave the fission spectrum $\chi(g)$, and the leakage terms $\mu \cdot \nabla$ unaffected. The latter effect is due to the fact that the leakage term in transport theory is number density independent. This differs from the diffusion theory, in which the leakage term contains the factor $D = 1/3 \sum_{tr}$, which is dependent on changes in number densities.

In those formulations of the transport theory which allow non-isotropic scattering, i.e., the P_1 and higher terms in the cross section expressions, the number density-dependent leakage terms reappear again as products $\phi_n \sum_{sn}$, and are again included in the perturbation matrices $\delta \underline{\underline{H}}$ and $\delta \underline{\underline{G}}$.

Since an isotropic scattering approximation has been used (but properly transport corrected), the leakage term will not appear in the derivation of the perturbation matrices.

The above considerations are consistent with the assumption of the first order perturbation theory, namely that the perturbed flux is so little changed that it can be replaced by its unperturbed form. Thus, the gradient-dependent part of leakage remains unperturbed.

4.3.4 Treatment of the transverse leakage Correction

The DOT code solves the multigroup discrete ordinate transport equation in x, y, r, γ , or $r-\theta$ geometry. In r, z geometry the total leakage from the reactor is handled directly. In x, y and $r-\theta$ geometry the leakage in the direction perpendicular (transverse) to the plane containing the coordinates x, y or $r-\theta$ is handled by increasing the total neutron absorption term by the factor, DB_T^2 , taken from diffusion theory

where $D = 1/3 \Sigma_{tr}$, $B_T^2 = (\frac{\pi}{H^*})^2$, and H^* is the extrapolated transverse direction:

$$H^* = H + 2 \times 0.71 \lambda_{tr}, \lambda_{tr} = 1/\Sigma_{tr}.$$

Thus the transverse leakage corrected Σ_{tr} becomes

$$\Sigma_{tr}^{LC} = \Sigma_{tr} + DB_T^2 = \Sigma_{tr} + \frac{B_T^2}{3 \Sigma_{tr}} \quad (23)$$

This term, when subject to perturbation, becomes

$$\delta(\Sigma_{tr}^{LC}) = \delta \Sigma_{tr} - \frac{B_T^2 \delta \Sigma_{tr}}{3(\Sigma_{tr})^2} = \delta \Sigma_{tr} \left[1 - \frac{B_T^2}{3(\Sigma_{tr})^2} \right] \quad (24)$$

This term, therefore, should replace $\delta \Sigma_{tr}$ in the perturbation equations.

4.3.5 Equations for Forward and Adjoint Flux

The solution of equations (1) and (2), with cross sections modified as shown in the preceding section, is carried out in the DOT code by the method of discrete ordinates. Energy, space and angle variables are discretized such that the following relations hold for the flux.

$$\int_0^V dV \int_0^\infty dE \int_0^{4\pi} d\Omega \phi(\underline{r}, E, \underline{\Omega}) = \sum_{i=1}^I V(i) \sum_{m=1}^M W(m) \sum_{g=1}^G N(i, m, g) \quad (25)$$

and the current

$$\int_0^V dV \int_0^\infty dE \int_0^{4\pi} d\Omega \underline{\Omega} \cdot \underline{\Omega} \phi(\underline{r}, E, \underline{\Omega}) = \sum_{i=1}^I V(i) \sum_{m=1}^M W(m) \mu(m) \sum_{g=1}^G N(i, m, g) \quad (26)$$

where

$V(i)$ - element of volume in space

$W(m)$ - weight in numerical quadrature over angular direction

$\mu(m)$ - cosine of the angle defining the discrete direction

$N(i, m, g)$ - angular neutron flux at spatial mesh i , direction m , and in energy group g .

For simplicity in notation, only one index for position in space and one for position in angular directions are given. In each case, the index denotes the average property applying at the center of space, direction, and energy mesh.

If the following partial sum is formed,

$$\phi(i, g) = \sum_{m=1}^M W(m) N(i, m, g) \quad (27)$$

the perturbation equation (20) can now be written in the following form. Terms in the numerator are:

$$\begin{aligned} & - \sum_{i=1}^I V(i) \sum_{g=1}^G \phi^+(i, g) \phi(i, g) \left\{ \delta \Sigma_{tr}(i, g) \left[1 - \frac{B_T^2}{3(\Sigma_{tr})^2} \right] - \right. \\ & \quad \left. - \sum_{g'=1}^G \delta \Sigma_s(i, g \rightarrow g') \right\} \quad \text{absorption + transverse leakage} \\ & - \sum_{i=1}^I V(i) \sum_{g=1}^G \phi^+(i, g) \phi(i, g) \sum_{g'=1}^G \delta \Sigma_s(i, g \rightarrow g') \quad \text{out-scatter up, down, and self} \end{aligned}$$

$$\begin{aligned}
 & + \sum_{i=1}^I v(i) \sum_{g=1}^G \phi^+(i, g) \sum_{g'=1}^g \delta \Sigma_s(i, g' \rightarrow g) \phi(i, g') && \text{In scatter from above and self} \\
 & + \sum_{i=1}^I v(i) \sum_{g=1}^G \phi^+(i, g) \sum_{g'=g+1}^G \delta \Sigma_s(i, g' \rightarrow g) \phi(i, g') && \text{In scatter from below} \\
 & + \sum_{i=1}^I v(i) \sum_{g=1}^G \phi^+(i, g) \chi(g) \sum_{g'=1}^G \frac{\delta \Sigma_f(i, g')}{K_0} \phi(i, g') && \text{Source from fission} \quad (28)
 \end{aligned}$$

The term in the denominator becomes

$$\sum_{i=1}^I v(i) \sum_{g=1}^G \phi^+(i, g) \chi(g) \sum_{g'=1}^G \frac{\delta \Sigma_f(i, g')}{K_0} \phi(i, g) \quad (29)$$

The above equations have been coded in PERT-2DW and constitute the numerical solution of equation (20) for the case of the transport corrected isotropic scattering approximation.

If equation (18) instead of (17) is subjected to a perturbation, the analogue of equations (28) and (29) is in the following form:

$$\begin{aligned}
 & - \sum_{i=1}^I v(i) \sum_{g=1}^G \phi(i, g) \phi^+(i, g) \left\{ \delta \Sigma_{tr}(i, g) \left[1 - \frac{B_T^2}{3(\Sigma_{tr})^2} \right] \right. \\
 & \quad \left. - \sum_{g'=1}^G \delta \Sigma_s(i, g \rightarrow g') \right\}
 \end{aligned}$$

$$- \sum_{i=1}^I v(i) \sum_{g=1}^G \phi(i, g) \phi^+(i, g) \sum_{g'=1}^G \delta \Sigma_s(i, g \rightarrow g')$$

$$+ \sum_{i=1}^I v(i) \sum_{g=1}^G \phi(i, g) \sum_{g'=1}^g \delta \Sigma_s(i, g \rightarrow g') \phi^+(i, g')$$

$$\begin{aligned}
& + \sum_{i=1}^I V(i) \sum_{g=1}^G \phi(i, g) \sum_{g'=g+1}^G \delta \Sigma_s(i, g \rightarrow g') \phi^+(i, g') \\
& + \sum_{i=1}^I V(i) \sum_{g=1}^G \phi(i, g) \frac{\delta \nu \Sigma_f(i, g)}{k_0} \sum_{g'=1}^G \chi(g') \phi^+(i, g)
\end{aligned} \tag{30}$$

and the denominator becomes

$$\sum_{i=1}^I V(i) \sum_{g=1}^G \phi(i, g) \frac{\nu \Sigma_f(i, g)}{k_0} \sum_{g'=1}^G \chi(g') \phi^+(i, g') \tag{31}$$

The two formulations (28) and (29), and (30) and (31) give identical total perturbation worth, $\delta \lambda_0$, when the perturbation is integrated over reactor volume and all energy groups. The individual group contributions are different.

This equation, (30) and (31), has also been included in PERT-2DW to serve as a check for equations (28) and (29) and the selection of technique is done by a control character in the input of PERT-2DW.

4.3.6 Calculation of Prompt Neutron Lifetime

Given the mean neutron velocities in each energy group, $\bar{V}(g)$, the quantities calculated for the perturbation equation can be used to obtain the prompt neutron lifetime, Λ , as follows:

$$\Lambda(\text{sec}) = \frac{1}{kD} \sum_{i=1}^I V(i) \sum_{g=1}^G \phi(i, g) \phi^+(i, g) / \bar{V}(g) \tag{32}$$

where

- k = k_{eff} of the unperturbed reactor
- D = denominator in the perturbation equation, eq. (29)
- $V(g)$ = logarithmic mean velocity (cm/sec) of neutrons in group g
- $V(i)$ = volume element about mesh point i .

The solution of this equation has been included in PERT-2DW capabilities.

4.4 ANGULAR FLUX INTERPOLATION TECHNIQUES

Discrete ordinate solutions of the transport equation, when evaluated at large distances from the source region in a void or in a medium of low scattering density, show the so-called "ray effects." The existence of these effects has been well documented in various applications of the discrete ordinate transport technique. (2,25,26)

These ray effects are caused by the superposition of the discretized components of the directed flux arriving at the detector plane from different source points, and produce "null" or low flux solutions in those mesh cells on the detector plane which are located away from points of intersection of that plane with the discrete directions of quadrature, and high flux solutions in the mesh cells subtending the discrete directions. Thus, the solution shows oscillatory effects in regions where, on physical grounds, the variation of the radiation field is expected to be a smooth function. For the above reasons, the direct application of the discrete ordinate methods to radiation transport through large voids leads to anomalous results.

The kernel methods of radiation transport through voids are free of ray effects per se, but require as input, detailed knowledge of the radiation source. When that source is taken as the surface leakage flux computed by the discrete ordinate method, any ray effects inherent in the discrete ordinate solution are propagated through the kernel transport solution as well.

The existence of the "ray effects" may be eliminated, or the magnitude of the variations may be reduced, by first converting the angular dependence of the leakage radiation flux at the midpoints of the mesh cells defining the r,z geometry from a discrete to a continuous domain through a suitable interpolation technique, and then carrying out the integrations over the surface to obtain the angular- and spatial-variation of flux at the detector surface points. The required interpolation should be carried out in functions with suitable orthogonal properties, and should satisfy the following conditions:

1. The values of the interpolant and the discrete ordinate fluxes should be identical at all discrete values of the angle ordinate.

2. The integrals over all directions of the interpolating continuous variable should equal the corresponding direction sums in the discrete variable. This implies using a Gaussian set of collocation points for the interpolating function.

This section describes the first part of the smoothing technique, namely, the theory and numerical formulation of the angular interpolation including examples of results using the technique. The future work will include the incorporation of this technique into the MAP code, which uses the kernel technique with the discrete direction angular flux without interpolation.

4.4.1 GEOMETRIC CONSIDERATIONS

The multidimensional solutions of the transport equation^(2,25) conventionally express the directional dependence of the neutron flux in terms of three angles between the coordinate axes and the discretized direction of the neutron motion. Figure 4-6 shows the orientation of the coordinate axes and the angles of interest for two locations of a radiation emitting point on the

1. top surface of the r, z problem
2. side surface of the r, z problem

In both cases the directions are measured with respect to the upward directed vertical (z axis) and the outward directed normal (x or r axis). The discrete ordinate directions are fixed in a discrete ordinate solution and define the position of vector $\underline{r}_m$ in a unit sphere at the point. In the MAP⁽¹³⁾ code, the direction vector $\underline{r}_c$ is obtained by connecting the points on the surface at which the radiation is emitted and the points on a detector surface.

The angular interpolation technique developed in this study is limited to interpolation in the angle ϕ (direction cosine η) between which the sets of discrete directions defined in each η level have minimum value of angle, α , i. e., having approximately

Figure 4-6. Geometry Used in MAP Calculations

the same value of the azimuthal angle, θ . In terms of the direction cosines of vectors $\underline{r}_c$ and $\underline{r}_m$ the requirement is

$$\min|\alpha| = \max |\cos \alpha| = \max |\mu_c \mu_m + \eta_c \eta_m + \xi_c \xi_m|$$

The +1 value of η is in the upward vertical direction and the range of the values of μ is given in Table 4-6.

On the basis of Table 4-6, it is seen that on the top and bottom surface of the r,z geometry results in interpolations in η over the half range. This is handled by assuming that a mirror image of the directed flux exists in the other half range. On the side of the reactor a full range in η of discrete ordinate angular flux is available for interpolation and is used.

TABLE 4-6

RANGES OF VARIATION OF ANGULAR PARAMETERS

Position on Reactor Surface	Cos of Zenith Angle, η	Cos of Azimuthal Angle (Projected on xy), μ
Top	+1, 0	+1, 0, -1
Side	+1, 0, -1	+1, 0
Bottom	0, -1	+1, 0, -1

4.4.2 TWO-DIMENSIONAL DISCRETE ORDINATE FLUX REPRESENTATION

The time-dependent transport equation in a direction variable, η , position variable, r , and energy, E , can be written as:

$$\eta \frac{\partial}{\partial r} N(E, \eta, r) + \frac{\beta}{2} \frac{(1-\eta^2)}{r} \frac{\partial}{\partial \eta} N(E, \eta, r) + \Sigma_t(E, r) N(E, \eta, r) = S(E, \eta, r) + \int_{-1}^{+1} \int_0^\infty \Sigma_s(E' \rightarrow E, \eta' \rightarrow \eta, r) N(E', \eta', r) d\eta' dE' \dots \quad (1)$$

where β is a constant dependent on geometry.

In the S_n method^(2,25) an approximate solution to (1) is obtained in the form of a histogram in the discretized position variable, r , at the space mesh, (i) , in the energy variable, E , at the energy mesh (g) , and in the direction variable, η , at the direction mesh, (m) . The solution provides at all values of (i) , (m) , and (g) the value of

$$\text{Directed flux} \quad N(i, m, g) \quad (2)$$

$$\text{Scalar flux} \quad \bar{N}(i, g) = \sum_{m=1}^n W(m) N(i, m, g) \quad (3)$$

$$\text{Vector current} \quad J(i, g) = \sum_{m=1}^n W(m) \eta(m) N(i, m, g) \quad (4)$$

The variable of interest here is the direction η in the interval $(+1, -1)$, which is divided into n parts, each associated with a fixed value of direction $\eta(m)$.

The upper and lower limits of the interval containing $\eta(m)$ are defined by the equations

$$\eta_{(m)}^U = 1 - \sum_{l=1}^{m-1} W(l) \quad (5)$$

$$\eta_{(m)}^L = 1 - \sum_{l=1}^m W(l) \quad (6)$$

Where $W(l)$, appearing in equations (3) through (6), is a suitably chosen weight of interval l for the quadrature in the direction variable, η . The method of computing the quadrature weights for the interpolating function will be given later.

4.4.3 LAGRANGIAN INTERPOLATION TECHNIQUE IN THE COSINE OF THE POLAR ANGLE

As explained in Section 4.4, a continuous angular distribution of the directed flux on the surface of a reactor is desired to remove the propagation of "ray effects." If this continuous distribution in direction is denoted by η (in place of the direction mesh index, m) in the argument of the directed flux, the following can be written

$$N(i, \eta, g) = \sum_{m=1}^n L_m^n(\eta) N(i, m, g) \dots \quad (7)$$

where $L_m^n(\eta)$ are the Lagrangian coefficients for interpolation in the direction variable, in quadrature order n , and applied to the m -th component of the directed flux, as obtained from a discrete ordinate solution (e.g., DOT-IIW).

The above interpolation coefficients can be obtained^(26,27) for each discrete direction, η_{nm}^0 , from the following relationship:

$$L_m^n(\eta) = \frac{1}{\left[\frac{dP_n(\eta)}{d\eta} \right]_{\eta = \eta_{nm}^0}} \times \frac{P_n(\eta)}{(\eta - \eta_{nm}^0)} \dots \quad (8)$$

In the above, the $P_n(\eta)$ are the Legendre polynomials of order n , and η_{nm}^0 are the direction cosines at which $P_n(\eta)$ has zero value. It will be recalled that each $P_n(\eta)$ has n such zeros, and that the quadrature directions, $\eta(m)$, used in discrete ordinate calculations, are not necessarily equal to the η_{nm}^0 .

To check that the interpolating function satisfies the first condition (namely that its value, when evaluated in a quadrature direction, be equal to the m -th component of the discrete ordinate flux solution) observe that for $\eta = \eta_{nm}^0$, $P_n(\eta_{nm}^0) = 0$, by definition of η_{nm}^0 . Therefore, since the term $\eta_{nm}^0 - \eta_{nm}^0 = 0$ appears in the denominator of equation (8), the indeterminate form $0/0$ may be avoided by applying L'Hospital's Rule to the fraction

$$L_m^n(\eta_{nm}^o) = \lim_{\eta \rightarrow \eta_{nm}^o} \left[\frac{1}{\frac{dP_n(\eta)}{d\eta}} \times \frac{\frac{dP_n(\eta)}{d\eta}}{\frac{d}{d\eta}(\eta - \eta_{nm}^o)} \right] = 1 \dots \dots \quad (9)$$

and from (9), we obtain as required:

$$N(i, \eta_{nm}^o, g) = N(i, m, g). \dots \quad (10)$$

The fulfillment of the second requirement on the interpolating function is discussed in the next section.

The Legendre functions and the derivatives appearing in equation (8) can be generated from $P_0(\eta) = 1$ and $P_1(\eta) = \eta$ by a repetitive application of the following recurrence relationships:

$$P_{n+1}(\eta) = \frac{1}{(n+1)} \left[(2n+1) \eta P_n(\eta) - n P_{n-1}(\eta) \right] \dots \quad (11)$$

$$\frac{d}{d\eta} P_n(\eta) = \frac{(n+1)}{(1-\eta^2)} \left[\eta P_n(\eta) - P_{n+1}(\eta) \right] \dots \quad (12)$$

Also note that $P_n(-\eta) = (-1)^n P_n(\eta)$, and the values of n which enter into consideration are always even, when applied to the order of quadrature used in both S_n and P_n calculations. The reasons for this choice are practical and derive from the fact each even, and its immediately higher odd, order of quadrature represents a system of coupled differential equations in the scalar and higher order moments of flux. Both the n and $n+1$ system may be reduced by successive substitutions to a single equation of higher order in the scalar flux, and the order of this equation is the source for both original n and original $n+1$ system. Thus, no increase of accuracy is expected from the odd $(n+1)$ order of quadrature as compared to the n th order, though solving the $n+1$ system is more laborious.

The values of the arguments of zeros of the first four even Legendre polynomials are given in Table 4-7 together with the values of the derivatives evaluated at these arguments, as required by equation (8). Zeros for higher order Legendre polynomials are given in Reference 28.

TABLE 4-7

ZEROS OF THE FIRST FEW LEGENDRE POLYNOMIALS,
PLUS THEIR DERIVATIVES AND CHRISTOFFEL NUMBERS

n	$\pm \eta_{nm}^{\circ}$	$\pm \frac{d}{d\eta} P_n(\eta_{nm}^{\circ})$	λ_{nm}
2	0.57735	1.73205	1.00000
4	0.86114	4.71675	0.34785
	0.33998	1.86215	0.65214
6	0.93247	9.45806	0.17132
	0.66121	3.13854	0.36076
	0.23862	2.12893	0.46791
8	0.96029	15.93141	0.10123
	0.79667	4.96175	0.22238
	0.52553	2.96782	0.31371
	0.18343	2.38882	0.36268

4.4.4 Direction Integrals and Quadrature Weights

Because of the orthogonal properties of the Legendre Polynomials, the direction integral of the interpolating function and its higher moments assume a particularly simple form. Thus, the k -th moment is, with substitution from (7)

$$\begin{aligned}
 N^k(i, g) &= \int_{-1}^{+1} N(i, \eta, g) \eta^k d\eta, \quad k = 0, 1, 2, \dots \\
 &= \sum_{m=1}^n N(i, m, g) \int_{-1}^{+1} L_m^n(\eta) \eta^k d\eta \\
 &= \sum_{m=1}^n W(m) N(i, m, g) (\eta_{nm}^0)^k \dots \dots \dots
 \end{aligned} \tag{13}$$

The integrals in (13) of $L_m^n(\eta)$ for the case of $k = 0$ are just the quadrature weights associated with the interpolating function. Thus, substituting from (8) for $L_m^n(\eta)$, we have

$$W(m) = \int_{-1}^{+1} L_m^n(\eta) d\eta = \int_{-1}^{+1} \frac{P_n(\eta) d\eta}{\frac{dP_n(\eta_{nm}^0)}{d\eta} (\eta - \eta_{nm}^0)} \dots \dots \tag{14}$$

The value of the integral above is known as the Christoffel number, λ_{nm} ,

$$W(m) = \lambda_{nm} = \frac{-2}{(n+1) \frac{dP_n(\eta_{nm}^0)}{d\eta} P_{n+1}(\eta_{nm}^0)} \dots \dots \tag{15}$$

The Christoffel numbers are always positive.

An alternative form of Christoffel numbers, and one that is easier to evaluate, can be obtained by applying the recurrence relation (12) to equation (15). This gives

$$\lambda_{nm} = \frac{2}{\left[1 - (\eta_{nm}^0)^2\right] \left[\frac{dP_n(\eta_{nm}^0)}{d\eta}\right]^2} \dots \dots \tag{16}$$

The significance of equations (13) and (15) lies in the fact that they provide the methods for evaluating direction integrals of the directed flux, equation (2), and directed current, equation (4), in terms of the sums of products of the directed flux with the Christoffel number

and either $(\eta_{nm}^0)^0 = 1$ or $(\eta_{nm}^0)^1 = \eta_{nm}^0$

For the case of the zeroth moment ($k = 0$) of the directed flux, the equation (13) shows that the second requirement placed on the interpolating function, namely that its space integral be equal to the properly weighted sum of the discrete ordinate components of the directed flux, is also satisfied.

The numerical values of the Christoffel numbers, λ_{nm} , are also given in Table 4-7 for the first few even zeros. For selected higher orders, they are given in Reference 28.

4.4.5 Evaluation of Lagrangian Interpolation Coefficients

The Lagrangian coefficients, defined by equation (8), were evaluated in the form resulting from application of the differential recurrence relation (12), namely in the form:

$$L_m^n(\eta) = \frac{[1 - (\eta_{nm}^0)^2]}{(n+1) [\eta_{nm}^0 P_n(\eta_{nm}^0) - P_{n+1}(\eta_{nm}^0)]} \times \frac{P_n(\eta)}{(\eta - \eta_{nm}^0)} \dots \dots \quad (17)$$

When written in this form, the coefficients consist of two parts: the constant first factor

$$A_m^n = \frac{[1 - (\eta_{nm}^0)^2]}{(n+1) [\eta_{nm}^0 P_n(\eta_{nm}^0) - P_{n+1}(\eta_{nm}^0)]} \dots \dots \quad (18)$$

and the η dependent second factor

$$B_m^n(\eta) = \frac{P_n(\eta)}{(\eta - \eta_{nm}^0)} \dots \dots \quad (19)$$

On theoretical grounds, the interpolation scheme requires that the S_n quadrature directions $\eta_{(m)}$ be exactly equal to the zeros of n -th order Legendre Polynomial, η_{nm}^0 . In this particular case, equation (18) simplifies to

$$A_m^n = \frac{[\eta_{nm}^o]^2 - 1}{(n+1) P_{n+1}(\eta_{nm}^o)} \cdot \dots \cdot \quad (20)$$

since, by definition, $P_n(\eta_{nm}^o) = 0$.

It is of interest, however, to evaluate the sensitivity of the angular interpolation scheme to the choice of quadrature directions, $\eta(m)$, other than the zeros of the Legendre polynomials. For this reason, the form of A_m^n given by equation (18) was mechanized in preference to form (20).

The value of the argument η , in the variable factor $B_m^n(\eta)$, is to be specified corresponding to the value of the direction cosine of the ray from the detector point to the midpoint of the surface mesh cell on the source plane.

4.4.6 Results from Application of Lagrangian Interpolation Technique

The interpolation scheme described above has been tested by applying it to the results of an S_8 calculation of radiation emitted from the outside surface of a cylindrical reactor mockup. The discrete ordinate solutions for the surface directed flux were converted to the continuous domain by the application of equation (7) and the interpolation coefficients, evaluated from (17). A fine, uniform mesh was chosen for the evaluation as a function of η .

Figures 4-7 through 4-11 show the plots of the directed flux in its discrete ordinate form from DOT and its corresponding continuous form obtained by Lagrangian interpolation. The results are given for selected mesh points located on the surface of the reactor at positions identified by circled numbers in Figure 4-6. For fluxes on the top of the reactor only, the range $+1 \geq \eta \geq 0$ is given, corresponding to the upward directed components, which are the only ones contributing to the radiation field at the detector. For the sides of the reactor, the full range $+1 \geq \eta \geq -1$ applies.

Examination of the figures reveals that the interpolating function oscillates about the discrete ordinate values, and in some ranges of η assumes negative values. If the negative values should be unacceptable for some reason, the parts between the interpolating function and the zero axis (i. e., the "negative areas") could be set equal to zero. To get some idea of the magnitude of error which such a procedure would introduce into the integral, over the η range, the fraction of the integrals under the zero axis, expressed as a percent of the total, is given in Table 4-8 and 4-9.

The Tables 4-8 and 4-9 contain also the integrals over the applicable η range for mesh points on the top and the side of the reactor for both the discrete ordinate and the interpolate, with the latter including the negative contributions. Excellent agreement is found between the integrals.

If the negative part of integrals of the interpolates is set equal to zero, to avoid ranges with negative values of interpolant, an error will be introduced into the integrals, equal in magnitude to the negative fraction of the integrals. This varies in magnitude between 0.85 and 2.86 percent for the top of the reactor, and 0.07 and 2.87 for the side. Although these are acceptable in magnitude, the final decision in the matter of treatment of the negative interpolant should be deferred until the results of the integrations over the angle subtended by the detector, as in the MAP code, are available for comparison.

4.4.7 Importance of Exact Gaussian Quadrature Directions

To test the sensitivity of the Lagrangian interpolation technique to the choice of values of the quadrature directions (collocation points on the η coordinate axis) use was made of equation (18) in calculating the coefficients of the interpolating function. In place of the exact Gaussian quadrature directions, such as those used in obtaining Figures 4-7 through 4-11, an alternative set has been used, taken from a well-known S_n calculation example. The two sets are listed for comparison in Table 4-10.

TABLE 4-8

COMPARISON OF INTEGRALS OF DIRECTED FLUX FROM DISCRETE ORDINATE SOLUTION
AND THE LAGRANGIAN INTERPOLATION, TOP OF THE REACTOR

Mesh Point	$10^2 \times \sum_{m=1}^4 N(m) \Delta \eta(m)$	$10^2 \int_0^{+1} N(\eta) d\eta$	$10^4 \int_0^{+1} N(\eta) d\eta < 0$	Negative Contribution, % of Total
1	1.25668	1.25818	1.32160	1.05
2	1.38450	1.38554	1.6646	1.20
3	1.47951	1.48051	2.6320	1.77
4	1.57693	1.57796	2.1710	1.37
5	1.63165	1.63275	2.9666	1.81
6	1.65867	1.65945	4.4578	2.68
7	1.71417	1.71434	3.0644	1.78
8	1.73405	1.73385	2.5795	1.48
9	1.74810	1.74764	2.1882	1.25
10	1.75709	1.75650	1.8372	1.04
11	1.66561	1.66251	1.3716	0.82
12	1.49215	1.48547	1.6824	1.13

4-67

TABLE 4-9

COMPARISON OF INTEGRALS OF DIRECTED FLUX FROM DISCRETE ORDINATE SOLUTION
AND THE LAGRANGIAN INTERPOLATION. SIDE OF THE REACTOR

Mesh Point	$10^2 \sum_{m=1}^8 N(m) \Delta\eta (m)$	$10^2 \int_{-1}^{+1} N(\eta) d\eta$	$10^4 \int_{-1}^{+1} N(\eta) d\eta < 0$	Negative Contribution, % of Total
1	2.68787	2.68383	4.561	1.69
2	3.48141	3.47694	2.135	0.61
3	4.67564	4.67128	0.890	0.19
4	5.89003	5.89742	0.610	0.10
5	6.68912	6.68783	0.316	0.04
6	6.83789	6.83622	0.799	0.11
7	6.36141	6.35946	0.495	0.07
8	5.33119	5.32736	0.740	0.14
9	4.16401	4.15914	1.269	0.40
10	3.29693	3.31507	3.811	1.14
11	2.82228	2.81820	5.907	2.09
12	2.52663	2.52255	3.917	1.55
13	2.29696	2.28157	1.670	0.73
14	2.15719	2.15827	0.604	0.28
15	1.90740	1.90867	1.338	0.70
16	1.69823	1.69176	3.301	1.95
17	1.50550	1.49794	4.252	2.89

Figure 4-7. Discrete Ordinate and Interpolated Flux. Mesh Point 1, Top of Reactor

Figure 4-8. Discrete Ordinate and Interpolated Flux. Mesh Point 8, Top of Reactor

Figure 4-9. Discrete Ordinate and Interpolated Flux. Mesh Point 12, Top of Reactor

Figure 4-10. Discrete Ordinate and Interpolated Flux. Mesh Point 10, Side of Reactor

TABLE 4-10

GAUSSIAN AND NON-GAUSSIAN COLLOCATION POINTS
USED IN TESTS OF THE INTERPOLATION TECHNIQUE

Gaussian $\pm \eta_{nm}^o$	Non-Gaussian $\pm \eta_{(m)}^*$
0.18343464	0.218218
0.52553240	0.57735
0.79666647	0.786796
0.96028985	0.95119

* (Taken from LA-3186)

Figure 4-11. Discrete Ordinate and Interpolated Flux, Mesh Point 6, Side of Reactor

The attempt to use the non-Gaussian quadrature directions in the interpolation routine has produced the wildly inaccurate results shown in Figure 4-12. The method is found to be very sensitive to the correct choice of the interpolating directions.

The reverse of the above statement is not true, however, namely the replacement of the non-Gaussian directions of Table 4-10 by the Gaussian set in the DOT calculations has a relatively minor effect.

In conclusion, the following statement can be made. The directed fluxes can be calculated in the S_n method with any quadrature directions reasonably approaching those of the Gaussian set, but the angular interpolation must use the exact Gaussian set, to produce accurate results.

4.4.8 Future Developments of the Technique

The immediate development need is the adaptation of the MAP code to handle the interpolating function in place of the discrete ordinate fluxes in the integration leading to the determination of the fluxes at the detector plane. The availability of this modification will provide the ultimate test of the interpolating routine.

Should the interpolation in one variable fail to remove the bulk of the "ray effect," an interpolation in two angle variables, η and μ may be attempted. Preliminary derivation of the bi-orthogonal functions $V_{nm}(\mu, \eta)$ has been done recently.³⁰ These functions are defined by

$$V_{nm}(\mu, \eta) = \frac{1}{n! m!} \frac{\partial^n}{\partial a^n} \frac{\partial^m}{\partial b^m} G_2(a, b, \mu, \eta) \dots \quad (21)$$

where

$$G_2(a, b, \mu, \eta) = \frac{1}{\sqrt{1 - 2a\mu - 2b\eta + a^2 + b^2}} \quad (22)$$

The functions have the properties of two-dimensional Legendre functions and define a surface in three-dimensional space as illustrated in Figure 4-13.

To use this technique in removing the ray effects, a two-dimensional interpolating technique, analogous to the method of Legendre, should be developed in which the place of the point zeros of the Legendre polynomials will be taken by the lines of intersection of the V_{nm} plane with the μ - η plane as shown in Figure 4-13.

Figure 4-12. Interpolation with Non-Gaussian Collocation Points

Figure 4-13. Surface Defining the Function $V_{nm}(\eta, \mu)$ and Locus of its Zeros ($n-m-4$)

5.0 DEVELOPMENT OF GEOMETRIC AND INVENTORY MODELS

5.1 PAX-E1 REACTOR CONFIGURATION

The PAX-E1 reactor assembly, built in support of the NRX-A6 reactor, consisted of a 90-degree mockup of NRX-A6 Build 2 fuel and a 270-degree rezoned PAX-D fuel loading as core, and the actual NRX-A6 beryllium reflector rings as reflector. The assembly has been documented in WANL-TME-1739.⁽³¹⁾ The PAX-E1 reactor configuration was selected for all r, θ analyses under Project 493 (SRT), since this assembly is being used in the evaluation of the WANL Integrated Nuclear, Radiation Shielding Standard Design Method (WISDM)⁽⁴⁾ and experimentally measured fission distribution data is available.⁽³¹⁾

The one-dimensional (radial) model of the PAX-E1 reactor configuration with the control vanes set at 105 degrees represented as an annular ring shown in Figure 5-1. This model of the PAX-E1 was used for all one-dimensional transport calculations (ANISN) and all azimuthally symmetric r, θ transport calculations (DOT-IIW) discussed under this project. Table A-1 (Appendix A) specifies in detail the radial mesh used in the PAX-E1 one-dimensional model.

Sixteen group cross section data was generated using the GAMB1T cross section averaging code.⁽³²⁾ The cross sections for each region were averaged over the appropriate PAX-E1 spectrum as calculated by the LINK system.⁽³⁴⁾ The sixteen group cross section data for the annular control vane ring was calculated using sixteen group microscopic boron-10 cross section data and the prescribed NERVA procedure.⁽²⁵⁾ Simulation of the NRX-A control vanes as an annular ring gives reasonable agreement with experimental measured edge power. The same sixteen group vane cross section data was used for all radial and azimuthally symmetric transport calculations discussed in this report.

The two-dimensional (r, θ) model of the PAX-E1 assembly differs only in the reflector from the one-dimensional (radial) model. Figure 5-2 describes the two-dimensional mockup of the PAX-E1 reflector for r, θ calculations and Table A-2 (Appendix A) specifies the corresponding atom density data. Sixteen group cross section data was generated using the GAMB1T code, in which the cross sections for each region were averaged over the appropriate PAX-E1 spectrum.

Figure 5-1. One-Dimensional (Radial) Model of PAX-E1 Reactor Configuration with Ring Vane 105 Degrees

<u>Region No.</u>	<u>Region Description</u>
1	Beryllium Reflector 1
2	Beryllium Reflector 2
3	Beryllium Reflector 3
4	Plungers
5	Springs
6	Titanium Tie Bolts
7	Control Vane
8	Void
9	Pressure Vessel

NOTE: Radial Dimensions in cm.
Azimuthal Dimensions in Degrees

Figure 5-2. Two-Dimensional Mockup of PAX-EI Reflector for r, θ Calculations

TABLE 5-1

PAX-E1 CONTROL VANE DATA*

VANE GEOMETRY:

Inner Radius of Control Drum	4.7625 cm.
Outer Radius of Control Drum	4.8895 cm.
Thickness of Vane	0.050 in.
Length of Plates	17.266 in.
Plates per Vane	3
Total Vanes, PAX-E1	12
Total Azimuthal Coverage of Vane	120 degrees
Radial Distance from Center of Core to Center of Control Drum	56.8325 cm

VANE MASSES:

Total Control Vane Mass	5146.434 grams
Total Mass Boron-10	1029.36 grams
Weight Fraction Boron-10 in Boron	0.9576

* References:

WANL-TME-1642, NRX-A6 Nuclear Subsystem Thermal and
Nuclear Design Data Book, November 15, 1967.

Drawing Number 909E267, Plate Control Drum.

5.2 EXPLICIT DEFINITION OF THE CONTROL VANES

The MERTH code (Mesh Evaluation in R, THETA) was used to develop an explicit definition of the control vanes in the PAX-EI reflector. (See Section 4.2.2 for a description of the MERTH code.) Table 5-1 specifies the PAX-EI control vane geometry and mass data. The PAX-EI reactor assembly has a periodicity of 30 degrees since it has twelve uniformly spaced control drums which move as a bank during normal operations, and therefore, a 30-degree sector of the reactor was analyzed in all r, θ calculations.

Figure 5-3 shows the input parameters to the MERTH calculation which explicitly defines a 100 mil thickness vane at an angle of 105 degrees. The actual physical thickness of the PAX-EI control vanes was 50 mils; however, a 100 mil vane was selected for use in this analysis since preliminary MERTH calculations showed that a very large number of r, θ mesh intervals would be required to mockup a 50 mil vane explicitly and continuously. A 100 mil control vane has been used in all previous analyses of the PAX-EI reactor, and consistent models were used in this analysis.

A series of MERTH calculations, using the geometry defined in Figure 5-3 were completed to determine the minimum fraction of an r, θ mesh interval area that should be vane material in order to assign that r, θ mesh interval to the control vane region. The criteria for the definition of the explicit vane are: (1) the explicit vane must be continuous,* and (2) the cross sectional area of the explicit vane should be in good agreement with the physical cross sectional area of the control vane. Using these criteria, an explicit control vane was selected, in which an r, θ mesh interval was assigned to the control vane region if 46 percent or more of the r, θ mesh interval area was vane. This explicit control vane had 49 r, θ mesh intervals, having a total area of 2.56656 cm^2 . The actual control vane has a cross sectional area of 2.56732 cm^2 , a difference of 0.03 percent from the $r-\theta$ mesh mockup.

*The requirement that the explicit control vane be continuous is defined to mean that at least one mesh point in every r, θ mesh interval assigned to the control vane region, must also be a mesh point in another r, θ mesh interval assigned to the control vane region.

Figure 5-3. MERTH (Mesh in R, Theta) Mockup of PAX-E1 Reflector Configuration for 100 Mil Vane at 105 Degrees

6.0 APPLICATIONS OF DOT-IIW CODE

The applications of the DOT-IIW code, as described in this section, used the PAX-EI reactor model and the version of the DOT-IIW code described in Section 4.1, except that the program tape used did not include the changes in the upscatter scaling technique noted in Section 4.1.5.

Figure 6-1 describes the method used in this analysis of the PAX-EI reactor, using DOT-IIW. This method is consistent with the discrete ordinate transport method for neutronics analysis. Section 4.0 and Appendix A describe the one- and two-dimensional model of the PAX-EI assembly. The LINK system was used to calculate the regionwise neutron spectrum of the PAX-EI, over which cross section data were averaged. GAMB1T calculations provided for all regions of interest the 16 group (11 fast, 5 thermal) transport corrected neutron cross sections, using the standard nuclear design cross section data tapes.

The DOT-IIW code does not have the capability of adding transverse (axial) leakage to the cross section data, as is required in r - θ calculations. Therefore, the SATURN cross section data processing code (see Section 4.2.1) was used to add DB^2 to the absorption and transport cross sections, based on an extrapolated height of 148 cm.⁷

The ANISN one-dimensional discrete ordinate transport code was used as a reference case for comparison to azimuthally symmetric DOT-IIW calculations and to provide 16 group transport corrected cross section data with upscatter data removed.

6.1 QUADRATURE DATA IN r, θ GEOMETRY

The Discrete Ordinate Quadrature computer code (DOQ) was used to calculate discrete ordinate quadrature coefficients (direction cosines and weights) given the point coordinates and symmetry conditions. Figure 6-2 shows the order of solution for an r, θ, S_6 cylindrical discrete ordinate transport calculation. In an r, θ calculation, the radial (μ) component of the angular flux is the largest component and thus, the error in flux solution may be minimized by solving for angular fluxes in the principal direction first. Figure 6-3 shows the order of solution for an r, z, S_6 calculation in which analogously axial (η) component most generally is the largest and, therefore, r, z problem quadratures are ordered to solve first in the η direction.

Figure 6-1. Discrete Ordinate Transport Method for Evaluation of DOT-IIW

Figure 6-2. r, θ Discrete Directions Quadrature Order = 6

Figure 6-3. r, z Discrete Directions Quadrature Order = 6

The quadrature data generated by the DOQ code is tabulated in Appendix B. The data includes the direction cosines in the r, z and θ directions (which are specified as μ, η and ξ , respectively, on the unit sphere) and weights for r, θ and r, z cylindrical geometry. Tables B-1, B-2, B-3 and B-4 present the completely symmetric Gauss-Legendre angular quadrature data in r, z cylindrical geometry for quadrature order two, four, six and eight, respectively. This quadrature data was used in all discrete ordinate transport calculations performed in this study.

The use of r, θ and r, z quadrature data in $r-\theta$ solutions did not provide any conclusive evidence that the order of solution was important. On azimuthally homogeneous problems, the identical answers were obtained for r, θ and r, z quadrature sets. This may not be the case for an azimuthally asymmetric problem with a local fixed source or absorbing region. However, this detailed analysis was not conducted due to the large cost in computer time required for such a detailed model.

6.2 COMPARISON OF RESULTS FROM ANISN AND DOT-IIW

A series of ANISN and azimuthally symmetric DOT-IIW problems were run, in order to show that under comparable conditions these transport codes gave comparable results. The PAX-E1 radial model used in these calculations is shown in Figure 5-1, and the azimuthally symmetric DOT-IIW calculations contain five uniformly spaced azimuthal mesh points, per radial mesh point, with no azimuthal variation in material. The results of these calculations are shown in Table 6-1. The described calculations had the same boundary conditions, the same convergence criteria (1.0×10^{-5} , 2.0×10^{-5} and 1.0×10^{-5} on eigenvalue, flux and upscatter, respectively) and the ANISN calculation started with a flat flux guess while the DOT started with a flux from an ANISN calculation in order to conserve computer time. Table 6-1 shows that the S_4 ANISN and DOT problems, both with and without upscatter, gave substantially the same results in eigenvalue and edge-to-center fission distribution ratio. The small difference shown (less than 5 cents in eigenvalue) can be attributed to the differences in convergence, negative flux fixup, or cross section logic between the one-dimensional code ANISN and two-dimensional code DOT-IIW.

Figure 6-4. r, z Discrete Directions Quadrature Order = 2

TABLE 6-1

COMPARISON OF ANISN AND AZIMUTHALLY SYMMETRIC DOT-IIW CALCULATIONS

Problem Number	Transport Code	Quadrature Order	Energy Groups			Eigenvalue		Fission Distribution Edge/Center Ratio	Computer Time (sec)**		
			Total	Upscatter	Downscatter	K	$\Delta K^*(\%)$		CP	PP	Total
14.208	ANISN	S ₄	16	4	9	1.0442	---	0.7332	148	37	185
14.309	DOT	S ₄	16	4	9	1.0439	-4.2	0.7338	807	497	1304
14.211	ANISN	S ₄	16	0	9	1.0462	---	0.7478	83	35	118
14.306E	DOT	S ₄	16	0	9	1.0461	-1.4	0.7481	523	83	606

* Change in eigenvalue relative to comparable ANISN calculation.

**CP - Central Processor time

PP - Peripheral processor time

6.3 CONVERGENCE PATTERNS IN DOT-IIW

The convergence patterns in DOT-IIW, with respect to acceleration techniques, quadrature data, boundary conditions, upscatter, convergence criteria and zones of convergence, were studied in azimuthally symmetric DOT calculations. These DOT calculations used the PAX-E1 radial model with a ring control vane at 105 degrees (Figure 5-1), 43 radial mesh points (Table A-1) and five uniformly spaced azimuthal mesh points, with no azimuthal variation in material.

6.3.1 Acceleration Techniques

The original DOT code had available only the normal power iteration technique of inner iteration convergence acceleration. DOT-IIW has available in addition, under user option, the space point scaling method, the successive overrelaxation method and the Chebyshev semi-iterative method. In order to check the operability of these methods in DOT-IIW, a simple 16 group, r,z eigenvalue DOT problem using zero upscatter cross sections was devised, which was run for only one outer iteration. The results of these calculations, using the four acceleration techniques, is shown in Table 6-2. This initial test problem indicated that the space point scaling method required fewer inner iterations to achieve convergence than was required by the other methods, and this fact was generally substantiated by later, more complex, calculations. However, the improved speed of convergence by the Chebyshev acceleration technique over the normal technique, was not substantiated by later calculations.

The four acceleration techniques were then tested in 16 group, S_2 azimuthally symmetric DOT-IIW eigenvalue problem using the PAX-E1 model. The results of these calculations are shown in Table 6-3. The four problems considered have the same convergence criteria and the input differs only in the inner iteration convergence acceleration technique selected. The calculation using Chebyshev acceleration did not converge, or even approach convergence, during the allotted central processor computer time (1000 seconds). The problems using the other three acceleration techniques: normal, successive overrelaxation, or space point scaling, converged to almost the same eigenvalue and edge-to-center fission distribution ratio, requiring about the same number of outer iterations and computer time. Figures 6-5, 6-6

TABLE 6-2

COMPARISON OF ACCELERATION TECHNIQUES
IN R,Z DOT-IIW CALCULATIONS

Single Outer Iteration Problem
16 Group, Zero Upscatter, Cross Sections

<u>Acceleration Technique</u>	<u>Number of Inner Iterations*</u>
Normal	351
Successive Overrelaxation	245
Chebyshev	214
Space Point Scaling	118

* The computer time required for a design DOT-IIW calculation is proportional to the total number of inner iterations.

TABLE 6-3

COMPARISON OF ACCELERATION TECHNIQUES IN S_2 AZIMUTHALLY SYMMETRIC DOT-IIW CALCULATIONS

Problem Number	Acceleration Technique	Convergence Criteria			Eigenvalue		Fission Distribution Edge/Center Ratio	Total Outer Iterations	Computer Time (sec)***		
		Eigenvalue	Flux	Upscatter	K	ΔK^{**}			CP	PP	Total
14.314A	Normal	10^{-4}	2×10^{-5}	5×10^{-4}	1.048478	---	0.70974	9	543	315	858
14.314B	Successive Overrelaxation	10^{-4}	2×10^{-5}	5×10^{-4}	1.048597	+1.7%	0.70936	9	517	314	831
14.314C	Space Point Scaling	10^{-4}	2×10^{-5}	5×10^{-4}	1.048466	-0.2%	0.70963	8	640	286	926
14.314D	Chebyshev Acceleration*	10^{-4}	2×10^{-5}	5×10^{-4}	1.067120	---	---	6*	---	---	---

* The DOT-IIW calculation using Chebyshev Acceleration did not converge during the allotted CP time, 1000 seconds. The result quoted is for the last completed outer iteration, number six.

** Change in eigenvalue relative to DOT calculation using Normal Acceleration.

*** CP - Central processor time

PP - Peripheral processor time

Figure 6-5. Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculation First Outer Iteration - Group One

Figure 6-6. Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculation First Outer Iteration - Group Seven

Figure 6-7. Comparison of Convergence Patterns in S_2 Azimuthally Symmetric DOT-IIW Calculations First Outer Iteration - Group Fifteen

and 6-7 show graphically for groups one, seven and sixteen, respectively, the convergence patterns of these azimuthally symmetric DOT-IIW problems, during the first outer iteration. In each case the maximum pointwise flux error is plotted for the inner iteration number prior to scaling. The apparent discontinuities in the convergence pattern (i. e. , the flux error), which occurs for all four acceleration techniques and each group shown, occurs at the "corners" of the problem (i. e. , at the first and last azimuthal mesh intervals for the last radial mesh interval in an r,θ problem). This discontinuity appears to be caused by an interaction between negative flux fix-up and the implicit boundary conditions (the azimuthal boundary conditions are periodic).

6.3.2 Quadrature Data

In order to study the convergence pattern of DOT-IIW calculations, a series of azimuthally symmetric DOT-IIW problems were run in which only one input parameter was changed at a time. The key results of these calculations are detailed in Table 6-4. In all these DOT-IIW problems a radial flux guess from an ANISN calculation and a uniform azimuthal flux guess was used.

To determine the effect of quadrature order, S_2 , S_4 , S_6 and S_8 azimuthally symmetric DOT-IIW problems were run. Comparison of the results obtained from these problems (lines 1, 2, 3 and 4, respectively, of Table 6-4) shows that eigenvalue problems of quadrature order two and quadrature order four yield different results in eigenvalue, fission distribution and scalar flux, while problems of quadrature order six and eight substantially agree with the S_4 problem and the S_8 problem required 55 percent longer than the S_6 problem. It should, however, be noted that in r,θ DOT-IIW calculations, where there is an azimuthal variation in material, and the angular flux is an important output parameter, problems of quadrature order greater than four may be required.

*Based on $\beta_{eff} = 0.0071$.

TABLE 6.0-4

CONVERGENCE PATTERNS IN AZIMUTHALLY SYMMETRIC DOT-IIW CALCULATIONS

Line	Problem Number	Quadrature		Boundary Condition		Upscatter	Convergence Criteria			Eigenvalue	Fission Distribution Edge/Center Ratio	Total Outer Iterations	Computer Time (sec)**		
		Order	Geometry	Top	Bottom		Eigenvalue	Flux	Upscatter				CP	PP	Total
1	14.301	2	R, θ	periodic	periodic	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.04848	0.70965	13	585	412	997
2	14.302	4	R, θ	periodic	periodic	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.04393	0.73378	11	806	455	1261
3	14.303	6	R, θ	periodic	periodic	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.04377	0.73629	10	1438	593	2031
4	14.304	8	R, θ	periodic	periodic	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.01384	0.73707	10	2393	763	3156
5	14.313	2	R, θ	periodic	periodic	Yes	10^{-4}	2×10^{-5}	10^{-4}	1.04848	0.70974	9	532	297	829
6	14.307	4	R, Z	periodic	periodic	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.04392	0.73383	11	642	484	1132
7	14.305	4	R, θ	reflective	reflective	Yes	10^{-5}	2×10^{-5}	10^{-5}	1.01100	0.73341	11	762	483	1245
8	14.306E	4	R, θ	periodic	periodic	No	10^{-5}	2×10^{-5}	---	1.04611	0.74907	2	523	83	606
9	14.308	4	R, θ	periodic	periodic	Yes	10^{-3}	2×10^{-3}	10^{-3}	1.03628	0.77481*	3	167	159	326
10	14.311B	4	R, θ	periodic	periodic	Yes	10^{-3}	2×10^{-5}	10^{-3}	1.04346	0.73402*	4	686	200	886
11	14.311A	4	R, θ	periodic	periodic	Yes	10^{-4}	2×10^{-5}	10^{-4}	1.04338	0.73381	7	722	321	1043
12	14.312A	4	R, θ	periodic	periodic	Yes	10^{-4}	2×10^{-5}	5×10^{-4}	1.04388	0.73381	7	748	336	1084
13	14.312B	4	R, θ	periodic	periodic	Yes	10^{-4}	2×10^{-5}	1×10^{-4}	1.04389	0.73381	7	749	336	1085
14	14.312C	4	R, θ	periodic	periodic	Yes	10^{-4}	2×10^{-5}	2×10^{-5}	1.04393	0.73383	10	781	458	1239

*Due to the convergence criteria selected for this problem, the fission distribution is azimuthally asymmetric and the value noted is an average for this calculation.

**CP--Central processor time

PP--Peripheral processor time

To compare the results in azimuthally symmetric DOT problems when using r,θ and r,z geometry quadrature data, S_4 calculations were performed using the quadrature data in Tables B-2 and B-6 (Appendix B), respectively. The results of these two calculations (lines 2 and 6, Table 6-4) showed that in azimuthally symmetric problems r,θ and r,z quadrature data give substantially the same results, while the calculation using the r,z data required slightly less total computer time (10 percent) than the calculation using r,θ data. However, a more definitive test of r,θ vs r,z quadrature data in an r,θ DOT problem, is a DOT calculation having an azimuthal variation in material. This calculation was not performed under this project during CY '69 due to limitations on the available computer time.

6.3.3 Boundary Conditions

This study of DOT-IIW convergence specified the top and bottom (i. e. , azimuthal) boundary conditions to be periodic. An S_4 azimuthally symmetric DOT calculation using reflective top and bottom boundary conditions (line 7, Table 6-4) showed that the reflective boundary condition is operational in DOT-IIW and produces substantially the same results and requires about the same total computer time as a comparable problem with periodic boundary conditions.

6.3.4 Upscatter

The previously described DOT-IIW calculations used sixteen group cross section data with four upscatter and nine downscatter groups. An azimuthally symmetrical DOT-IIW problem using sixteen group cross sections with upscatter collapsed in previous ANISN calculation, showed different results than a comparable problem which included upscatter. Comparing the DOT problems with and without upscatter (lines 2 and 8, respectively, Table 6-4), shows that the problem without upscatter had a 31 percent higher eigenvalue and a higher edge-to-center fission distribution ratio than the comparable problem with upscatter; while the problem without upscatter required fewer outer iterations (two as compared to eleven) and 52 percent less total computer time than the problem with upscatter; r,θ DOT-IIW eigenvalue calculations performed later in this study (see Table 6-7) confirm the fact that zero upscatter DOT-IIW problems have a higher eigenvalue than a comparable problem with upscatter.

6.3.5 Convergence Criteria

A series of azimuthally symmetric DOT-IIW eigenvalue calculations, with and without upscatter, were performed to establish appropriate convergence criteria in DOT-IIW calculations.

6.3.5.1 Flux Convergence

To determine an appropriate flux convergence a series of zero upscatter, S_4 , azimuthally symmetric DOT-IIW calculations were performed, the results of which are shown in Table 6-5. DOT problems using zero upscatter cross sections were selected in order to conserve computer running time. The results from the DOT problems were compared to a reference ANISN calculation (line 1, Table 6-5) since previous analysis had shown (Section 6.2) that comparable DOT and ANISN problems yield comparable results. The flux convergence in the problems was varied from 2×10^{-3} to 10^{-5} , and it was found that a flux convergence of 2×10^{-5} gave eigenvalue and edge-to-center fission distribution results in substantial agreement with the reference ANISN calculation. It was also noted that tightening the flux convergence from 2×10^{-5} to 1×10^{-5} did not significantly change the results, while it did increase the total computer running time.

6.3.5.2 Eigenvalue Convergence

Having selected a flux convergence of 2×10^{-5} , the eigenvalue convergence was varied from 10^{-3} to 10^{-5} (lines 6, 7, and 8, Table 6-5). It was seen that reducing the eigenvalue convergence from 10^{-5} to 10^{-4} gave substantially the same results and gave a small saving in total computer time, while further reducing the eigenvalue convergence from 10^{-4} to 10^{-3} caused no change in either the results or the total computer time. Therefore, an eigenvalue convergence of 10^{-4} was selected as appropriate.

6.3.5.3 Upscatter Convergence

Unlike previous versions of the DOT code, the DOT-IIW code permits the user to specify a convergence factor on upscatter. Earlier versions of DOT internally set the upscatter convergence equal to the eigenvalue convergence (see Section 4.1.4). In three, S_4 , azimuthally symmetric DOT-IIW calculations, the upscatter convergence was varied from

TABLE 6-5
EFFECT OF CONVERGENCE CRITERIA IN ZERO UPSCATTER, S_4 ,
AZIMUTHALLY SYMMETRIC DOT-IIW CALCULATIONS

Line	Problem Number	Transport Code	Convergence Criteria		Eigenvalue		Fission Distribution Edge/Center Ratio	Computer Time (sec)**		
			Eigenvalue	Flux	K	$\Delta K^*(\%)$		CP	PP	Total
1	14.211	ANISN	10^{-5}	2×10^{-5}	1.0462	---	0.7478	83	35	118
2	14.306A	DOT	10^{-3}	2×10^{-3}	1.0396	-93.0	0.7928	151	105	256
3	14.306B	DOT	10^{-4}	2×10^{-4}	1.0455	- 9.9	0.7522	361	84	445
4	14.306C	DOT	10^{-4}	10^{-4}	1.0458	- 5.6	0.7498	391	84	475
5	14.306D	DOT	10^{-4}	10^{-5}	1.0461	- 1.4	0.7479	587	84	671
6	14.306E	DOT	10^{-5}	2×10^{-5}	1.0461	- 1.4	0.7481	523	83	606
7	14.306F	DOT	10^{-4}	2×10^{-5}	1.0461	- 1.4	0.7481	503	88	591
8	14.306G	DOT	10^{-3}	2×10^{-5}	1.0461	- 1.4	0.7481	502	88	590

* Change relative to ANISN problem.

**CP - Central processor time.

PP - Peripheral processor time

2×10^{-5} to 5×10^{-4} (lines 12, 13, and 14, Table 6-4), without any significant change occurring in the eigenvalue, edge-to-center fission distribution ratio and scalar flux, while the number of outer iterations were reduced from 10 to 7 and there was a 13 percent reduction in total computer time. Therefore, an upscatter convergence of 5×10^{-4} was selected. Further study, particularly in r, θ azimuthally asymmetric problems, may show that a further reduction in the upscatter convergence factor is possible without a substantial reduction in precision.

6.3.6 Zones of Convergence

Previous versions of the DOT code have required convergence at each mesh point in each region (zone) of the problem. The DOT-IIW code permits the user to require either pointwise or integral convergence in any one or more zones of the problem (see Section 4.1.4). Integral convergence is indicated by setting the flux convergence factor equal to 0.0. A zone of convergence option has the advantage that under this option a great deal of computer time need not be spent to converge the flux in peripheral zones of the problem (e.g., the pressure vessel), where its solution is of no interest.

Table 6-6 describes a series of S_4 , azimuthally symmetric DOT-IIW calculations using normal and space point scaling acceleration. In the calculations using the normal acceleration technique, the problems requiring convergence in all zones, except the void and pressure vessel (at the edge of the system), did not change the calculated results (eigenvalue and edge-to-center fission distribution ratio) and slightly reduced the central processor computer time* (0.5 percent). Meanwhile the problem that only required convergence in the nine core regions also showed no significant change in the calculated results while the central processor time was reduced by 20.5 percent. Similarly, the DOT-IIW calculations using the space point scaling technique showed that by only requiring convergence in the nine core zones, a very large reduction in central processor computer time is achieved (33.2 percent), while no significant change occurs in the calculated eigenvalue and edge-to-center fission distribution ratio. The substantial advantage of the zones of convergence option in DOT-IIW is, therefore, evident and use was made of this in the r, θ DOT-IIW calculations performed

*Since the total number of outer iterations remained unchanged, there was no significant change in the peripheral processor computer time.

TABLE 6-6
EFFECT OF ZONES OF CONVERGENCE OPTION IN AZIMUTHALLY SYMMETRIC DOT-IIW CALCULATIONS

Problem Number	Zones of Convergence*	Acceleration Technique	Convergence Criteria			Eigenvalue	Fission Distribution Edge/Center Ratio	Total Outer Iterations	Computer Time (sec.)**			Percent Change in CP Time***
			Eigenvalue	Flux	Upscatter				CP	PP	Total	
14.312A	1 - 19	Normal	10^{-4}	2×10^{-5}	5×10^{-4}	1.04388	0.73381	7	748	336	1084	---
14.316A	1 - 17	Normal	10^{-4}	2×10^{-5}	5×10^{-4}	1.04386	0.73385	7	744	337	1081	-0.5
14.318A	1 - 9	Normal	10^{-4}	2×10^{-5}	5×10^{-4}	1.04386	0.73389	7	595	335	930	-20.5
14.317A	1 - 19	Space Point Scaling	10^{-4}	2×10^{-5}	5×10^{-4}	1.04393	0.73355	8	747	386	1133	---
14.316B	1 - 17	Space Point Scaling	10^{-4}	2×10^{-5}	5×10^{-4}	1.04392	0.73368	7	687	335	1022	-8.0
14.318B	1 - 9	Space Point Scaling	10^{-4}	2×10^{-5}	5×10^{-4}	1.04390	0.73353	7	499	332	831	-33.2

* Zones 1 - 19: All zones in the calculation.

Zones 1 - 17: All zones in the calculation, except the void and pressure vessel regions.

Zones 1 - 9: All core zones only.

** CP--Central processor time

PP--Peripheral processor time

*** Relative to the calculation using the same acceleration technique and all zones are converged.

under this project during CY '69. To further reduce the computer running time of r, θ DOT-IIW calculations, convergence was only required in those zones at the edge of the core; that is, Zones 7, 8 and 9 (36.689 cm to 43.804 cm in the homogenized core), since these are the major zones of interest in calculating the eigenvalue and fission distribution (fissions/gram).

6.4 r, θ DOT-IIW EIGENVALUE CALCULATIONS

Using the explicit control vane model that was developed with the aid of the MERTH code (Section 5.2), a number of detailed r, θ DOT-IIW eigenvalue calculations were performed, which are described in Table 6-7. The number of these detailed calculations was limited, due to limitations on the available computer time.

6.4.1 Quadrature Order

Previous experience in the running of r, z DOT calculations (using an earlier version of the code), had shown that it was advantageous with respect to computer time to first run a problem of quadrature order 2, followed by a higher order calculation using as a flux guess the fluxes calculated in the S_2 problem. With this in mind, an S_2 r, θ DOT-IIW problem was run (line 1, Table 6-7), and subsequently, an S_4 problem was completed (lines 3 and 4, Table 6-7). The very high computer running time of the S_2 problem, and the still substantial running time of S_4 problems, appears to indicate that in r, θ DOT-IIW calculations no advantage is gained by first calculating an S_2 flux guess. This statement is substantiated by the fact that an S_4 problem which started from a flat flux guess (line 5, Table 6-7) and which approached but did not reach convergence, required only a little more computer time than the comparable S_2 problem (line 1, Table 6-7).

It can also be noted by comparing the S_2 and S_4 problems (line 1 and 4, Table 6-7), that the S_2 calculation yields a higher eigenvalue than the S_4 problem. This is consistent with the results shown for the azimuthally symmetric DOT-IIW calculations (e.g., lines 1 and 2, Table 6-4).

6.4.2 Acceleration Technique

To obtain a comparison between the normal and space point scaling acceleration techniques in r, θ DOT-IIW calculations, S_2 calculations were performed using these techniques

(lines 1 and 2, Table 6-7). In these two problems, as in all the detailed r, θ DOT-IIW calculations, convergence in only the edge core zones (Zones 7, 8, and 9) was required. Also, the two problems had slightly different convergence criteria; that is, in an effort to conserve computer time, the problem using space point scaling had looser eigenvalue and upscatter convergence criteria. The results of these problems show that the calculation using space point scaling has a somewhat lower eigenvalue (76 cents) and a substantially lower total computer running time (63 percent). The reason for the large change in running time can be seen by comparing the convergence patterns of these problems. Figures 6-8, 6-9, and 6-10 present this comparison for groups one, seven and fifteen of the first outer iteration.

The frequency of space point scaling in inner iterations (the scale cycle), is determined by the value of the dominance ratio, computed for the solution matrix at the start of the calculation. Figure 6-8 shows that after scaling, a sharp change occurs in the convergence rate of group one (the dominance ratio dependent scale cycle is 3 for group one). Thus, during the first outer iteration, group one is converged after the fifth inner iteration using space point scaling, as compared to the eleventh inner iteration using the normal acceleration technique. The dominance ratio dependent scale cycle is eleven for group seven, and, therefore, as shown in Figure 6-9 the two acceleration schemes generally show the same convergence patterns since convergence is reached prior to scaling. Figure 6-10 describes the convergence pattern for group fifteen, which has a dominance ratio dependent scale cycle of nine. Therefore, as in the case for group one, the group fifteen convergence pattern using space point scaling is sharply changed after scaling and is converged after 14 inner iterations as compared to 24 inner iterations for the normal acceleration technique.

It should be noted from Figures 6-5, 6-9, and 6-10 that when the zones of convergence option is used in DOT-IIW and no converged solution is attempted in the "corners" of the problems, there are then no discontinuities in the convergence pattern, as was the case when pointwise convergence was required everywhere in the system, as previously shown in Figures 6-5, 6-6, and 6-7. (The apparent discontinuity in Figure 6-10 in the flux error at the ninth inner iteration, is due to overambitious scaling; note that the scale cycle for group fifteen is nine.)

TABLE 6-7
SUMMARY TABLE OF r, θ DOT-IIW EIGENVALUE CALCULATIONS FOR THE PAX-EI REACTOR

Line	Problem Number	Quadrature Order	Cross Sections	Acceleration Technique	Source of Flux Guess	Convergence Criteria			Eigenvalue	Upscatter Scale Factor	Total Outer Iterations	Computer Time (sec.) ⁽²⁾		
						Eigenvalue	Flux ⁽¹⁾	Upscatter				CP	PP	Total
1	14,339	2	with upscatter	Normal	Flat	10^{-4}	0.0	5×10^{-4}	1.0564	1.0004	16	8203	2434	10637
2	14,340	2	with upscatter	Space Point Scaling	Flat	2×10^{-3}	0.0	2×10^{-3}	1.0510	0.9986	13	1970	1986	3956
3	14,342	4	with upscatter	Normal	problem 14,339	10^{-3}	0.0	10^{-3}	1.0264	0.9991	12	2428	2138	4566
4	14,346	4	with upscatter	Normal	problem 14,342	10^{-4}	0.0	10^{-3}	1.0402	0.9997	18	6166	3150	9316
5	14,347	4	with upscatter	Normal	Flat	10^{-4}	0.0	10^{-3}	1.0501	1.0030	15 ⁽³⁾	9078	2641	11719
6	14,348	4	zero upscatter	Normal	Flat	10^{-4}	0.0	—	1.0482	—	8	4516	870	5386

(1) A flux convergence criteria of 0.0 indicates integral convergence.

(2) CP - Central processor time
PP - Peripheral processor time

(3) Problem exited upon reaching the maximum allowed number of outer iterations for this calculation.

Figure 6-8. Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation
First Outer Iteration - Group One

Figure 6-9. Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation

Figure 6-10. Comparison of Convergence Patterns in S_2 R, θ DOT-IIW Calculation
First Outer Iteration - Group Fifteen

6.4.3 Eigenvalue

As previously stated, Table 6-7 describes the r, θ DOT-IIW eigenvalue calculations in which the reflector contains an explicit control vane model at 105 degrees. Problem 14.346 (line 4, Table 6-7) is the most tightly converged of the S_4 DOT problems with upscatter cross sections, and is a restart of problem 14.342 (line 3). The results of these DOT-IIW calculations can be compared to the results obtained from a comparable EXTERMINATOR-2 calculation.⁹ The DOT-IIW and EXTERMINATOR-2 calculations both contained an explicit control vane at 105 degrees and used the same cross section data; however, the meshing of the control vane differed in the two calculations.

In the EXTERMINATOR-2 problem an eigenvalue of 1.0326 was calculated, as compared to 1.0402 in the DOT-IIW problem (line 4, Table 6-7). The cause of this 1.07% difference in eigenvalue has not been determined, but it may indicate that the DOT-IIW calculation should be run to a pointwise flux convergence, since the problem in question was only run to an integral flux convergence in the edge core zones (Zones 7, 8 and 9). Previous analysis of the PAX-E1 reactor has shown⁽⁹⁾ that when corrected for factors not included in the calculation, the eigenvalue calculated by EXTERMINATOR-2 is in reasonable agreement with the experiment. The difference in the eigenvalues as calculated by DOT-IIW and EXTERMINATOR-2 does not appear to be due to differences in the two-dimensional PAX-E1 model used in the problems, since the only substantial difference exists in the explicit control vane model which should not cause a large difference in the calculated absolute reactivity. This fact is further substantiated by a comparison of the calculated and experimentally measured fission distribution (see Section 6.4.4).

As an additional point of reference, an r, θ DOT-IIW eigenvalue calculation was performed, using cross section data in which upscatter had been removed by a previous ANISN calculation (line 6, Table 6-7). The eigenvalue calculated by the zero upscatter DOT-IIW problem was 1.13% higher than that calculated by a comparable S_4 r, θ DOT-IIW using cross section data with four upscatter groups. This is consistent with previous experience, which has shown that DOT-IIW problems without upscatter calculate higher eigenvalues than comparable DOT-IIW problems with upscatter (e. g., see Table 6-4).

Figure 6-11. Comparison of Calculated and Experimentally Measured Fissions Per Gram in PAX-EI Reactor - Radial Traverse Between Drums

Figure 6-12. Detailed Comparison Between 35 and 43.8 cm, of Calculated and Experimentally Measured Fission per Gram in PAX-E1 Reactor - Radial Traverse Between Drums

6.4.4 Fission Distribution

Figure 6-11 compares, for a radial traverse between the drums, the fissions per gram as calculated by DOT-IIW (problem 14.346, line 4, Table 6-7) by EXTERMINATOR-2,⁹ and as experimentally measured in the PAX-E1 reactor.¹ Figure 6-12 presents the same data in greater detail near the core edge, 35 to 43.8 cm. The experimental data has been normalized to give the same average as the DOT-IIW calculation.

These fissions per gram results show that in this radial traverse between the drums, the DOT-IIW calculation gives better agreement with experiment at the edge of the homogenized core (43.8 cm) than the EXTERMINATOR-2 results. For this traverse between the drums, the EXTERMINATOR-2 calculation is about 7 percent lower than the experiment, while DOT-IIW is 3 percent higher.

Figure 6-13 compares, for an azimuthal traverse at the edge of the homogenized core (43.8 cm), the fissions per gram as calculated by DOT-IIW (problem 14.346, line 4, Table 6-7) and EXTERMINATOR-2.⁹ The experimentally measured fissions per gram data is not presented on this figure, since the azimuthally asymmetric groups of graphite elements (both filler strip and support) at the edge of the PAX-E1 core perturb the fission pattern and thus the DOT-IIW calculated results, which assume a uniformly cylindrical core edge, cannot be directly compared to the experimental data at the irregular core periphery. The data presented in Figure 6-13 shows the DOT-IIW calculated fissions per gram. A comparison of the group 16 thermal flux at the edge of the homogenized core as calculated by DOT-IIW and EXTERMINATOR-2, Figure 6-14, shows in more detail the irregularity of the flux solution in the region of the control vane (15 to 20 degrees). This apparently "unconverged" solution is due to diamond difference breakdown in DOT-IIW and should be rectified by coding changes to DOT-IIW during the recommended CY '70 program.

To obtain a direct comparison of the DOT-IIW calculated and the experimentally measured fissions per gram, use must be made of the PFENCER program which compares the experimental and calculated fissions per gram value and computes their ratio (NC_f). This PFENCER analysis was not within the scope of this study, and prior to such analysis the

PFENCER program will have to be recoded to accept fluxes in the DOT-IIW format since at present PFENCER can only accpet fluxes in the EXTERMINATOR-2 format.

Figure 6-13. Calculated Fissions Per Gram in PAX-E1 Reactor Azimuthal Traverse at Edge of Cylindricized Core (43.8 cm)

Figure 6-14. Comparison of Group 16 Thermal Flux in DOT-IIW and EXTERMINATOR-2 Calculations
Azimuthal Traverse at Edge of Cylindricized Core (43.8 cm)

7.0 REFERENCES

1. L. I. Ortenberg, "Evaluation of the WANL Integrated Nuclear, Radiation and Shielding Standard Design Method (WISDM)," WANL-TME-2689, September 1970
2. F. R. Mynatt, "Development of Two-Dimensional Discrete Ordinates Transport Theory for Radiation Shielding," Ph.D. Thesis, University of Tennessee, February 1969
3. F. R. Mynatt, "A Users' Manual for DOT," K-1694, (to be published).
4. F. R. Mynatt, "DOT Two-Dimensional Discrete Ordinates Transport Code," RSIC-CCC-89, 1970
5. R. G. Soltesz and R. K. Disney, "One-Dimensional Discrete Ordinates Transport Technique," WANL-PR(LL)-034, Volume 4, August 1970
6. G. Collier and G. Gibson, "GAMBIT Program," WANL-TME-1752, April 1968
7. R. G. Soltesz, R. K. Disney, and S. L. Zeigler, "Cross Section Generation and Data Processing Techniques," WANL-PR(LL)-034, Volume 3, August 1970, p.5-1.
8. R. G. Soltesz, R. K. Disney, and S. L. Zeigler, "Cross Section Generation and Data Processing Techniques," WANL-PR(LL)-034, Volume 3, August 1970, p.2-1.
9. R. G. Soltesz, R. K. Disney, and S. L. Zeigler, "Cross Section Generation and Data Processing Techniques," WANL-PR(LL)-034, Volume 3, August 1970, p.3-1.
10. R. G. Soltesz, R. K. Disney, J. Jedruch, and S. L. Zeigler, "Two-Dimensional, Discrete Ordinates Transport Techniques," WANL-PR(LL)-034, Volume 5, August 1970
11. R. K. Disney and J. Jedruch, (to be published)
12. R. K. Disney, (to be published)
13. R. K. Disney, R. G. Soltesz, J. Jedruch, and S. L. Zeigler, "Code Description and Users' Manual for the MAP Radiation Transport Computer Code," WANL-TME-2706, August 1970
14. R. S. Kaiser, "LINK Users' Manual," (Internal Memorandum) NRD-70-287, September 1970
15. B. J. Jacob, L. I. Ortenberg, C. P. Saalbach, "Users' Manual - PFENCER-1, PFENCER-2, PFENCER-3," (Internal Memorandum) WANL-TMI-1999, January 1970

16. R. G. Soltesz, R. K. Disney, and S. L. Zeigler, "Cross Section Generation and Data Processing Techniques," WANL-PR(LL)-034, Volume 3, 1970, p.4-1.
17. R. K. Disney and S. L. Zeigler, "Point Kernel Techniques," WANL-PR(LL)-034, Volume 6, August 1970
18. R. S. Varga, Matrix Iterative Analysis, Prentice Hall, Publ., Englewood Cliffs, N. J. 1962.
19. K. D. Lathrop, "DTF-IV, A FORTRAN-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering," LA-3373, November 1965
20. Personal Communication, G. Laliti, NASA-Lewis Research Laboratory, Cleveland, Ohio, 1969
21. B. G. Carlson and G. I. Bell, "Solution of the Transport Equation by the S_n Method," Proc. Second Intern. Conf. Peaceful Uses of Atomic Energy, Geneva, 16, 535, 1958
22. T. E. Murley, J. W. Silliamson, "STØER, A One-Dimensional Perturbation Code," WARD-71, 1969
23. R. W. Hardie, W. W. Little, Jr., "PERT-IV, A Two-Dimensional Perturbation Theory Code in FORTRAN-IV," BNWL-409, April 1967
24. D. A. Sargis, "GAPER, A Transport Perturbation Theory Program," GA-8667, April 1968
25. B. G. Carlson, Numerical Formulation and Solution of Neutron Transport Problems," LA-2226, April 1964
26. P. M. Campbell, "A Numerical Method for Discrete Ordinate and Moment Equations in Radiative Transfer," Int. J. Heat Mass Transfer 12, 497 - 507, 1969
27. Z. Kopal, Numerical Analysis, Chapman and Hall, Publishers, London, 1955, p. 369
28. M. Abramowitz, I. A. Stegun, Editor, Handbook of Mathematical Functions, National Bureau of Standards, Washington, D. C., 1964
29. H. Bateman, Higher Transcendental Functions, McGraw-Hill, New York, Chapter 10, p. 161, 1953
30. K. D. Lathrop, N. S. Demuth, "Bi-Orthogonal Angular Polynomial Expansion of the Two-Dimensional Transport Equation," Nucl. Sci. Eng. 32, 120 - 130, 1968

31. WANL-TME-1739, "WANEF Critical Experiments in Support of NERVA, Quarterly Report - 3rd Quarter CY '67," January 1968
32. "The Evaluation of the WANL Integrated Nuclear, Radiation and Shielding Standard Design Method (WISDM)," to be published
33. WANL-TME-1751, "GAMBIT Users' Manual," W. H. Gray, G. Collier, February 1968
34. E. Iwinski, personal communication
35. DRM-51105, "Flow Charts for an Integrated Nuclear and Radiation, Thermal and Structural Analysis Procedure and Identification and Description of Computer Codes," February 1969
36. P. J. Sipush, Internal Memorandum (WANL-TMI-1505), "Improved One-Dimensional NRX-A Control Vane Representation," August 13, 1965
37. WANL-TME-1642, "NRX-A6 Nuclear Subsystem Thermal and Nuclear Design Data Book," November 15, 1967
38. L. I. Ortenberg, R. S. Kaiser, Internal Memorandum (NRD-69-107), "Preliminary Results from EXTERMINATOR-2 Calculations for PAX-E1," April 2, 1969

APPENDIX A

PAX-E1 MODEL DESCRIPTION

TABLE A-1

ONE-DIMENSIONAL PAX-E1 MODEL WITH RING VANE PRESCRIPTION AT 105°

<u>Radial Mesh Line</u>	<u>Zone</u>	<u>Radius (cm)</u>	<u>ΔR (cm)</u>	<u>Region Description</u>
1	1	0.0	7.0	Core Region-1
2	1	7.0	5.0	Core Region-1
3	1	12.0	3.747	Core Region-1
4	2	15.747	4.698	Core Region-2
5	3	20.445	4.946	Core Region-3
6	4	25.391	3.559	Core Region-4
7	4	28.950	3.541	Core Region-4
8	5	32.491	1.803	Core Region-5
9	6	34.294	2.395	Core Region-6
10	7	36.689	1.411	Core Region-7
11	7	38.100	1.380	Core Region-7
12	8	39.480	0.746	Core Region-8
13	8	40.226	0.747	Core Region-8
14	8	40.973	0.746	Core Region-8
15	9	41.719	0.516	Core Region-9
16	9	42.235	0.515	Core Region-9
17	9	42.750	0.527	Core Region-9
18	9	43.277	0.527	Core Region-9
19	10	43.804	0.685	Filler Strip
20	10	44.489	0.685	Filler Strip
21	11	45.174	0.652	Lateral Support-1
22	11	45.826	0.652	Lateral Support-1
23	12	46.478	0.6765	Lateral Support-2
24	12	47.1545	0.6765	Lateral Support-2
25	13	47.831	0.9525	Be-1
26	13	48.7835	0.9525	Be-1
27	14	49.736	1.140	Be-2
28	15	50.876	1.124	Be-3
29	15	52.0	1.2	Be-3
30	15	53.2	1.2	Be-3
31	15	54.4	1.2	Be-3
32	15	55.6	0.764	Be-3
33	16	56.364	0.101	Vane
34	16	56.465	0.101	Vane

TABLE A-1 (Continued)

<u>Radial Mesh Line</u>	<u>Zone</u>	<u>Radius</u>	<u>ΔR</u>	<u>Region Description</u>
35	17	56.566	0.934	Be-3
36	17	57.5	1.4	Be-3
37	17	58.9	1.4	Be-3
38	17	60.3	1.3	Be-3
39	17	61.6	1.214	Be-3
40	18	62.814	0.369	Void
41	19	63.183	0.8505	Pressure Vessel
42	19	64.0335	0.8505	Pressure Vessel
43		64.884		

APPENDIX B

DISCRETE ORDINATES QUADRATURE DATA
FOR r,θ and r,z GEOMETRIES

TABLE B-1

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R, θ) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 2

R-DIRECTION -----	θ -DIRECTION -----	Z-DIRECTION -----	WEIGHT -----
-0.81650	0.00000	+0.57735	0.00000
-0.57735	-0.57735	+0.57735	0.25000
+0.57735	-0.57735	+0.57735	0.25000
-0.81650	0.00000	+0.57735	0.00000
-0.57735	+0.57735	+0.57735	0.25000
+0.57735	+0.57735	+0.57735	0.25000

TABLE B-2

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,θ) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 4

R-DIRECTION -----	θ-DIRECTION -----	Z-DIRECTION -----	WEIGHT -----
-0.936741778	0.000000000	+0.350021200	0.000000000
-0.868890280	-0.350021200	+0.350021200	0.083333333
-0.350021200	-0.868890280	+0.350021200	0.083333333
+0.350021200	-0.868890280	+0.350021200	0.083333333
+0.868890280	-0.350021200	+0.350021200	0.083333333
-0.495004728	0.000000000	+0.868890280	0.000000000
-0.350021200	-0.350021200	+0.868890280	0.083333333
+0.350021200	-0.350021200	+0.868890280	0.083333333
-0.936741778	0.000000000	+0.350021200	0.000000000
-0.868890280	+0.350021200	+0.350021200	0.083333333
-0.350021200	+0.868890280	+0.350021200	0.083333333
+0.350021200	+0.868890280	+0.350021200	0.083333333
+0.868890280	+0.350021200	+0.350021200	0.083333333
-0.495004728	0.000000000	+0.868890280	0.000000000
-0.350021200	+0.350021200	+0.868890280	0.083333333
+0.350021200	+0.350021200	+0.868890280	0.083333333

TABLE B-3

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,θ) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 6

R-DIRECTION -----	θ-DIRECTION -----	Z-DIRECTION -----	WEIGHT -----
-0.963797442	0.000000000	+0.266635500	0.000000000
-0.926180879	-0.266635500	+0.266635500	0.044031561
-0.681507707	-0.681507707	+0.266635500	0.039301772
-0.266635500	-0.926180879	+0.266635500	0.044031561
+0.266635500	-0.926180879	+0.266635500	0.044031561
+0.681507707	-0.681507707	+0.266635500	0.039301772
+0.926180879	-0.266635500	+0.266635500	0.044031561
-0.731810935	0.000000000	+0.681507707	0.000000000
-0.681507707	-0.266635500	+0.681507707	0.039301772
-0.266635500	-0.681507707	+0.681507707	0.039301772
+0.266635500	-0.681507707	+0.681507707	0.039301772
+0.681507707	-0.266635500	+0.681507707	0.039301772
-0.377079540	0.000000000	+0.926180879	0.000000000
-0.266635500	-0.266635500	+0.926180879	0.044031561
+0.266635500	-0.266635500	+0.926180879	0.044031561
-0.963797442	0.000000000	+0.266635500	0.000000000
-0.926180879	+0.266635500	+0.266635500	0.044031561
-0.681507707	+0.681507707	+0.266635500	0.039301772
-0.266635500	+0.926180879	+0.266635500	0.044031561
+0.266635500	+0.926180879	+0.266635500	0.044031561
+0.681507707	+0.681507707	+0.266635500	0.039301772
+0.926180879	+0.266635500	+0.266635500	0.044031561
-0.731810935	0.000000000	+0.681507707	0.000000000
-0.681507707	+0.266635500	+0.681507707	0.039301772
-0.266635500	+0.681507707	+0.681507707	0.039301772
+0.266635500	+0.681507707	+0.681507707	0.039301772
+0.681507707	+0.266635500	+0.681507707	0.039301772
-0.377079540	0.000000000	+0.926180879	0.000000000
-0.266635500	+0.266635500	+0.926180879	0.044031561
+0.266635500	+0.266635500	+0.926180879	0.044031561

TABLE B-4

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,θ) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 8

R-DIRECTION -----	θ-DIRECTION -----	Z-DIRECTION -----	WEIGHT -----
-0.975900071	0.000000000	+0.218217900	0.000000000
-0.951189727	-0.218217900	+0.218217900	0.030246915
-0.786795790	-0.577350269	+0.218217900	0.022685185
-0.577350269	-0.786795790	+0.218217900	0.022685185
-0.218217900	-0.951189727	+0.218217900	0.030246915
+0.218217900	-0.951189727	+0.218217900	0.030246915
+0.577350269	-0.786795790	+0.218217900	0.022685185
+0.786795790	-0.577350269	+0.218217900	0.022685185
+0.951189727	-0.218217900	+0.218217900	0.030246915
-0.816496581	0.000000000	+0.577350269	0.000000000
-0.786795790	-0.218217900	+0.577350269	0.022685185
-0.577350269	-0.577350269	+0.577350269	0.023148144
-0.218217900	-0.786795790	+0.577350269	0.022685185
+0.218217900	-0.786795790	+0.577350269	0.022685185
+0.577350269	-0.577350269	+0.577350269	0.023148144
+0.786795790	-0.218217900	+0.577350269	0.022685185
-0.617213403	0.000000000	+0.786795790	0.000000000
-0.577350269	-0.218217900	+0.786795790	0.022685185
-0.218217900	-0.577350269	+0.786795790	0.022685185
+0.218217900	-0.577350269	+0.786795790	0.022685185
+0.577350269	-0.218217900	+0.786795790	0.022685185
-0.308606714	0.000000000	+0.951189727	0.000000000
-0.218217900	-0.218217900	+0.951189727	0.030246915
+0.218217900	-0.218217900	+0.951189727	0.030246915
-0.975900071	0.000000000	+0.218217900	0.000000000
-0.951189727	+0.218217900	+0.218217900	0.030246915
-0.786795790	+0.577350269	+0.218217900	0.022685185
-0.577350269	+0.786795790	+0.218217900	0.022685185
-0.218217900	+0.951189727	+0.218217900	0.030246915
+0.218217900	+0.951189727	+0.218217900	0.030246915
+0.577350269	+0.786795790	+0.218217900	0.022685185
+0.786795790	+0.577350269	+0.218217900	0.022685185
+0.951189727	+0.218217900	+0.218217900	0.030246915
-0.816496581	0.000000000	+0.577350267	0.000000000
-0.786795790	+0.218217900	+0.577350267	0.022685185
-0.577350269	+0.577350269	+0.577350267	0.023148144
-0.218217900	+0.786795790	+0.577350267	0.022685185
+0.218217900	+0.786795790	+0.577350267	0.022685185
+0.577350269	+0.577350269	+0.577350267	0.023148144
+0.786795790	+0.218217900	+0.577350267	0.022685185
-0.617213403	0.000000000	+0.786795790	0.000000000
-0.577350269	+0.218217900	+0.786795790	0.022685185
-0.218217900	+0.577350269	+0.786795790	0.022685185
+0.218217900	+0.577350269	+0.786795790	0.022685185
+0.577350269	+0.218217900	+0.786795790	0.022685185
-0.308606714	0.000000000	+0.951189727	0.000000000
-0.218217900	+0.218217900	+0.951189727	0.030246915
+0.218217900	+0.218217900	+0.951189727	0.030246915

TABLE B-5

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,Z) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 2

R-DIRECTION -----	Z-DIRECTION -----	θ -DIRECTION -----	WEIGHT -----
-0.81650	-0.57735	0.00000	0.00000
-0.57735	-0.57735	-0.57735	0.25000
+0.57735	-0.57735	-0.57735	0.25000
-0.81650	+0.57735	0.00000	0.00000
-0.57735	+0.57735	-0.57735	0.25000
+0.57735	+0.57735	-0.57735	0.25000

TABLE B-6

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,Z) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 4

R-DIRECTION -----	Z-DIRECTION -----	θ-DIRECTION -----	WEIGHT -----
-0.495004728	-0.868890280	0.000000000	0.000000000
-0.350021200	-0.868890280	+0.350021200	0.083333333
+0.350021200	-0.868890280	+0.350021200	0.083333333
-0.936741778	-0.350021200	0.000000000	0.000000000
-0.868890280	-0.350021200	+0.350021200	0.083333333
-0.350021200	-0.350021200	+0.868890280	0.083333333
+0.350021200	-0.350021200	+0.868890280	0.083333333
+0.868890280	-0.350021200	+0.350021200	0.083333333
-0.495004728	+0.868890280	0.000000000	0.000000000
-0.350021200	+0.868890280	+0.350021200	0.083333333
+0.350021200	+0.868890280	+0.350021200	0.083333333
-0.936741778	+0.350021200	0.000000000	0.000000000
-0.868890280	+0.350021200	+0.350021200	0.083333333
-0.350021200	+0.350021200	+0.868890280	0.083333333
+0.350021200	+0.350021200	+0.868890280	0.083333333
+0.868890280	+0.350021200	+0.350021200	0.083333333

TABLE B-7

COMPLETELY SYMMETRIC ANGULAR QUADRATURES
(R,Z) CYLINDRICAL GEOMETRY
QUADRATURE ORDER = 6

R-DIRECTION -----	Z-DIRECTION -----	θ-DIRECTION -----	WEIGHT -----
-0.377079540	-0.926180879	0.000000000	0.000000000
-0.266635500	-0.926180879	-0.266635500	0.044031561
+0.266635500	-0.926180879	-0.266635500	0.044031561
-0.731810935	-0.681507707	-0.000000000	0.000000000
-0.681507707	-0.681507707	-0.266635500	0.039301772
-0.266635500	-0.681507707	-0.681507707	0.039301772
+0.266635500	-0.681507707	-0.681507707	0.039301772
+0.681507707	-0.681507707	-0.266635500	0.039301772
-0.963797442	-0.266635500	0.000000000	0.000000000
-0.926180879	-0.266635500	-0.266635500	0.044031561
-0.681507707	-0.266635500	-0.681507707	0.039301772
-0.266635500	-0.266635500	-0.926180879	0.044031561
+0.266635500	-0.266635500	-0.926180879	0.044031561
+0.681507707	-0.266635500	-0.681507707	0.039301772
+0.926180879	-0.266635500	-0.266635500	0.044031561
-0.377079540	+0.926180879	0.000000000	0.000000000
-0.266635500	+0.926180879	-0.266635500	0.044031561
+0.266635500	+0.926180879	-0.266635500	0.044031561
-0.731810935	+0.681507707	0.000000000	0.000000000
-0.681507707	+0.681507707	-0.266635500	0.039301772
-0.266635500	+0.681507707	-0.681507707	0.039301772
+0.266635500	+0.681507707	-0.681507707	0.039301772
+0.681507707	+0.681507707	-0.266635500	0.039301772
-0.963797442	+0.266635500	0.000000000	0.000000000
-0.926180879	+0.266635500	-0.266635500	0.044031561
-0.681507707	+0.266635500	-0.681507707	0.039301772
-0.266635500	+0.266635500	-0.926180879	0.044031561
+0.266635500	+0.266635500	-0.926180879	0.044031561
+0.681507707	+0.266635500	-0.681507707	0.039301772
+0.926180879	+0.266635500	-0.266635500	0.044031561

TABLE B-8
 COMPLETELY SYMMETRIC ANGULAR QUADRATURES
 (R,Z) CYLINDRICAL GEOMETRY
 QUADRATURE ORDER = 8

R-DIRECTION -----	Z-DIRECTION -----	θ -DIRECTION -----	WEIGHT -----
-0.308606714	-0.951189727	0.000000000	0.000000000
-0.218217900	-0.951189727	-0.218217900	0.030246915
+0.218217900	-0.951189727	-0.218217900	0.030246915
-0.617213403	-0.786795790	0.000000000	0.000000000
-0.577350269	-0.786795790	-0.218217900	0.022685185
-0.218217900	-0.786795790	-0.577350269	0.022685185
+0.218217900	-0.786795790	-0.577350269	0.022685185
+0.577350269	-0.786795790	-0.218217900	0.022685185
-0.816496581	-0.577350269	0.000000000	0.000000000
-0.786795790	-0.577350269	-0.218217900	0.022685185
-0.577350269	-0.577350269	-0.577350269	0.023148144
-0.218217900	-0.577350269	-0.786795790	0.022685185
+0.218217900	-0.577350269	-0.786795790	0.022685185
+0.577350269	-0.577350269	-0.577350269	0.023148144
+0.786795790	-0.577350269	-0.218217900	0.022685185
-0.975900071	-0.218217900	0.000000000	0.000000000
-0.951189727	-0.218217900	-0.218217900	0.030246915
-0.786795790	-0.218217900	-0.577350269	0.022685185
-0.577350269	-0.218217900	-0.786795790	0.022685185
-0.218217900	-0.218217900	-0.951189727	0.030246915
+0.218217900	-0.218217900	-0.951189727	0.030246915
+0.577350269	-0.218217900	-0.786795790	0.022685185
+0.786795790	-0.218217900	-0.577350269	0.022685185
+0.951189727	-0.218217900	-0.218217900	0.030246915
-0.308606714	+0.951189727	0.000000000	0.000000000
-0.218217900	+0.951189727	-0.218217900	0.030246915
+0.218217900	+0.951189727	-0.218217900	0.030246915
-0.617213403	+0.786795790	0.000000000	0.000000000
-0.577350269	+0.786795790	-0.218217900	0.022685185
-0.218217900	+0.786795790	-0.577350269	0.022685185
+0.218217900	+0.786795790	-0.577350269	0.022685185
+0.577350269	+0.786795790	-0.218217900	0.022685185
-0.816496581	+0.577350269	0.000000000	0.000000000
-0.786795790	+0.577350269	-0.218217900	0.022685185
-0.577350269	+0.577350269	-0.577350269	0.023148144
-0.218217900	+0.577350269	-0.786795790	0.022685185
+0.218217900	+0.577350269	-0.786795790	0.022685185
+0.577350269	+0.577350269	-0.577350269	0.023148144
+0.786795790	+0.577350269	-0.218217900	0.022685185
-0.975900071	+0.218217900	0.000000000	0.000000000
-0.951189727	+0.218217900	-0.218217900	0.030246915
-0.786795790	+0.218217900	-0.577350269	0.022685185
-0.577350269	+0.218217900	-0.786795790	0.022685185
-0.218217900	+0.218217900	-0.951189727	0.030246915
+0.218217900	+0.218217900	-0.951189727	0.030246915
+0.577350269	+0.218217900	-0.786795790	0.022685185
+0.786795790	+0.218217900	-0.577350269	0.022685185
+0.951189727	+0.218217900	-0.218217900	0.030246915

Fold
or Cut

TITLE ANNUAL REPORT FOR CONTRACT YEAR 1969 SUPPORTING RESEARCH AND TECHNOLOGY PROJECT 493	
	DOCUMENT NO. WANL-TME-2704	DATE February 4, 1971
ABSTRACT Advances in the methods for neutronic and radiation design of NERVA are described. The transport code DOT-IIW was improved in the acceleration of convergence, handling of boundary conditions and tape operations, and extensively tested for flux and eigenvalue convergence at different orders of quadrature and in r, θ geometry. Satellite codes for preparation of cross sections, and geometry were developed. Reduction of ray effects through Lagrangian interpolation in discrete ordinate fluxes was achieved. Improvements in two-dimensional perturbation code were made.		
DATA ITEM NO. N/A	SECURITY CLASSIFICATION OF DOCUMENT Unclassified	
CDRL LINE NO N/A	TOTAL NO OF PAGES 160	
KEY WORDS Two-dimensional transport theory NERVA nuclear and radiation design Angular Flux interpolation Two-dimensional perturbation theory		
AUTHOR/EDITOR R. K. Disney, J. Jedruch, R. G. Soltesz, R. S. Kaiser, S. L. Zeigler		PREPARING DEPT NRD
W Form 59943 DOCUMENT INFORMATION SUMMARY		

Fold
or Cut