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VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion-Theory Approximation to Neutron Transport, Version II

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OAK RIDGE NATIONAL LABORATORY
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VENTURE: A CODE BLOCK FOR SOLVING MULTIGROUP NEUTRONICS PROBLEMS APPLYING THE FINITE-DIFFERENCE DIFFUSION-THEORY APPROXIMATION TO NEUTRON TRANSPORT, VERSION II

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for the
DEPARTMENT OF ENERGY

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*This effort began in the ORNL Reactor Division.

**Member of the Computer Sciences Division, Union Carbide Nuclear Division.

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ABSTRACT

This report documents the computer code block VENTURE designed to solve multigroup neutronics problems with application of the finite-difference diffusion-theory approximation to neutron transport (or alternatively simple P_1) in up to three-dimensional geometry. It uses and generates interface data files adopted in the cooperative effort sponsored by the Reactor Physics Branch of the Division of Reactor Research and Development of the Energy Research and Development Administration. Several different data handling procedures have been incorporated to provide considerable flexibility; it is possible to solve a wide variety of problems on a variety of computer configurations relatively efficiently. The programming in Fortran is straightforward, although data is transferred in blocks between auxiliary storage devices and main core, and direct access schemes are used. The size of problems which can be handled is essentially limited only by cost of calculation since the arrays are variably dimensioned and several data handling modes are programmed; the memory requirement is held down while data transfer during iteration is increased only as necessary with problem size.

The more common orthogonal coordinate systems arising in reactor analysis applications have been treated in from one through three dimensions. These include the slab, the cylinder, Θ-R, Θ-R-Z, and hexagonal and triagonal coordinate systems in two and three dimensions. Only the mesh-centered finite difference formulation has been programmed. There is provision for the more common boundary conditions including the repeating boundary, 180° rotational symmetry, and the rotational symmetry conditions for the 90° slab and the 60° and 120° triangular grids on planes.

A variety of type of problem may be solved: the usual eigenvalue problem, a direct criticality search on the buckling, on a reciprocal velocity absorber (prompt mode), or on nuclide concentrations, or an indirect criticality search on nuclide concentrations, or on dimensions. First-order perturbation analysis capability is available at the macroscopic cross section level.

COMPUTER CODE ABSTRACT

1. Program Identification: VENTURE, A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion or a Simple P_1 Theory Approximation to Neutron Transport, Version II.[a]
2. Function: This code solves usual neutronics eigenvalue, adjoint, fixed source, and criticality search (direct and indirect) problems, treating up to three geometric dimensions, maps power density and does first order perturbation analysis at the macroscopic cross section level. The code is used as a module of a local computation system.[b]
3. Method of Solution: An inner, outer iteration procedure is used with several different data handling schemes programmed in parallel. Restrained line overrelaxation is used, and succeeding iterate flux sets may be accelerated by the Chebyshev process, and asymptotic extrapolation done when distinct error modes establish. Normally the eigenvalue of a problem is estimated each outer iteration from an overall neutron balance; however, source ratios are used in some situations. The difference equation is mesh centered point. Advanced capability is incorporated, as to treat direction-dependent diffusion coefficients and zone-dependent fission source distribution functions. Macroscopic nuclear properties are calculated from microscopic cross sections and nuclide concentrations.
4. Related Material: Standard interface data file specifications adopted in the ERDA Reactor Physics code coordination effort are used. Input data must be read by a separate processor. Other codes using the same interface files will couple directly with this one, including several in routine use locally, as for exposure calculations to treat depletion.

5. Restrictions: This code is quite thoroughly variably dimensioned. Generally the larger the problem, the more Input/Output required for iteration. One-dimensional problems have been solved treating thousands of mesh points or more than one-hundred energy groups within a 50,000 short-word total fast computer memory.
6. Computer: This code has been run on IBM computers including the 360/91, the 360/75, and 360/195, and on the CDC-7600 computer after the required conversion step. A separate version is expected to be made available for long-word, small fast memory computers having large extended slow memories.
7. Running Time: Running time is directly related to problem size and inversely proportional to some measure of central processor and data transfer speeds. The basic rate of solution of eigenvalue problems is about 500 space energy points per second of central processor time on an IBM 360/195; this rate falls off approximately as $(10/N)^{0.7}$ where N is the average number of points in one dimension, less when the amount of data transfer is low, and more when it is high, excepting one-dimensional problems. Thermal reactor lattice and cell problems normally require more time by perhaps a factor of two. Problems involving significant upscatter (multithermal-group treatment) require additional computer time by a factor of about two.
8. Programming Languages: The programming is basically in the ASA 1966 FORTRAN language excepting certain extensions, especially those required for unindexed, mixed type block data transfers and direct access of data by record from disc. Known limitations of manufacturer's current compilers are not exceeded: for example, arrays are limited to three dimensions, dummy arguments in subroutines to

sixty, and subscripted subscripts are not used. Special routines are used for certain functions including memory allocation, support of the data transfer procedures and to make available elapsed computer time for executing certain user options; these would require replacement for compatibility with a different operating system. The source deck consists of about 40,000 statements (VENTURE proper), and the transmission package about 80,000.

9. Operating System: The basic OS-360 IBM operating system has been used under HASP and ASP with a FORTRAN IV, H level compiler version 21.6. Access capability of programs in the modular sense is essential to use the system of codes.

10. Machine Requirements: A 32,000 word core is needed, and preferably one much larger; auxiliary storage of the disc or drum type is essential, preferably several on different data channels. The programming is included for three-level hierarchy data storage for efficient use of an extended slow memory for large three-dimensional problems when such a memory is available. Typically the code uses 27 logical units.

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12. References:

a. D. R. Vondy et al., "VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion-Theory Approximation to Neutron Transport, Version II," ERDA Report, ORNL-5062, revision 1 (1977).

b. D. R. Vondy et al., "A Computation System for Nuclear Reactor Core Analysis," ERDA Report, ORNL-5158 (1977).

c. G. E. Bosler et al., "LA SIP-III, A Generalized Processor for Standard Interface Files," ERDA Report, LA-6280 MS (April 1976).

d. D. R. Vondy et al., "Input Data Requirements for Special Processors in the Computation System Containing the VENTURE Neutronics Code," ERDA Report, ORNL-5229, (1976).

e. D. R. Vondy et al., "Reference Test Problems for the VENTURE Neutronics and Related Computer Codes," ERDA Report ORNL/TM-5887 (1977).

13. Material Available: The package submitted to the Argonne Code Center includes Fortran card image source decks for a control module, the VENTURE neutronics code, a cross section processor code, a reaction rate calculation code, input data processors, a code system driver, a control module, assembly language routines for use on a compatible computer, and an input data deck for sixteen sample problems plus the edit from the computer run for these. New modules will be added to the package as they can be made available, including the BURNER exposure module.

GENERAL DISCUSSION

The code block VENTURE is designed to solve multi-neutron-energy-group, multi-dimensional neutronics problems. The finite-difference diffusion or a simple P_1 theory approximation to neutron transport is applied. Usual eigenvalue problems may be solved to determine the multiplication factor and the neutron flux distribution. The adjoint problem may be solved. Fixed source problems are treated and a variety of criticality search problems. Perturbation results based on macroscopic cross sections are produced by option.

The code treats scattering from one energy group to any other, including upscattering, internal black absorber zones, and a variety of boundary conditions including periodic and the more important rotational symmetry conditions.

The method of solution implemented is an inner, outer iteration process with rather involved acceleration procedures.

The loose-leaf form of this report with sections in short blocks was chosen to facilitate updating to account for revisions.

Background

The procedures implemented in the VENTURE code represent a background of effort which can be traced back to the late 1950's, to the work of M. L. Tobias[a] and others. Over this period of time a large number of problems have been solved in routine reactor analysis effort at ORNL and at other installations by the methods which were evolving during this period. It seems noteworthy that although theoretical considerations have played a role, this has been primarily an engineering development directed

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[a]See ORNL-4078 for example.

at economical solution of problems encountered in analysis. The previous code programmed in this effort was CITATION.[a]

Many individuals have worked on developing and implementing procedures for solving diffusion theory neutronics problems, especially at the ERDA National Laboratories,[b] but also in private companies[c] and in other countries.[d] We are aware of much of this work, and acknowledge that published information and discussions with several individuals have made direct contributions to this effort.

The Procedure of Calculation

A flow chart for the code is presented in Fig. 001-1. This shows the general flow through the procedures of calculation.

An inner, outer iteration scheme is used to solve problems. New flux values are calculated from finite-difference, neutron balance equations for a row of points simultaneously, and each new value is driven in the direction of the change from the old value. This procedure is continued over the space problem at one energy; it is repeated for a number of inner iterations, and the calculation proceeds to the next energy. At each energy the inscattering source and the fission source are determined. After a complete sweep of the problem, the eigenvalue is estimated either from an overall neutron balance, summed neutron balance equations, or from the source ratio, and the calculation is continued to satisfy specified convergence criteria. For an indirect criticality search, an

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[a] T. B. Fowler, D. R. Vondy, and G. W. Cunningham, "Nuclear Reactor Core Analysis Code: CITATION," ORNL-TM-2496, Revision 2, Oak Ridge National Laboratory (July 1971).

[b] See WAPD-TM-678, BNWL-1264, ANL-7716, and LASL-4396.

[c] See GA-6540.

[d] See AEEW-R682, TRG-229(R).

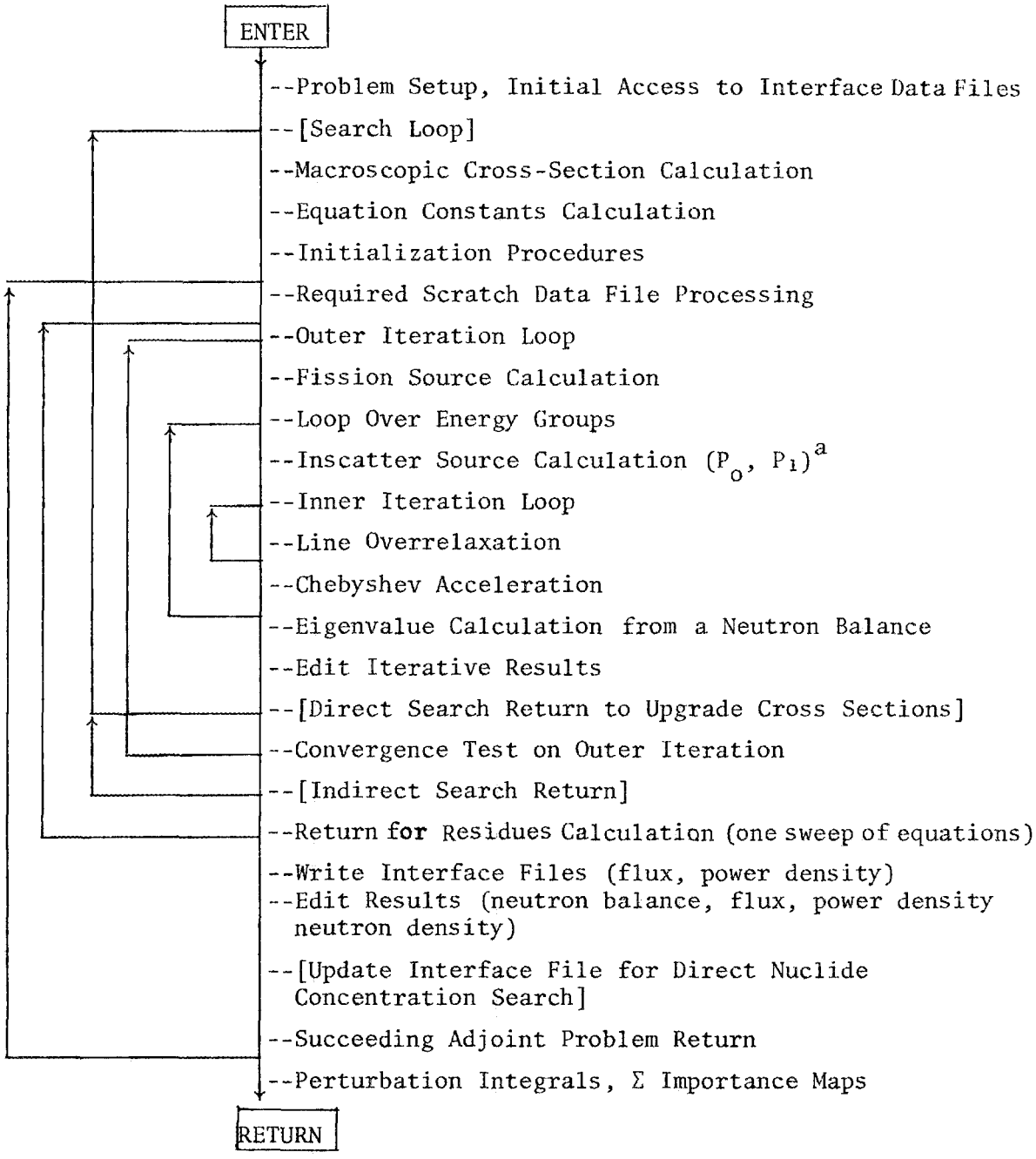

Fig. 001-1. User flow chart, VENTURE finite-difference diffusion theory neutronics code block.

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[a]The inscatter source calculation is normally done outside the inner iteration loop; however in one data handling mode this source is calculated inside the inner iteration loop to minimize data transfer.

additional outer iterative loop is required to adjust the desired parameters, nuclide concentrations or dimensions, to effect a desired solution.

If there is one main feature which stands out in the VENTURE code, it is the direct search procedure. As carried over from the CITATION code, an iteration procedure is implemented to move the iterate flux estimate directly toward a solution by determining the eigenvalue of the problem when certain parameters are adjusted. Perhaps only the analyst who has experienced the frustrations of and relatively high cost of obtaining solutions by indirect methods can fully appreciate the utility of this direct search capability. For a direct criticality search problem, the relative buckling, reciprocal velocity loss term, or relative change in the search nuclide concentrations is treated as the eigenvalue of the problem. No outer iteration loop is required.

The calculation of macroscopic cross sections, from the nuclide densities and microscopic cross sections and of equation constants is done in the head end of the code. As shown in the flow chart of Fig. 001-1, returns are made to this part of the program for recalculation of this macroscopic data to account for the effects from adjustments to the parameters in a criticality search problem. To initiate a succeeding adjoint problem which involves no changes in the parameters for a regular problem which has been solved, the data for the regular problem is simply reprocessed, and the procedure for the regular problem is used. Subsequent calculations, as of conversion ratio and perturbation integrals, are done using the macroscopic data generated initially without reaccess of the microscopic data.

Alternative Procedures and Large Problems

The code contains parallel procedures, different ways of handling data, involving varying amounts of data transfer between memory and auxiliary storage within a flexible, basic iterative procedure. Automatic selection between these allows effective application with different computer hardware configurations to solve a variety of problem sizes with use of a reasonable amount of computer memory. Still, modifications may well be required to most effectively use a particular facility, especially if it has a hierarchy of auxiliary storage devices which have quite different data transfer rates. The necessary changes should not be extremely hard to make if a preferred structuring can be identified.

The VENTURE code represents a considerable extension over the CITATION code in the size of problems which may be treated. One thousand point one-dimensional problems have been solved, and the extent in the other two dimensions is not limited. However, selection of a practical problem requires consideration of the cost of the calculation and justification of the expenditure in computer time. On many computers, especially so the IBM 360/91, the extra cost associated with the increased amount of data Input/Output required to solve the larger problems is indeed significant. Also, adequate on-line auxiliary storage is required for a problem to be solved, which increases directly with the number of space-energy points considered.

Standard Interfacing

This code block was programmed specifically to operate (interface) with other programs developed under rules established in a cooperative effort between several installations, an effort sponsored by the Reactor

Physics Branch of the Division of Reactor Research and Development of the Energy Research and Development Administration. For example, all user input data is processed by separate code blocks. This neutronics code block only interfaces binary data files. It uses microscopic cross sections supplied in a standard interface format from any source;[a] other code blocks are being programmed elsewhere to generate this data, and yet others to use the results from the neutronics calculation. This coupling between major code blocks is effected by satisfying hard interface data file specifications.

We believe this code block satisfies the primary objective of this effort: to develop a neutronics code which uses and generates interface data files having standardized formats; one which can be converted from one computer to run on another relatively easily and permit effective and efficient utilization of computers having a variety of hardware configurations.

Programming

The programming is done in the Fortran language. Basically, ASA 1966 standard Fortran as generally implemented was used with a few extensions; data are transferred in blocks of mixed data type and direct access is used, for example. Known limits on the major computers using current manufacturer's compilers have quite generally not been exceeded. For example, the maximum number of dimensions of any variable is three, the number of arguments in subroutine statements is limited to sixty, and subscripts are not subscripted. Both short- and long-word storage of data are used for effective execution on IBM 360, 370 series computers (very low accuracy is associated with use of short words, single precision,

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[a]Locally with the AMPX Code Systems, ORNL-TM-3706.

carrying less than the equivalence of seven significant decimal digits), but this was done in such a way that conversion to such a machine as a CDC-7600 should not be too difficult if the comment instructions for this conversion included in this program are followed. However, special local system routines have been used to allocate memory, and to set up direct access file specifications dynamically, and to use the system data transfer routines directly outside of Fortran. Also, certain key subroutines have been written in machine language (not essential) to improve performance on the local computers.

Status

The VENTURE and related codes are in routine production use locally and via remote terminal from other installations as modules in a local computation system.[a] Production use has contributed directly by information feedback to the developed capability and reliability. Some of the individuals involved in application are E. J. Allen in the Energy Division, Neutron Physics Division Staff members, S. C. Crick at General Electric (Sunnyvale), and D. Lancaster at Westinghouse (Madison). Testing of an early version of the code at LASL by G. E. Bosler and R. D. Odell on a CDC-7600 computer and by D. E. Ferguson at ANL made contribution.

A major code block is generally not free of bugs, especially when complicated options tend to have overlapping control. Still we have used an unusually large number of test problems for which reliable solutions are available. This testing gives us confidence that most problems will be properly solved. Part of this confidence comes from

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[a]ORNL-5158.

the nature of the effort, a straightforward extension of capability which has had wide application on a production basis.

This document presents basic information about the code including descriptions of the procedures and mathematical equations. Certain modules used with this code are discussed in the appendices. Requirements for input data processors are documented elsewhere.[a,b]

END OF SECTION

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[a]ORNL-5158.

[b]ORNL-5229.

COMPUTER REQUIREMENTS

In the following discussion, information is presented which may be needed by a user for effective application of the code. The required files must be made available, and there must be adequate space allocated on each logical unit for the data carried on it. Much of the user burden regarding allocation of space is relieved by use of a reference catalog procedure available to the operating system; however, especially for solving large problems, it will be necessary to change the allocations by overriding those provided. The code is used as a loaded module which cannot be altered by a user, satisfying basic quality assurance requirements of a large user community.

VENTURE as a Module

The VENTURE code block is a module for solving neutron transport problems by application of diffusion theory. It is structured for use in a modular code system; other modules which serve the same role may parallel it in a system. The code does not read user input cards. Data it requires must be available in binary interface data files. Results from the code are placed on other interface data files on demand for subsequent use. The code contains routines to produce elaborate edits of results on demand and always edits key results.

Locally the code is used under a resident driver and a primary control module as discussed in another report.[a] The code is placed in executable load module form incorporating an overlay structure, assembled. The codes in this system are available on disc which may or may not be on-line. A catalog procedure stored on disc contains basic job control instructions

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[a]ORNL-5158.

with provision for changing the space allocations and data blocking factors. Changes to the program, to the Fortran language compiler instructions, cannot be done simply because reloading is necessary and are not allowed by the user community. The code is used on a production basis locally and remotely from other installations via remote terminal. Therefore, modifications must be carefully assessed and proofed prior to general use, and ongoing analysis effort not disrupted.

Other computation modules are in use in this system. These include a cross section processor, a code to produce reaction rates and related results, and an exposure module. Special input data processors are also in use which generate data files. New modules will be phased into the system as they become developed and adequately tested to assure reliable application.

Machine Time Requirements and Charging

Of primary concern here are central processor (cp) time, clock time, and costing. Clock time is quite dependent on what tasks are being performed; it increases with the number of Input/Output operations performed during any task, execution of a job, or computation. If a large fraction of the memory available for computation is used by a job, then the multitasking system cannot effectively overlap calculation and data transfer.

A reference rate of fast reactor problem solution is 500 space-energy points per second IBM-360/195 central processor time. This rate falls off approximately as $(10/N)^{0.7}$ where N is the average number of points in one dimension, less when the amount of data transfer is low and more when it is high, excepting one-dimensional problems. Certain types of problems require more time, especially when upscattering is treated or the problem is for a large thermal reactor or a cell with reflecting boundaries.

Relative processor time for the IBM-360/91 is about twice that for the /195. Clock time is three to six times the processor time when a job is run in the multitasking mode using less than half the computer memory.

Memory Requirements

Memory requirements for the code block are discussed here. Separate storage is required to satisfy four requirements:

1. Program (machine instructions and variables not variably dimensioned) — The storage is minimized by an effective overlay scheme.

2. Library Routines — These are provided by the system and range from arithmetic functions to the data Input/Output package.

3. Buffer Area — This storage is required in most modes of data transfer to allow block transfer. Careful allocation of the buffer storage is important for effective machine utilization. The best allocation depends on the problem and the available facility, so experience must be a guide to reasonable allocation. Generally, the larger the problem, the more data which must be transmitted and the larger the buffers required. However, if a large allocation of buffers causes degrading of the mode of data handling during iteration, the performance can be expected to be degraded. A special situation exists when extended slow memory is used for buffer storage of data being transferred requiring consideration. The main scratch files are used in a direct access mode with automatic allocation of buffer size.

4. Variably Dimensioned Data — Most data arrays in the code are variably dimensioned. The required memory size depends on an involved combination of the primary variables of a problem, the options exercised, and the mode of data handling automatically selected.

There are six data handling modes programmed (see Section 225); the one used by the code depends on the problem and the available memory.

Additional capability is automated to reduce the amount of data transfer automatically when memory space permits, as to default scratch data files to reside in memory.

The code edits a table of data storage requirements for all the applicable data handling modes when a job is executed, and automatically selects that mode involving the least amount of data Input/Output unless overridden by user control. Also edited are data file storage requirements which presents some of the information required in the job control instructions.

Basic Requirements (IBM short word, 4-byte)

Program	30,000
Library Routines	8,200
Buffer Area	5,000-30,000
Minimum Data	5,000

When operated under a resident assembly language driver, about 6,000 additional words of memory are required.

Auxiliary Storage

In solving a large problem, this code may well tax available capability for fast access storage. A 2.5×10^6 space-energy point problem requires 5×10^6 short-word (2.5×10^6 long-word) storage for one set of the flux values. Not only must three sets of these be stored, but also the equation constants requiring about four times as much space as one set of flux values. This storage space must be available, generally on disc units, preferably separated between control channels for efficient

data transfer. When one disc surface is inadequate to hold a file, the data must span two or more surfaces. Details of the files are discussed in Section 204.

To exercise control over the interface data files, a user must have information about these; refer to Section 204 and to the computation system documentation, ORNL-5158.

END OF SECTION

PROGRAMMING INFORMATION

In the following sections, the information needed for a comprehensive understanding of the program is presented. This information is directed at the programmer making modification to the code or converting it from one computer to another, and is intended only to supplement the source deck FORTRAN listing which contains informative comments. Primary data arrays are defined on comment lines and conversion notes are included.

The source language is FORTRAN, primarily the standard ASA 1966 FORTRAN. However, block transfer of data of mixed type is done without indexing in the guise of the REAL type, and the direct access mode of data transfer is used. Local system routines are used to allocate memory and to define the direct access files and access parameters dynamically, and also to obtain time and computer model; the functions of these routines would have to be satisfied or the requirements and associated capability bypassed. Certain key routines are also available in assembly language to reduce computation time on IBM-360, 370 model machines.

END OF SECTION

Section 201: Information About Subroutines

Here principal information is provided about the subroutines. Where practical, they are grouped into sets to identify those which are used together to perform some well-defined function.

FIGURE 201-1. VENTURE SUBROUTINES.

THE ACCESS, CONTROL, AND GENERAL PURPOSE ROUTINES

```
MAIN   ENTRY POINT TO THE VENTURE NEUTRONICS CODE BLOCK
            CALLS ERRSET, TIMER, DOPC, IONO, VENT, DRIV
IONO   ASSIGNS INPUT/OUTPUT UNIT NUMBERS
VENT   ACCESSES CODE BLOCK CONTROL INFORMATION
            CALLS SKER, FERR
DRIV   PASSES INFORMATION TO THE CONTROLLER ROUTINE
       ALLOCATES CORE STORAGE
            CALLS GETCOR, ROXX, ROXY, DIFF, DOPC, FRECOR
DIFF   CONTROLS THE CALCULATION
            CALLS CORE, MAC1, CON1, PHIA, ORLX, COMC, LCAL, FLXR,
                  FXSR, BSQV, AJNT, PROS, DOPC, OUTR, DSDF, DCID,
                  DIMS, AJDS, FLRD, ADN1, EDIT, SAV1, PERT, JERT,
                  FERR, TIMER
CORE   DETERMINES STORAGE REQUIREMENTS AND DATA HANDLING MODES
            CALLS CORI, CORP, GNAM, CORD, CORB, DDSP, DASU, SKER,
                  JPRT, FERR
CORI   OBTAIN FILE SPECIFICATION RECORD FROM INTERFACE FILES NDXSRF,
       ZNATDN, GRUPXS, AND GEODST
            CALLS SKER
DASU   SETUP DIRECT ACCESS FILES
            CALLS DOPC, FERR
EASU   SETUP DIRECT ACCESS FILES
            CALLS DOPC, FERR
TIMER  SERVICE ROUTINE FOR COMPUTER TIME ETC.
STOR   SERVICE ROUTINE FOR MOVING DATA IN MAIN MEMORY
SKER   FILE MANAGEMENT RELATED ERROR MESSAGES
FERR   ALL OTHER FATAL ERROR MESSAGES
KEEP   DUMMY SUBROUTINE USED TO OUTFOX THE OPTIMIZING COMPILER
```

THE INPUT/OUTPUT ROUTINES

```
DOPC   INITIALIZES, OPENS, AND CLOSES DATA FILES
         ENTRY ROXY   COMMUNICATES DATA ARRAYS
            CALLS SEEK, RITE, DEFILE, CLOSDA, (FBSAM AND ENTRIES)
RITE   DATA TRANSFER MANAGER AND WRITES DATA (FORTRAN WRITE) -
       CALLED BY MOST ROUTINES
         ENTRY REED   READS DATA (FORTRAN READ) - CALLED BY MOST
                      ROUTINES
         ENTRY ROXX   COMMUNICATES DATA ARRAYS
            CALLS CRIT, CRED, (FBSAM AND ENTRIES)
SEEK   INTERFACE DATA FILES MANAGER
            CALLS RITE, REED
CRIT   ASSEMBLY LANGUAGE ROUTINE FOR CORE TO EXTENDED CORE DATA
       TRANSFER (SEE SECTION 203 FOR THE FORTRAN EQUIVALENT)
         ENTRY CRED   EXTENDED CORE TO CORE DATA TRANSFER
```

(CONT)

DEFILE ASSEMBLY LANGUAGE ROUTINE TO EXECUTE THE FORTRAN DEFINE FILE STATEMENT USING PROBLEM DEPENDENT VARIABLES (OPENS DIRECT ACCESS FILES) - ACCESSES SYSTEM ROUTINE IHCEDIOS

CLOSDA ASSEMBLY LANGUAGE ROUTINE TO CLOSE DIRECT ACCESS FILES

FBSAM LOCAL I/O ROUTINE USED ALONG WITH THE IBM I/O PACKAGE TO PRODUCE SPECIAL CAPABILITY

THE CALCULATION OF MACROSCOPIC CROSS SECTIONS

MAC1 CONTROLS MACROSCOPIC CROSS SECTION CALCULATION
CALLS MACA, MACB, MAC2, SCAL, MAC3, MAC5, CHDM, MAC4, MAC6, SKER, FERR

MACA INITIAL PROCESSING OF GRUPXS
CALLS STOR

MACB CHECK NAMES AND CLASSES ON NDXSRF AND GRUPXS FOR AGREEMENT

MAC2 CALCULATE MACROSCOPIC PRINCIPAL CROSS SECTIONS

SCAL LOCATES POSITION OF SCATTERING RECORDS ON GRUPXS

MAC3 CALCULATE MACROSCOPIC SCATTERING CROSS SECTIONS

MAC5 ADJUST DIFFUSION CONSTANT AND SCATTERING DATA FOR P1 CALC.

CHDM CHECK DIMENSION SEARCH DATA
CALLS SKER

MAC4 CALCULATE MACROSCOPIC SEARCH DATA

MAC6 EDIT MACROSCOPIC CROSS SECTIONS

THE CALCULATION OF EQUATION CONSTANTS

CON1 CONTROLS EQUATION CONSTANTS CALCULATION
CALLS MSH0, NRCF, MSH1, CON2, GEOQ, CON3, MSH3, CKCT, CON4, CON5, CON7, CON9, STOR, SKER, FERR

MSH0 SETUP COARSE MESH PARAMETERS FOR 1D AND 2D CASES

NRCF CONVERT REGION ASSIGNMENTS BY COARSE MESH TO FINE MESH

MSH1 CALCULATE FINE MESH DISTANCES

CON2 SETUP BOUNDARY CONSTANTS AND BUCKLING

GEOQ CHANGE FROM 3D TO 2D CASE

CON3 RESTRUCTURE MACROSCOPIC DATA AND ZERO ROD CROSS SECTIONS
CALLS NROD, STOR

MSH3 EDIT FINE MESH DISTANCES

CKCT SETUP INDEXING FOR DIFFUSION CONSTANTS

CON4 CALCULATES LEAKAGE CONSTANTS
CALLS NROD, BNDY

CON5 CALCULATES LEAKAGE CONSTANTS (TRIAGONAL)
CALLS NROD, BNDY

CON7 CALCULATES LEAKAGE CONSTANTS (HEXAGONAL)
CALLS NROD, BNDY

CON9 CALCULATE ZONE VOLUMES FROM REGION VOLUMES AND DETERMINE ZONE WITH MAXIMUM NU*SIGF*VOL
CALLS NROD

NROD FUNCTION TO DETERMINE INTERNAL BLACK ABSORBER ZONES

BNDY FUNCTION TO CALCULATE NON-RETURN LEAKAGE CONSTANT

(CONT)

THE INITIALIZATION PROCESS

ORLX CONTROLS ITERATIVE PROCESS PARAMETER INITIALIZATION
CALLS ORLA, ORLB, ORLC, ORLD, ORLE, ORLF, BATG, ORLR, CON6, FERR, RCOV

ORLA LOCATES A REFERENCE POINT IN MESH TO USE AS A BASIS FOR INITIALIZATION PROCEDURES (2,3-D PROBLEMS ONLY)
CALLS MUCK

ORLB DETERMINES AN ENERGY DISTRIBUTION FUNCTION FROM EQUATION CONSTANTS AT THE REFERENCE POINT (2,3-D PROBLEMS ONLY)
CALLS KEEP

ORLC SETUP 1-D EQUATION CONSTANTS ALONG THE ROW CONTAINING THE REFERENCE POINT (2,3-D PROBLEMS ONLY)
CALLS KEEP

ORLD SETUP DATA FOR THE 1-D INITIALIZATION CALCULATION (2,3-D PROBLEMS ONLY)
CALLS NROD

ORLE SETUP CROSS SECTIONS FOR THE 1-D INITIALIZATION CALCULATION (2,3-D PROBLEMS ONLY)

ORLF SOLVES THE 1-D PROBLEM FOR INNER AND OUTER ITERATION BEHAVIOR (2,3-D PROBLEMS ONLY)
CALLS LAXR, LAXP

BATG CALCULATE OVERRELAXATION COEFFICIENTS AND INNER ITERATIONS AND CHEBYSHEV PARAMETER AND SETS DEFAULT OPTIONS (2,3-D PROBLEMS ONLY)
CALLS LUCK

ORLR BYPASS INITIALIZATION DURING SEARCH OR PERTURBATIONS ONLY CALCULATIONS (2,3-D PROBLEMS ONLY)

RCOV RECOVERS DATA FOR SUCCESSIVE NEUTRONICS PROBLEMS

LAXR LINE RELAXATION FOR 1-D INITIALIZATION CALCULATION

LAXP POINT RELAXATION FOR 1-D INITIALIZATION CALCULATION

MUCK FUNCTION TO LOCATE REFLECTED BOUNDARY

LUCK FUNCTION TO DETERMINE MESH DEPENDENT PARAMETER FOR LAMBDA

CON6 PREPARE MACROSCOPIC CROSS SECTIONS AND OTHER DATA FOR ITERATIVE PROCESS

PHIA CONTROLS FLUX INITIALIZATION
CALLS PHI1, PHI7, PHI2, PHI3, FERR

PHI1 INITIAL FLUX IS CONSTANT
CALLS NROD

PHI7 INITIAL FLUX IS SYNTHESIZED FROM THE RESULT OF THE 1-D INITIALIZATION CALCULATION (2,3-D PROBLEMS ONLY)
CALLS SDBN, TOIP, NROD

TOIP SIMPLE LINEAR INTERPOLATION

PHI2 INITIAL FLUX IS A FUNCTION OF SPACE AND ENERGY
CALLS EDBN, SDBN, NROD

EDBN CALCULATE ENERGY DISTRIBUTION FUNCTION

SDBN CALCULATE SPATIAL DISTRIBUTION FUNCTIONS

PHI3 PROCESS INITIAL FLUX FROM FLUX INTERFACE (MAY BE EXPANDED TO NEW MESH EXCEPT FOR HEXAGONAL GEOMETRY)
CALLS PHI4, PHI5 ,PHI6, GRXP, PAN1, PAN2, NROD, SKER

PHI4 1D FLUX EXPANSION

PHI5 2D FLUX EXPANSION
CALLS PBND, PC2D

(CONT)

```
PHI6   3D FLUX EXPANSION
            CALLS PBND, PC2D, PC3D
GRXP   GROUP EXPANSION
PAN1   TRIANGULAR EXPANSION ON PLANES
PAN2   TRIANGULAR EXPANSION BETWEEN PLANES
PBND   FUNCTION TO DETERMINE ARTIFICIAL FLUX POINT
PC2D   FUNCTION TO DETERMINE ARTIFICIAL CORNER POINT - 2D
PC3D   FUNCTION TO DETERMINE ARTIFICIAL CORNER POINT - 3D
            CALLS PC2D
```

THE ITERATIVE PROCESS

```
COMC   UTILITY ROUTINE
LCAL   CALCULATES STARTING ADDRESSES IN DATA ARRAY
            CALLS FERR
FLXR   OBTAINES INITIAL FLUX
FXSR   OBTAINS A FIXED SOURCE
            CALLS SKER
BSQV   SEARCH CALCULATION UTILITY ROUTINE
AJNT   SETS UP INPUT/OUTPUT FILES FOR THE ADJOINT PROELEM
            CALLS REV1
REV1   PROCESSES SCATTERING DATA FOR ADJOINT PROBLEM
PROS   SETS UP INPUT/OUTPUT FILES
            CALLS ZIO3, FEFS
ZIO3   PROCESSES PRINCIPAL CROSS SECTIONS
FEFS   SETS INITIAL FLUX TO FIXED SOURCE WHEN FIXED SOURCE LT 0
DSDF   CALCULATES INDIRECT NUCLIDE SEARCH CHANGE EIGENVALUE
DCID   CONTROLS SEARCH CALCULATION EXIT OPTIONS
DIMS   CALCULATES DIMENSION SEARCH CHANGE FACTOR
ADJS   CONTROLS DIMENSION SEARCH CHANGES
            CALLS DIM1, DIM2, DIM3
DIM1   READS COARSE MESH MODIFIERS FROM SEARCH INTERFACE FILE
DIM2   CONTROLS COARSE MESH AND VOLUME CHANGES - WRITES NEW GEODST
            CALLS CMES, CRGV
DIM3   CONTROLS CHANGE ZONE VOLUMES - WRITES NEW NDXSRF INTERFACE
            CALLS ZVRV
ZVRV   CHANGES ZONE VOLUMES
FLRD   READS GEODST FOR FINAL EDIT OF MESH - DIMENSION SEARCH
            CALLS FLMH
CMES   CHANGES COURSE MESH
CRGV   CALCULATE REGION VOLS FROM POINT VOLS
            CALLS CHVL
CHVL   CHANGES REGION VOLUMNS
FLMH   EDITS FINAL MESH - DIMENSION SEARCH
OUTR   OUTER ITERATION CONTROLLER
            CALLS DOIN, ZINS, FSOR, SSOR, FLUX, PSOR, JUSB, BALC, XTRP
                  , WRES, RRES, PREC, MUEX, CHEV, ETR1, ETR2
                  , ATED, SGDA, FERR
BALC   NEUTRON BALANCE CALCULATION
ZINS   CALCULATES THE DIRECT SEARCH PROBLEM EIGENVALUE
CHBF   CHEBYSHEV ACCELERATION ROUTINE
```

(CONT)

```
CHEV   CHEBYSHEV ACCELERATION ROUTINE
RDAB   CALCULATES ROD ABSORPTIONS
LTRG   CALCULATES IN-LEAKAGE FOR TRIANGULAR GEOMETRY
XTRP   ASSESSES FLUX CONVERGENCE
            CALLS FFGG, BHAV
BHAV   CALCULATES ITERATIVE CONVERGENCE PARAMETERS
JUSB   OVERRELAXATION COEFFICIENT CONTROL
ATED   EDITS ITERATION DATA
FFGG   CALCULATES FLUX EXTRAPOLATION FACTORS
RDUE   RESIDUE ESTIMATE OF THE MULTIPLICATION FACTOR
RELX  SOLVES FOR THE FLUX VALUES ALONG A ROW AND OVERRELAXES THEM
OELX  SOLVES FOR THE FLUX VALUES ALONG A ROW NO OVERRELAXATION
NEWB  CALCULATES NEW OVERRELAXATION FACTORS
FSOR   FISSION SOURCE CALCULATION CONTROLLER
            CALLS FOU1, FOU2, FOU3, FOU4, FOU5, FOU6
SSOR   SCATTERING SOURCE CALCULATION CONTROL
            CALLS SOU1, SOU2, SOU3, SOU4, SOU5, SOU6
PSOR   P-1 SCATTERING SOURCE CALCULATION CONTROL
            CALLS POU1, POU2, POU3, POU4, POU5
FLUX   INNER ITERATION CONTROL
            CALLS INR1, INR2, INR3, INR4, INR5, INR6, INRX, BHAV
MUEX   EXTRAPOLATION PARAMETER PROCESSING
ETR1   SINGLE ERROR MODE FLUX EXTRAPOLATION
ETR2   DOUBLE ERROR MODE FLUX EXTRAPOLATION
SGDA   SAVES AND RETRIVES DATA DURING DIRECT NUCLIDE SEARCH
DOIN   FLUX CALCULATION UTILITY ROUTINE
RRES   READS RESTART FILE
WRES   WRITES RESTART FILE
PREC   CALCULATES ONE-DIMENSIONAL SWEEP PARAMETERS
ADN1   CONTROLLER FOR UPDATING ATOMIC DENSITIES
            CALLS ADN2, ADN3, FERR, SKER
ADN2   UPDATES ATOMIC DENSITIES
ADN3   EDITS ATOM DENSITIES

INR1   INNER ITERATION CONTROL (1 ROW STORED MODE)
            CALLS LOU1, RDUE, RELX, LEK1, CHEV, OELX, NEWB
LOU1   IN-LEAKAGE CALCULATION
FOU1   FISSION SOURCE CALCULATION
SOU1   SCATTERING SOURCE CALCULATION
POU1   P-1 SCATTERING SOURCE CALCULATION
LEK1   OUT-LEAKAGE CALCULATION

INR2   INNER ITERATION CONTROL (ALL DATA STORED MODE)
            CALLS LOU2, RDUE, RELX, LEK2, CHEV, RDAB, OELX, NEWB
FOU2   FISSION SOURCE CALCULATION
LOU2   IN-LEAKAGE CALCULATION
SOU2   SCATTERING SOURCE CALCULATION
POU2   P-1 SCATTERING SOURCE CALCULATION
LEK2   OUT-LEAKAGE CALCULATION

INR3   INNER ITERATION CONTROL (SPACE PROBLEM DATA STORED MODE)
            CALLS LOU3, RDUE, RELX, LEK3, CHEV, LTRG, RDAB, OELX, NEWB
```

(CONT)

```
LOU3    IN-LEAKAGE CALCULATION
FOU3    FISSION SOURCE CALCULATION
SOU3    SCATTERING SOURCE CALCULATION
POU3    P-1 SCATTERING SOURCE CALCULATION
LEK3    OUT-LEAKAGE CALCULATION
INR4    INNER ITERATION CONTROL (MULTIPLE PLANE DATA STORED MODE)
             CALLS LOU4, QDUE, QELX, LEK4, SOUX, J1C4, CHEV, LTRG, RDAB
                   NEWB
LOU4    IN-LEAKAGE CALCULATION
LTRG    SPECIAL IN-LEAKAGE CALCULATION FOR TRANGULAR GEOMETRY
FOU4    FISSION SOURCE CALCULATION
SOU4    SCATTERING SOURCE CALCULATION
SOUX    SCATTERING SOURCE CALCULATION
POU4    P-1 SCATTERING SOURCE CALCULATION
LEK4    OUT-LEAKAGE CALCULATION
J1C4    DEL DOT J CALCULATION
QDUE    ACCESSES RESIDUE CALCULATION
             CALLS RDUE
QELX    ACCESSES FLUX CALCULATION
             CALLS RELX, OELX

INR5    INNER ITERATION CONTROL (MULTI-ROW STORED MODE)
             CALLS LOU5, RDUE, RELX, LEK5, J1C5, CHEV, OELX, NEWB
LOU5    IN-LEAKAGE CALCULATION
FOU5    FISSION SOURCE CALCULATION
SOU5    SCATTERING SOURCE CALCULATION
POU5    P-1 SCATTERING SOURCE CALCULATION
J1C5    DEL DOT J CALCULATION
LEK5    OUT-LEAKAGE CALCULATION

INR6    CONTROLLER ROUTINE FOR THE SPECIAL ONE-DIMENSIONAL PROCEDURE
             CALLS CHEV
FOU6    FISSION SOURCE CALCULATION
SOU6    SCATTERING SOURCE CALCULATION
DELX    LINE RELAXATION WITHOUT OVERRELAXATION

INRX    INNER ITERATION CONTROL (MULTI-LEVEL DATA TRANSFER MODE)
             CALLS LOUX, RDUE, RELX, LEKX, SOUZ, J1CX, CHEV, RDAB, OELX
                   NEWB
LOUX    IN-LEAKAGE CALCULATION
FOUX    FISSION SOURCE CALCULATION
SOUY    SCATTERING SOURCE CALCULATION
SOUZ    SCATTERING SOURCE CALCULATION
POUX    P-1 SCATTERING SOURCE CALCULATION
LEKX    OUT-LEAKAGE CALCULATION
J1CX    DEL DOT J CALCULATION
```

THE EDIT ROUTINES
--- ---- --------

```
EDIT    CONTROLS EDITS
             CALLS NBAL, PNDN, FLXW, PERT, BSQS, FISS,JINT,PTVL,PTZF
CORP    EDIT PROBLEM DESCRIPTION
```

(CONT)

```
GNAM   EDIT GEOMETRY AND CHECK FOR VALIDITY
CORD   EDIT MAJOR PROBLEM PARAMETERS
JPRT   CALCULATES PERTURBATION STORAGE REQUIREMENTS
CORB   EDIT BOUNDARY INDICATORS AND CHECK FOR VALIDITY
DDSP   EDIT SYMBOLIC PARAMETERS FOR DISK SPACE (IBM 360 JCL)
JINT   CALCULATES AND EDITS ADJOINT ZONE FLUX RESULTS
POUT   PRINTS FLUX, POWER DENSITY, NEUTRON DENSITY
NBAL   PRINTS NEUTRON BALANCE
            CALLS SOBL, SKER
SOBL   CALCULATES NEUTRON BALANCE SCATTERING DATA
FISS   WRITES FISSION SOURCE INTERFACE (FISSOR)
            CALLS SKER
BSQS   CALCULATES BUCKLINGS IN 3-D PROBLEMS
PNDN   CALCULATES POWER AND NEUTRON DENSITY
            CALLS POUT, SKER
PTVL   GETS DATA FOR SUBROUTINE PTZF
PTZF   WRITES FLUXES FOR 2 ZONES ON RZFLUX FOR DEPLETION
FLXW   WRITES FLUX INTERFACE DATA FILE
            CALLS POUT, SKER
SAV1   SPECIAL DATA OUTPUT IN BCD FORM
            CALLS SAV2, SAV4, SAV6
SAV2   SPECIAL DATA OUTPUT IN BCD FORM (GEODST)
            CALLS SAV3
SAV3   SPECIAL DATA OUTPUT IN BCD FORM (GEODST)
SAV4   SPECIAL DATA OUTPUT IN BCD FORM (PWDINT)
            CALLS SAV5
SAV5   SPECIAL DATA OUTPUT IN BCD FORM (PWDINT)
SAV6   SPECIAL DATA OUTPUT IN BCD FORM (RTFLUX)
            CALLS SAV7
SAV7   SPECIAL DATA OUTPUT IN BCD FORM (RTFLUX)
```

THE PERTURBATION ROUTINES

```
QOUT  EDITS SPACE POINT IMPORTANCE MAPS
RTUB  WRITES INTERFACE FILE PERTUB
            CALLS SKER
MRPT  CALCULATES CHANGE IN KEFF DUE TO SIGMAS
PERO   EDITS PERTURBATION INTEGRALS
BBB2   PERTURBATION UTILITY ROUTINE
BBB1   PERTURBATION UTILITY ROUTINE
            (FOR ALL EXCEPT 1-ROW STORED MODE)
JERT   PERTURBATION CONTROL
            CALLS JAFA,JIFE,JUFY,PERO,JAPS,RTUB,QOUT,SKER,JGET
JAFA   SETS UP INPUT/OUTPUT FILES FOR PERTURBATION CALCULATION
JIFE   CALCULATES BASIC PERTURBATION INTEGRALS
JUFY   CALCULATES TRANSPORT PERTURBATION INTEGRALS
            CALLS BBB1,BBB2
JAPS   CALCULATES SPACE POINT IMPORTANCE MAPS
            CALLS JMAP
JMAP  CONTROLS EDIT OF IMPORTANCE MAPS
            CALLS QOUT
```

(CONT)

```
JGET   GETS DCONS (FOR 1-ROW STORED MODE)
PERT   PERTURBATION CONTROL
            CALLS DAFA,LIFE,TUFY,PERO,MAPS,RTUB,QOUT,SKER
DAFA   SETS UP INPUT/OUTPUT FILES FOR PERTURBATION CALCULATION
LIFE   CALCULATES BASIC PERTURBATION INTEGRALS
TUFY   CALCULATES TRANSPORT PERTURBATION INTEGRALS
            CALLS BBB1,BBB2
MAPS   CALCULATES SPACE POINT IMPORTANCE MAPS
            CALLS PMAP
PMAP  CONTROLS EDIT OF IMPORTANCE MAPS
            CALLS QOUT
```

SPECIAL ROUTINES

```
GETCOR ASSEMBLY LANGUAGE ROUTINE TO ALLOCATE CORE DYNAMICALLY FOR
       THE VARIABLY DIMENSIONED ARRAYS AT RUN TIME
FRECOR ASSEMBLY LANGUAGE ROUTINE TO FREE CORE ALLOCATED BY GETCOR
ERRSET   SUPPLIES THE LEVEL OF ERROR STOPS TO THE SYSTEM
```

LABEL COMMON BLOCKS

```
CNTRL
VCTRL
MGMTIO
IOUNT
AFLUY
AOSUB
LIMTS
ADRES
FSWAP
DEASU
COMSAM
USRID
```

END OF SECTION 201

Section 203: Transferring Data

To facilitate any changes which might be required to the method of data transfer between memory and auxiliary storage, the routines REED and RITE with known functions have been used. REED transfers data from auxiliary storage into memory, RITE moves data from memory onto auxiliary storage. These transfers are made in relatively large blocks of binary data, always under the guise of 4-byte IBM floating point short word, often mixed type.

Sequential Access

A record is kept of the access position of each logical unit in the service routine. Upon any request for a data transfer operation, the access position for that unit is checked with the reference record number provided. If properly positioned, the transfer is made with a Fortran READ or WRITE statement. If not properly positioned, repositioning is done to a higher record number or a rewind is done and repositioning done from the start. (The backspace capability is not used; trouble with this technique has simply caused us an inordinate amount of trouble locally and on conversion to distant facilities, and has been a costly penalty in analysis effort on projects.) Thus for transfers which are made sequentially, the tasks are performed directly.

It is noted that the technique implemented may discourage carrying an access position from one routine to another. This practice is generally deemed to be undesirable, that is, to read to some point in a data file in one routine and then continue reading in another routine, because it restrains sequencing routes. The access position data is carried in an array in a labeled common block in the service routines and not accessed in the primary coding nor tinkered with.

REWIND capability is provided. Also there is protection against reading data which has not been written, especially useful for the debugging phase of program development. An END OF FILE is usually placed on the unit after it has been written by a special call. The position flags for the units accessed sequentially are initially set to zero; an attempt to access data before it has been written will cause an error message edit, but not an abort.

Direct Access

It is true that all data transfers could be made in either the direct access mode or the sequential access mode by repositioning. However, we find generally that when data is moved sequentially, sequential access is the most efficient. The multiple repositioning associated with accessing records out of order is a serious penalty when sequential access is used on many systems. The solution to this problem with storage on disc units is to carry a record accounting in the operating system and transmit a single positioning order, the direct access mode. In the direct access by record mode, only fixed length, unformatted records are moved.

To allow both sequential and direct access modes of operation in a program requires identification of the mode for each logical unit. This could be done by (1) using different routines or set flags in the program, (2) defining a range of logical units for one type of access, or (3) providing hidden flags. We reject (1) as inhibiting interchange, and (2) as an undesirable and not a sufficiently general scheme. The scheme selected allows the same logical unit to be used one way at one point in a calculation and another way later; for example, a file containing the flux values may be blocked with all values at one group for the iterative calculation in a record, but only one plane of data in a record for the calculation of regular, adjoint flux integrals.

For efficent execution, parameters such as record length must be made problem dependent. This is done with routines adapted locally which are accessed for "opening" prior to use.

Capability to use a local implementation of the IBM system data transfer routines is implemented (outside of Fortran), available on option.[a] We have not found a significant gain in total computer efficiency, but clock time for a run is significantly reduced when large records of data are involved (many points on a plane) by using this scheme, and buffer space is eliminated.

Core-to-Core

An implementation was adopted which allows data files to be stored in memory (extended core) if space allows. In this mode, the data is simply moved from one location to another directly.

Asynchronous Operations

The routines provide for asynchronous operations to allow overlap of input/output operations with calculation. Special routines are required on a computer to provide this capability locally.

Multilevel I/O Hierarchy

Capability in the routines provides for storage of data in an extended (slow) core and input/output with both disc and memory. This capability admits simulation and testing of procedures programmed for hierarchy storage by assigning the slow memory space to fast memory.

---

[a]W. A. Rhoades, "The FBSAM Data Transmission Package for IBM 360/370 Computers," ERDA Report, ORNL-TM-5199 (January 1976).

The Input/Output Service Routines

We expect compromises to be made in the cooperative inter-installation effort for a scheme to admit a variety of input/output techniques to be used in a code. This code uses an early implementation of such capability developed locally. Documentation is provided in ORNL-5158, but the concerned programmer should refer to the Fortran listing of the routines actually distributed. The capability included in these, including both the local implementation of the computer system data input/output routines (non-Fortran) and the defaulting of files to memory, is operational in the present version of this code.

END OF SECTION

Section 204: Input/Output File Requirements

In this discussion, the data files which must be resident on auxiliary storage devices are identified as Standard Interface files[a] or scratch files. It is assumed that the scratch files are each assigned a logical unit number in the range 21-65 and units 1-9 are reserved for special purposes. Our normal logical devices are unit 5 input and unit 6 output. Unit 4 is used to contain a collection of the results for export (BCD, tape). (Assignments may be simply changed at the front end of the code to satisfy other local requirements at another installation.)

Interface Data Files Used

GRUPXS — Group ordered microscopic cross sections

GEODST — Geometry description

NDXSRF — Nuclide to cross section referencing data

ZNATDN — Zone nuclide atomic densities

SEARCH — Search data (required only for search)

FIXSRC — Fixed source (required for a fixed source problem only)

RTFLUX — Total neutron flux (if supplied and for successive cases)

ATFLUX — Total adjoint neutron flux (if supplied)

RZFLUX — Zone average total neutron flux (for successive cases)

Interface Data Files Generated by Option

RTFLUX — Total neutron flux

ATFLUX — Total adjoint flux

RZFLUX — Zone average total neutron flux

PWDINT — Point power density

GEODST — Geometry description upon dimension search

---

[a]Version III Specifications, LASL report, LA-6280-MS; see remarks about files SEARCH and FIXSRC on page 204-24.

NDXSRF — Nuclide to cross section referencing data upon dimension search

ZNATDN — Zone nuclide atomic densities upon concentration search

FIXSRC — Fixed source result

PERTUB — Regular, adjoint flux integrals

RSTRTR — Data for problem restart

FISSOR — Special Fixed Source Data

Scratch Data Files by Unit Number

21	Macroscopic scattering cross sections
22	Principal macroscopic cross sections
23 (Direct access)[a]	Equation coupling constants in space, normally not used
24 (Direct access)	Total neutron flux
27 (Direct access)	Flux Copy
28 (Direct access)	Flux Copy
29 (Direct access)	$\nabla \cdot J$ times volume (current in the P_1 sense)
40 (Direct access)	Equation constants
41	Fixed source
42	Fission source
43	Total source
44	Neutron balance data
45	Miscellaneous[b]
46	Miscellaneous
47	Search data, misc.

---

[a]Unless noted otherwise, files are accessed sequentially; by direct access is meant write and read of disc files at random by record.

[b]By miscellaneous is meant that these files are generally used to store different information at different stages of a calculation, but the required storage space is usually not large relative to those for which requirements are given in detail.

48	Miscellaneous
49	Point volume data
50, 51, 52	Cross section data
53	Mesh data

Certain files contain a large fraction of the data to be stored. Note that the product of the record length and number of records is the total amount of data to be stored in a file for direct access.

Let J = points in a row

I = number of rows in a plane

L = number of planes

K = number of groups

W = 1 for long-word machines, 2 for short word

R = 0 for one-dimensional, 2 for two-dimensional, 4 for three-dimensional cases

H = 1 for hexagonal, 0 otherwise

M = number of zones (m refers to zone)

A record on unit 40 (or 23 when required) contains the following data for a row or a plane of points: total loss terms including leakage, regions, element volumes, left leakage constants, top and bottom leakage constants, front and back leakage constants, extra leakage constants for hexagonal geometry data terminated as appropriate for few-dimension problems.

The primary cross sections are carried on units 21 and 22 as follows, where M refers to the number of zones and K to the number of groups, N to the number of black absorber zones, and I the number of dimensions.

Units	Record Length (Words)	Number of Records	Notes
23	[3 + W(1+2H)](J+1) + RJ	ILK	Needed only for the "row-stored" mode (see Section 103).
24,27,28,29	WJI	LK	
40	(R+W)JI + (2+H)JI + (1+H)(J+L) + H	LK	For "plane-stored" mode only.
40	(3+W+H)JIL + (1+H)(J+I)L + JI + HL	K	For "mesh-stored" mode only.
40	{[3 + W(1+2H)](J+1) + RJ} I	LK	For the "multilevel data transfer" mode only.
41	WJI	L	
42	WJI	L	
43	WJI	L	
44	WMK	2	
45	WJI	L	
46[a]	WJI	L	
47	WMK	1	
48	WMK	K	
49	WJ	IL	
50-53	Variable but small	Variable	

[a]For the case when the initial fluxes are read from the standard interface RTFLUX, number of records is LK.

Unit	Record Length	Number of Records	Contents
21	M[N(k)]	K	Inscattering $\sum_s^0(k' \to k,m)$; for the P_1 calculation, the data for each k follows the $\sum_s^0$ data in a separate record, increasing the number of records to 2K, $D(k,m)\sum_s^1(k' \to k,m)$
22	MK	1	Fission source distribution $\chi(m,k)$
	MK	1	Sink term $\sum_a(m,k) + D_\perp B_\perp^2(m,k)$
	MK	1	Buckling loss $D_\perp B_\perp^2(m,k)$
	MK	1	Production $\nu\sum_f(m,k)$
	MK	1	Search production $\nu\sum_p(m,k)$
	MK	1	Search absorption $\sum_q(m,k)$
	MK	1	Energy per unit flux W(m,k)
	MK	1	Reciprocal velocity Z(m,k)
	2K	1	Inscatter range, location of in-group term N(k),NJ(k)
	N	1	Black absorber zone list, if N > 0
	M	1	Zone volumes V(m)
	K	1	Number of inner iterations, if I > 1
	K	1	Spectral radius, if I > 1
	K	1	Overrelaxation factors, if I > 1
	MK	1	Removal cross sections (only with P_1 treatment)
	MK	1 to 4	Diffusion coefficients by zone, as well as the coordinate-direction dependent values when available from GRUPXS except with P_1 treatment
	2J+2I +2L+3	1	Distances to flux points and fine mesh interval interfaces

Unit	Record Length	Number of Records	Contents
	7K	1	External and internal boundary condition constants.
	MK	1	$\Sigma a(m,k)$ fissile
	MK	1	$\Sigma c(m,k)$ fertile

It should be noted that microscopic cross sections are used in a group-ordered form. A processor code block is required to recast the data into this form from a reference broad-energy-group library in the nuclide-ordered format defined by the specification for file ISOTXS.

Code-Dependent Data Files

Figure 204-1 shows the content of special interface files CONTRL, PERTUB, RSTRTR, and FISSOR. Also shown are the contents of the BCD file on unit 4 used to transfer data to other installations.

CONTRL is a file containing code module control instructions in records.

PERTUB is generated by otpion by the code and contains the basic perturbation integrals.

RSTRTR is a restart file which is written by option and may be supplied to the code to continue a previous calculation.

FISSOR is a fission source interface file written on option.

Also, certain data is placed on the end of the file RZFLUX for recovery of iteration information when successive problems are solved, as in depletion calculations. This file also will contain local flux values when used for auxiliary exposure calculations. Additional data is also placed in a record at the end of file FIXSRC when generated by the VENTURE code for subsequent recovery and use.

FIGURE 204-1. SPECIAL DATA FILE SPECIFICATIONS

```
C*********************************************************************
CN          DATE 3-15-77
C
CF          CONTRL
C
CE          CODE-BLOCK-DEPENDENT DATA UNDER CONTROL OF THE DRIVER
C*********************************************************************

CS           A FILE IDENTIFICATION RECORD ALWAYS FIRST
CS          THE FOLLOWING ARE CONTROL DATA RECORDS, ONE FOR EACH CODE
CS          DATA BLOCK, LENGTH 101*MULT+100 WORDS, 201 LONG, 302 SHORT
CS
CS          RECORD NAME    CODE BLOCK (MODULE)            REQUIREMENT
CS          -----------    -------------------            -----------
CS            PROINS       (PROBLEM INFORMATION)          ALWAYS FIRST
CS            DVRINS       (MODULE DRIVING INFORMATION)   ALWAYS
CS            XCPINS       CROSS SECTION PROCESSOR      AS NEEDED
CS            DTNINS       NEUTRONICS (VENTURE)         AS NEEDED
CS            RRTINS       REACTION RATE                AS NEEDED
CS            BLANK        (CLOSURE)                      ALWAYS LAST
CS          MUCH OF THE DATA IN THE INDIVIDUAL INSTRUCTION RECORDS IS
CS          NOT DEFINED, IT BEING RESERVED FOR FUTURE USE AND DEFINITION
C
C-------------------------------------------------------------------
CR          FILE IDENTIFICATION
C
CL    HNAME,(HUSE(I),I=1,2),IVERS
C
CW          3*MULT + 1
C
CD    HNAME          FILE NAME (A6) 'CONTRL'
CD    HUSE           USER IDENTIFICATION (A6)
CD    IVERS          FILE VERSION NUMBER
C
CN    MULT           1 FOR LONG WORD, 2 FOR SHORT WORD MACHINES
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          PROBLEM INFORMATION
C
CL    PROINS, (XX(I),I=1,100), (IX(I),I=1,100)
C
CW    101*MULT + 100
C
CD    PROINS         PROBLEM INFORMATION DATA IDENTIFIER (6HPROINS)
CD    XX(1-24)       PROBLEM OR CASE TITLE (A6)
CD    XX(25)         USER LABEL (JOBNAME) FOR INTERFACE DATA FILES (A6)
CD    XX(26)         USER LABEL (DATE) FOR INTERFACE DATA FILES (A6)
C
C-------------------------------------------------------------------
```

(CONT)

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C-----------------------------------------------------------------------
CR          MODULE DRIVING INFORMATION
C
CL    DVRINS, (XX(I),I=1,100), (IX(I),I=1,100)
C
CW    101*MULT + 100
C
CD    DVRINS          MODULE DRIVING INFORMATION IDENTIFIER (6HDVRINS)
CD    XX(1-100)       RESERVED
CD    IX(1)           PRIMARY MEMORY ALLOCATION, WORDS
CD    IX(2)           RESERVED
CD    IX(3)           RESERVED
CD    IX(4)           MAXIMUM BLOCK SIZE FOR DIRECT ACCESS DATA FILES,
CD                        WORDS, BEST VALUE DEPENDS ON SEVERAL THINGS
CD                        INCLUDING DISC TRACK LENGTH, OVERRIDE THE
CD                        AUTOMATED PROCEDURE ASSIGNMENT IF NON-ZERO
CD    IX(5)           TOTAL PROCESSOR TIME ALLOWED FOR THE RUN, MINUTES
CD    IX(11)          STAND-ALONE FLAG -
CD                        0 - MODULES ARE ACCESSED IN A TRUE MODULAR SENSE
CD                        1 - MODULES ARE ACCESSED AS IF EACH IS A
CD                            STAND-ALONE CODE (NOT RECOMMENDED)
C
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          CROSS SECTION PROCESSOR INSTRUCTIONS
C
CN    THIS DATA REQUIRED BY THE CROSS SECTION PROCESSOR
C
CL    XCPINS, (XX(I),I=1,100), (IX(I),I=1,100)
C
CW    101*MULT + 100
C
CD    XCPINS          CROSS SECTION PROCESSOR DATA IDENTIFIER (6HXCPINS)
CD    XX(1-100)       RESERVED
CD    IX(1-2)         RESERVED
CD    IX(3)           OPTION ON INPUT CROSS SECTION FILE PROCESSING
CD                        0 - NO PROCESSING REQUIRED
CD                        1 - GENERATE NEW NUCLIDE-ORDERED FILE FROM
CD                              THE FILE OR FILES HAVING FORMAT IX(5)
CD                              (REQUIRES INTERFACE FILE CXSPRR FOR
CD                              ADDITIONAL INFORMATION)
CD    IX(4)           OPTION TO GENERATE A GROUP-ORDERED FILE FROM
CD                        A NUCLIDE-ORDERED FILE
CD                        0 - NO
CD                        1 - YES
CD    IX(5)           FORMAT OF INPUT CROSS SECTIONS FOR IX(3) EQ 1
CD                        0 - NUCLIDE-ORDERED FILE
CD                        1 - CITATION CROSS SECTION SETS
CD                        2 - MERGE TWO NUCLIDE-ORDERED FILES
```

(CONT)

```
CD     IX(6)          OPTION ON PRINCIPAL CROSS SECTION DATA
CD                        FOR IX(4) EQ 1
CD                        0 - RETAIN ALL DATA
CD                        1 - REDEFINE (N,GAMMA) CROSS SECTION TO BE
CD                              THE CAPTURE CROSS SECTION = (N,GAMMA) +
CD                              (N,ALPHA) + (N,P) + (N,D) + (N,T) - (N,2N)
CD     IX(7)          OPTION ON SCATTERING DATA FOR IX(4) EQ 1
CD                        0 - RETAIN ALL DATA
CD                        1 - RETAIN THE TOTAL SCATTERING ONLY
CD     IX(8)          OPTION ON SCATTERING ORDER FOR IX(4) EQ 1
CD                        0 - RETAIN ALL DATA
CD                        N - RETAIN ORDERS UP TO (N-1) ONLY
CD     IX(9)          OPTION ON SCATTERING RECORD BLOCKING FACTOR
CD                        FOR IX(4) EQ 1
CD                        0 - NSBLOK = 1
CD                        N - NSBLOK = N, IF (NISO/N)*N EQ NISO,
CD                              OTHERWISE NSBLOK = NISO
CD                              WHERE NISO IS THE NUMBER OF NUCLIDES
CD     IX(10)         OPTION TO COMPUTE THE TOTAL SCATTERING MATRIX
CD                        FROM THE COMPONENTS FOR IX(4) EQ 1
CD                        TOTAL = ELASTIC + INELASTIC + N2N
CD                        (THIS MUST BE DONE IF THE GRUPXS FILE IS TO BE
CD                         USED BY VENTURE AND THERE IS NO TOTAL
CD                         SCATTERING DATA PRESENT)
CD                        0 - NO
CD                        1 - YES
CD                        2 - YES AND MULTIPLY N2N SOURCE BY 2.0
CD     IX(11)         OPTION TO CREATE ISOTOPE MIXTURES AFTER PROCESSING
CD                        SPECIFIED BY IX(3) AND IX(5), IF ANY
CD                        0 - NO
CD                        1 - YES (REQUIRES INTERFACE FILE CXSPRR FOR
CD                              ADDITIONAL INFORMATION)
CD     IX(12-22)      RESERVED
CD     IX(23)         OPTION TO EDIT LATEST NUCLIDE-ORDERED FILE
CD                        0 - NO
CD                        1 - YES
CD     IX(24)         OPTION TO EDIT GROUP-ORDERED FILE
CD                        0 - NO
CD                        1 - YES
CD     IX(25-100)     RESERVED
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           NEUTRONICS INSTRUCTIONS
C
CL     DTNINS, (XX(I),I=1,100), (IX(I),I=1,100)
C
CD     DTNINS              NEUTRONICS CONTROL IDENTIFIER, A(6)
CD     XX(1)               REFERENCE REAL TIME, DAYS
CD     XX(2)               MACHINE TIME ALLOWED FOR SOLUTION, MIN
CD                           (ITERATION TERMINATED IF TIME EXCEEDED)
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(CONT)

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CD     XX(3)                CYCLE TIME IN MINUTES TO WRITE RESTART DATA
CD                             NOT DONE IF 0, ALWAYS DONE AT END IF NON-ZERO
C
CN           NOTE THAT VARIABLES NOT DEFINED ARE RESERVED FOR LATER USE
C
CD     XX(4)                POWER LEVEL OF REACTOR, WATTS THERMAL
CD                           IF 0, NORMALIZATION IS TO ONE SOURCE NEUTRON
CD                           (WATT-SEC/FISS DEFAULTED TO 3.2E-11 IF ZERO)
CD     XX(5)                ENERGY CONVERSION FACTOR, FISSION TO THERMAL
CD     XX(6)                FRACTION OF REACTOR TREATED
CD     XX(7)                SPECIFIED MULTIPLICATION FACTOR FOR SEARCH IF
CD                            NON-ZERO
CD     XX(8)                SPECIFIED OVERRELAXATION COEFFICIENT IF NON-ZERO
CD     XX(9)                ESTIMATE OF THE EIGENVALUE FOR CHEBYCHEV
CD                            ACCELERATION ON OUTER ITERATIONS
CD     XX(10)               ESTIMATE OF THE LOWER LIMIT OF THE SPECTRUM OF
CD                            EIGENVALUES FOR CHEBYCHEV ACCELERATION
CD     XX(11)               CONVERGENCE CRITERIA ON INTEGRAL QUANTITIES
CD                             MAXIMUM RELATIVE CHANGE ON OUTER ITERATION
CD     XX(12)               CONVERGENCE CRITERIA ON LOCAL OR POINT VARIABLES
CD                             MAXIMUM RELATIVE POINT FLUX CHANGE ON OUTER
CD                             ITERATION (.00005)
CD     XX(13)               CONSTANT BUCKLING VALUE WHICH OVERRIDES THE DATA
CD                             IN GEODST FILE IF NON-ZERO
CD     XX(14) - XX(100)     RESERVED
C
CD     IX(1)                INDICATOR THAT THE CODE BLOCK HAS INPUT DATA
CD                             NOT CONTAINED IN THE STANDARD INTERFACE FILES
CD                              OTHER THAN THIS BLOCK OF DATA IF .GT.0
CD     IX(2)                RESTART OPTIONS-  RESTART USING DATA FROM AN
CD                             OLD CASE IF .GT. 0, REQUIRES SPECIAL RESTART
CD                             DATA FILE
CD     IX(3)                REFERENCE COUNT ON PROBLEMS (CYCLE NUMBER)
CD     IX(4)                FORMULATION OPTIONS
CD                           VENTURE, MESH CENTERED FINITE-DIFFERENCE
CD                            0- DIFFUSION THEORY
CD                            1- SIMPLE P1 APPROXIMATION
CD                           VANCER, MESH EDGE (2- AND 3-D SLAB INFO SHOWN )
CD                            0,1 SELECTED DEFAULT
CD                            2- LINEAR FINITE DIFFERENCE (8, 10 NEIGHBORS)
CD                            3- EXTENDED TAYLOR SERIES (8, 10 NEIGHBORS)
CD                            4- LINEAR FINITE ELEMENT (8, 10 NEIGHBORS)
CD                            5- SIMPLE TAYLOR SERIES (8, 10 NEIGHBORS)
CD                            6- USUAL FINITE DIFFERENCE (4, 6 NEIGHBORS)
CD                            7- COMPROMISE (8, 10 NEIGHBORS)
CD                            8- COMPROMISE (4, 6 NEIGHBORS)
CD                            9- COMPENSATED DIFFERENCE (4, 6 NEIGHBORS)
CD     IX(5)                TYPE OF PROBLEM
CD                              0- DETERMINE SOURCE MULTIPLICATION FACTOR
CD                              1- SEARCH PROBLEM (FILE OF SEARCH DATA IS
CD                                 REQUIRED, SEE OPTION IX(10))
CD                              2- FIXED SOURCE PROBLEM
CD                              3- ADJOINT PROBLEM ONLY
CD                              4- BUCKLING SEARCH
CD                              5- PROMPT MODE ALPHA CALCULATION, 1/V SEARCH
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CD     IX(6)          ADJOINT PROBLEM OPTIONS
CD                        0 - NO ADJOINT PROBLEM TO BE DONE
CD                        1 - EIGENVALUE TYPE PROBLEM
CD                            (NORMALLY FOLLOWING A FORWARD PROBLEM)
CD                        2 - FIXED SOURCE TYPE PROBLEM
CD     IX(7)          OPTION TO USE THE LOCAL IMPLEMENTATION OF THE
CD                      OPERATING SYSTEM DATA TRANSFER ROUTINES
CD                      (REQUIRES MEMORY SPACE)
CD     IX(8)          OPTION TO FORCE DATA HANDLING MODE (FOR TESTING)
CD                      -1   OPTION TO TERMINATE IF MEMORY ALLOCATION
CD                           IS TOO SMALL FOR EFFICIENT EXECUTION (THE
CD                           SPACE PROBLEM CANNOT BE STORED IN TWO-
CD                           DIMENSIONS OR ENOUGH PLANES OF DATA CAN
CD                           NOT BE STORED TO AVOID EXCESS TRANSFER
CD                           IN THREE-DIMENSIONS)
CD                      0- AUTOMATED TO MINIMIZE INPUT/OUTPUT
CD                      1- BASE PROBLEM CORE CONTAINED
CD                      2- SPACE PROBLEM AT EACH ENERGY CONTAINED
CD                      3- ONE ROW CONTAINED IN CORE
CD                      4- ONE OR MORE SPACE PLANES CONTAINED IN CORE
CD                      5- MULTIPLE ROWS STORED FOR TWO DIMENSIONAL
CD                      6- MULTI-LEVEL DATA TRANSFER
CD     IX(9)          OPTIONS ON FLUX INITIALIZATION
CD                      -1 SET ALL FLUX VALUES EQUAL
CD                       0 AUTOMATED PROCEDURE
CD                       1 POINT ENERGY MODEL, COSINE IN SPACE
CD                       2 USE AVAILABE SCALAR FLUX FILE
CD     IX(10)         IDENTIFIES SEARCH DATA IN SEARCH FILE, IX(5)=1
CD     IX(11)         IDENTIFIES SECONDARY SEARCH DATA IN SEARCH FILE
CD                      TO BE USED IF CONSTRAINTS FOR FIRST SET ARE
CD                      NOT SATISFIED, AND SECOND SEARCH IS TO BE DONE
CD     IX(12)         SPECIFIES THAT A 2-D (OR 1-D) PROBLEM IS TO BE
CD                       SOLVED FOR THIS PLANE (OR ROW) OF A 3-D
CD                       (OR 2-D) DESCRIPTION IF NON-ZERO
CD     IX(13)         ORDER IN THE CROSS SECTION FILE OF THE DIRECTION
CD                      DEPENDENT TRANSPORT CROSS SECTION TO BE USED
CD                      FOR THE FIRST CORRDINATE DIRECTION (USUALLY 0)
CD     IX(14)         DITTO, SECOND COORDINATE DIRECTION
CD     IX(15)         DITTO, THIRD COORDINATE DIRECTION
CD     IX(16)         INSTRUCTION NORMALLY EXERCISED BY CONTROL MODULE
CD                      TO INFORM THE NEUTRONICS MODULE TO RECOVER
CD                      DATA FOR INITIALIZATION FROM FILES RZFLUX AND
CD                      RTFLUX
CD     IX(17)         FORCE KEFF. CALC. BY SOURCE RATIO IF GT 0
CD     IX(18)         FISSION SOURCE DISTRIBUTION FUNCTION OPTION
CD                      0- SET VALUES TO BE USED (SAME IN EACH ZONE)
CD                      1- REGION DEPENDENT VALUES TO BE USED
CD     IX(19)         FISSION SOURCE DISTRIBUTION NORMALIZATION OPTION
CD                      0- LEAVE UNNORMALIZED
CD                      1- NORMALIZE EACH SET TO SUM TO UNITY
CD     IX(20)         CONSTRAINT ON OUTER ITERATIONS(MAX ALLOWED)
CD                      (SET BY THE CODE IF NOT SPECIFIED)
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CD     IX(21)              INNER ITERATION OPTION
CD                           0- USE AUTOMATED PROCEDURE(RECOMENDED)
CD                           N- REFERENCE NUMBER OF INNERS = N
CD                            SET BY THE CODE IF NOT SPECIFIED
CD                              (IF 1 .LE. N .LE. 4, CHEBYSHEV ACCELERATION
CD                              WILL NOT BE DONE ON OUTER ITERATIONS
CD                              AS THE AUTOMATED PROCEDURE)
CD     IX(22)              OPTION TO REESTIMATE OVERRELAXATION FACTORS BY
CD                          L1 NORM FOR ZERO SOURCE PROBLEM, SPECIAL INNER
CD                          ITERATIONS ARE DONE (MAKE LARGE TO OVERRIDE
CD                         THE AUTOMATED PROCEDURE WHICH EMPLOYS THIS)
CD     IX(23)              INITIALIZATION OPTIONS FOR PROCEDURES, CHOICE OF
CD                           OVERRELAXITION COEFFICIENTS AND ITERATIONS
CD                           -2  DONT DO ONE-DIMENSIONAL CALCULATION
CD                                FOR INITIALIZATION
CD                           -1 DONT USE 1-D OVERRELAXATION COEFFICIENTS
CD                           0- USE AUTOMATED PROCEDURE, SOLVES 1-D PROBLEM
CD                              CHEBYSHEV COEFFICIENTS ON OUTER ITERATIONS
CD                              IF THE NUMBER OF INNERS IS .LT. 5
CD                              EXCEPT WHEN CHEBYSHEV FLUX ON OUTERS
CD                           1- SAME AS 0 BUT DO NOT CHEBYSHEV
CD                              OVERRELAXATION COEFFICIENTS
CD                           2- FIX THE NUMBER OF INNER ITERATIONS
CD                           3- FIX NUMBER OF INNERS, NO CHEBYSHEV
CD                           4- FIXED INNERS AND INITIAL COEFFICIENTS
CD                           5- FIXED INNERS AND COEFFICIENTS, NO CHEBYSHEV
CD                           6- SAME AS 4 BUT DONT USE 1-D COEFFICIENTS
CD                           7- SAME AS 5 BUT DONT USE 1-D COEFFICIENTS
CD     IX(24)              INNERITERATION SWEEP ORDER
CD                           -1 NORMAL ORDERED
CD                            0 AUTOMATED (SIGMA-1 IF AVAILABLE, USUALLY)
CD                            1 SIGMA-1 ORDERED IF AVAILABLE
CD     IX(25)              OUTER ITERATION CHEBYCHEV ACCELERATION OPTIONS
CD                           .LT. 0 START AT THIS ITERATION
CD                           0- USE AUTOMATED PROCEDURE
CD                           1- APPLY ONLY AFTER THE FIRST EXTRAPOLATION
CD                           2- APPLY CONTINUOUSLY FROM THE START
CD                           3- DONT APPLY THE PROCESS
CD                           .GT.100- THE PROCESS IS STARTED AT ITERATION
CD                              IX(25)-100 USING AN L1 NORM EIGENVALUE
CD     IX(26)              ASYMPTOTIC OUTERITERITION EXTRAPOLATION OPTIONS
CD                          -1 SINGLE ERROR MODE ONLY
CD                           0- USE AUTOMATED PROCEDURE
CD                           1- SINGLE ERROR MODE USING DATA FOR ALTERNATE
CD                              ITERATIONS
CD                           2- NOT ALLOWED
CD                           3- WE ARE TRYING TO FIGURE OUT WHAT THIS DOES
CD     IX(27)              FORCED DELAY IN ASYMPTOTIC EXTRAPOLATION
CD                            N- NOT ALLOWED FOR THIS MANY OUTER ITERATIONS
CD                            (IF NEGATIVE, A FORCED PROCEDURE MAY BE
CD                            EXECUTED EARLIER)
C
CN         EDITS GENERALLY ARE NOT DONE WHEN FLAG IS ZERO
C
CD     IX(28)              OPTION FOR CONDENSED EDIT (TERMINAL) IF .GT. 1
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CD      IX(29)          OPTION TO EDIT THE PRINCIPAL MACRCSCOPIC
CD                        CROSS SECTIONS BY ZONE
CD      IX(30)          OPTION TO EDIT THE MACROSCOPIC SCATTERING
CD                        CROSS SECTIONS BY ZONE
CD      IX(31)          OPTIONS ON ITERATION DATA EDITS
CD                        -1- NO EDITS DURING ITERATION
CD                        0, OR 1- PRIMARY OUTER ITERATION DATA ONLY
CD                        2- GETS DETAILS EDITED FOR TESTING
CD                        3- REQUESTS EXTENDED EDIT FOR DEBUGGING
CD      IX(32)          OPTION TO EDIT OVERALL NEUTRON BALANCE BY GROUP
CD      IX(33)          OPTION TO EDIT NEUTRON BALANCE BY ZONE
CD      IX(35)          OPTION TO EDIT SCALAR NEUTRON FLUX BY POINT
CD      IX(37)          OPTION TO EDIT ZONE-AVERAGE FLUX BY GROUP
CD                      IF .GT. 1, ALSO EDIT THE ZONE,GROUP ADJOINT FLUX
CD      IX(38)          OPTION TO EDIT POWER DENSITY MAP BY INTERVAL
CD      IX(39)          OPTION TO EDIT POWER DENSITY TRAVERSES THRU PEAK
CD      IX(40)          OPTION TO EDIT NEUTRON DENSITY MAP (1/V FLUX
CD                         WEIGHTING)
CD      IX(41)          OPTION TO EDIT NEUTRON DENSITY T-AVE-SES
CD      IX(42)          OPTION TO EDIT SCALAR ADJOINT FLUX
CD      IX(44)          OPTION TO EDIT ATOMIC DENSITIES WHEN SEARCHING
CD                         0- NO EDIT
CD                         1- MINIMUM EDIT AT END
CD                         2- MAXIMUM EDIT DURING CALCULATION
CD      IX(45)          PERTURBATION OPTIONS - IF NEGATIVE, FILES RTFLUX
CD                         AND ATFLUX ARE SUPPLIED AND NO NEUTRONICS
CD                         CALCULATION IS DONE - OTHERWISE THE REGULAR
CD                         AND/OR ADJOINT SOLUTION IS OBTAINED AS
CD                         SPECIFIED ABOVE AND EITHER FLUX FILE NOT
CD                         GENERATED MUST BE SUPPLIED
CD                        0- NO PERTURBATION CALCULATION
CD                        1- CALCULATE AND EDIT BASIC REGULAR*ADJOINT
CD                           FLUX INTEGRALS EXCEPT TRANSPORT
CD                        2- ALSO CALCULATE AND EDIT TRANSPORT INTEGRALS
CD                           (REQUIRED FOR COMPLETE PERTURBATION EFFECT)
CD                        3- ALSO EDIT MACROSCOPIC ABSORPTION CROSS
CD                           SECTION SPACE POINT IMPORTANCE MAP
CD                        4- ALSO EDIT MACROSCOPIC PRODUCTION CROSS
CD                           SECTION SPACE POINT IMPORTANCE MAP
CD                           PLUS ABS-PROD MAP
CD                        5- ALSO EDIT 1/V SPACE POINT IMPORTANCE MAP
CD      IX(46)          EDIT RESULTS FOR A 100 PERCENT CHANGE IN MACRO
CD                         CROSS SECTIONS, ONLY IF IX(45).NE.0
CD      IX(47)          OPTION TO WRITE POINT FLUX VALUES FOR EXPOSURE
CD                       (EXERCISED ONLY IF IX(53) .GT. 0)
CD                        .GT. 0  WRITE DATA FOR POINTS IN THIS ZONE
CD                        -1 WRITE ONLY THE SPECTRUM FOR THE POINT WHERE
CD                           THE POWER DENSITY IS A MAXIMUM INITIALLY
CD                       -2 WRITE DATA FOR THE POINTS IN THE ZONE WHERE
CD                           THE POWER DENSITY IS A MAXIMUM INITIALLY
CD                        -3 WRITE ONLY THE SPECTRUM FOR THE POINT WHERE
CD                           THE FIRST GROUP FLUX IS A MAXIMUM INITIALLY
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CD                          -4 WRITE DATA FOR THE POINTS IN THE ZONE WHERE
CD                              THE FIRST GROUP FLUX IS A MAXIMUM INITIALLY
C:                           .LT.-4  WRITE SPECTRUM FOR THIS MESH POINT
CD     IX(48)              ANOTHER ZONE NUMBER FOR WHICH THE POINT FLUX
CD                           VALUES ARE TO BE WRITTEN FOR EXPOSURE IF .GT. 0
CD     IX(49)              OPTION TO EDIT THE DIRECT CONTRIBUTION TO CHANGE
CD                         IN CONVERSION RATIO FROM UNIT CHANGE IN FERTILE
CD                           CAPTURE AND FISSILE ABSORPTION (MACROSCOPIC)
CD     IX(51)              OPTION TO WRITE THE POINT SCALAR FLUX FILE
CD                             0- NO
CD                             1- REWRITE THE LATEST VERSION OF AN OLD FILE
CD                                (IF THERE IS NONE, WRITE A NEW ONE)
CD                             2- WRITE NEW FILE
C
CN          OPTIONS ABOVE ARE TYPICAL FOR EACH FILE COVERED BELOW
C
CD     IX(52)              OPTION TO WRITE THE POINT FISSION SOURCE FILE
CD     IX(53)              OPTION TO WRITE ZONE-AVERAGE SCALAR FLUX FILE
CD     IX(54)              OPTION TO WRITE POINT POWER DENSITY FILE
CD     IX(55)              WRITE THE CONVERSION RATIO ADJOINT IMPORTANCE
CD                           FIXED SOURCE FILE (ALWAYS ADDS A FILE OR TWO)
CD                         .GT.0- WRITE COMBINED FILE (HAS NEGATIVE DATA)
CD                         .LT.0- WRITE TWO FILES, ALL POSITIVE
CD     IX(56)              OPTION TO WRITE THE ZONE POWER DENSITY FILE
CD     IX(57)              OPTION TO WRITE THE ADJOINT ZONE AVERAGE FLUX
CD                             FILE AZFLUX
CD     IX(58)              OPTION TO WRITE SCALAR ADJOINT FLUX FILE
CD                           APPLICABLE ONLY IF AN ADJOINT PROBLEM WAS DONE
CD     IX(59)              OPTION TO WRITE PERTURBATION INTEGRALS ON FILE
CD                           PERTUB. IX(45) MUST BE NON-ZERO. TRANSPORT
CD                           INTEGRALS ARE INCLUDED IF ABS(IX(45)) GT 2.
CD     IX(60)              OPTION TO WRITE SPECIAL FORMATTED DATA FILE
CD                           (LOGICAL 4) AT THE END OF A CASE - SEE SECTION 204
CD                           OF THE VENTURE REPORT
CD     IX(61)              A PLANE NUMBER AT WHICH ZONE AND GROUP BUCKLINGS
CD                           ARE TO BE CALCULATED
CD     IX(62)              A SECOND PLANE NUMBER FOR THE BUCKLING CALCULATION
CD     IX(63)              OPTION TO WRITE A POINTWISE FIXED SOURCE FILE
CD                             AS (DB**2) TIMES FLUX
CD     IX(70)              FORCE DATA TRANSFER IN INITIALIZATION (TO TEST
CD                           PROCEDURES)
CD     IX(73)              OVERRIDE DEFAULT OF FILES TO MEMORY (TO TEST
CD                           PROCEDURES)
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          REACTION RATE MODULE INSTRUCTIONS
C
CL     RRTINS, (XX(I),I=1,100), (IX(I),I=1,100)
C
CW     101*MULT + 100
C
CD     RRTINS          REACTION RATE MODULE DATA IDENTIFIER (6HRRTINS)
CD
CC     NOTE- UNDEFINED DATA ARE RESERVED FOR FUTURE USE.
CC     NOTE- THE VALUE OF ZERO IS A DEFAULT MEANING THAT THE OPTION TO
CC           PERFORM THE TASK IS NOT EXERCISED.  CONSIDERABLE DATA
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CC          HANDLING MAY BE INVOLVED AND MUCH PAPER PRINTED, SO CARE
CC          SHOULD BE TAKEN TO OBTAIN ONLY THOSE RESULTS NEEDED.
CC    NOTE- QUITE GENERALLY THE FILES -NDXSRF- AND -ZNATDN- ARE NEEDED
CC          AND USUALLY -GRUPXS-
CD    XX(1)          DESIRED POWER LEVEL IF NON-ZERO (USUALLY NEW)
CD    XX(3)          WEIGHTING FACTOR DISCUSSED BELOW
CD    XX(4)          WEIGHTING FACTOR DISCUSSED BELOW
C
CD    IX(3)          OPTION TO EDIT PROGRAMMER INFORMATION FOR DEBUGGING
CD    IX(6)          OPTION TO COMPUTE AND EDIT REACTION RATES,
CD                       INVENTORIES, AND POWER PRODUCTION
CC    NOTE- INDEPENDENT OF THE OPTIONS WHICH FOLLOW, SUMMARY TABLES
CC          ARE ALWAYS EDITED ON THIS OPTION
CD    IX(9)          OPTION TO EDIT BY ZONE AND SUBZONE FOR EACH UNIQUE
CD                       NUCLIDE NAME
CD                       1 - YES (WILL BE DONE ONLY IF THERE ARE
CD                                SUBZONES)
CC    NOTE- IN THIS EDIT, ZONE RESULTS EXCLUDE SUBZONE CONTRIBUTIONS
CD    IX(10)         OPTION TO EDIT BY ZONE FOR EACH UNIQUE NUCLEDE NAME
CD                       NOTE - ZONES WILL INCLUDE SUBZONE CONTRIBUTIONS
CD    IX(11)         OPTION TO EDIT BY ZONE CLASS FOR EACH UNIQUE
CD                       NUCLIDE NAME
CD    IX(14)         OPTION TO WEIGHT SUMMARY REACTION RATES BY NUCLIDE
CD                       ENERGY GENERATION
CD                       1- FISSION ENERGY ONLY
CD                       2- FISSION PLUS CAPTURE ENERGY
CD    IX(15)         OPTION FOR ADDITIONAL RESULTS WITH ALTERNATIVE
CD                       WEIGHTINGS (SUMMARY TABLES ONLY)
CD                       1- BY NET NEUTRON PRODUCTION (GENERATION MINUS
CD                          ABSORPTION)
CD                       2- BY CAPTURE RATE IF FERTILE AND ABSORPTION
CD                          RATE IF FISSILE
CD    IX(16)         REPEAT THE CALCULATIONS OF REACTION RATES INDICATED
CD                       ABOVE (IX(6).GT.0) USING FLUX, ADJOINT WEIGHTING
CD                       REQUIRING FILE -PERTUB-
C
CN          THE FOLLOWING ARE PRELIMINARY, NOT IMPLEMENTED
C
CD    IX(21)         OPTION TO EDIT REACTION RATE MAPS USING FILE -RTFLUX
CD                       .GT.0- SPECIFIES A PLANE OF A 3-D PROBLEM OR
CD                              A ROW OF A 2-D PROBLEM
CD                       -1-    THE PLANE OR ROW IS TO CONTAIN THE
CD                              LOCATION OF MAXIMUM POWER DENSITY
CD    IX(22)         MAP PRINCIPAL REACTION RATES FOR FISSILE NUCLIDES
CD                       1- ABSORPTION
CD                       2- ABSORPTION AND PRODUCTION
CD                       3- CAPTURE AND FISSION
CD                       4- CAPTURE, FISSION AND PRODUCTION PER
CD                          ABSORPTION
CD    IX(23)         MAP PRINCIPAL REACTION RATES FOR FERTILE NUCLIDES
CD                       1- CAPTURE
CD                       2- ABSORPTION ONLY
CD    IX(24)         MAP ABSORPTION RATES FOR NUCLIDES OF THIS CLASS
CD    IX(26)         REPEAT THE MAPPING WITH WEIGHTING ON ADJOINT FLUX
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CD                          USING FILE -PERTUB
CD     IX(31)          OPTION TO EDIT REACTIVITY COEFFICIENTS FOR UNST
CD                          CHANGES IN FISSILE NUCLIDE CONCENTRATIONS
CD     IX(32)          OPTION TO EDIT REACTIVITY COEFFICIENTS FOR UNIT
CD                          CHANGES IN FERTILE NUCLIDE CONCENTRATIONS
CD     IX(33)          OPTION TO EDIT REACTIVITY COEFFICIENTS FOR UNIT
CD                          CHANGES IN NUCLIDE CONCENTRATIONS OF THIS CLASS
CD     IX(37)          OPTION TO PRODUCE DELAYED NEUTRON PROPERTIES WITH
CD                          FLUX, ADJOINT WEIGHTING USING FILE -PERTUB- AND
CD                          -DLAYXS-
CD     IX(41)          OPTION TO COLLAPSE CROSS SECTIONS IN ENERGY, FILE
CD                          -ISOTXS-TO-ISOTXS- USING THE ENERGY STRUCTURE
CD                          GIVEN AS GROUP LOWER BOUNDS DESCENDING EV, DATA
CD                          IN ARRAY XX STARTING AT XX(21) TERMINATING WITH
CD                          A ZERO ENTRY FOR THE LAST GROUP
CD                          1- PRODUCE MACROSCOPIC CROSS SECTIONS FOR PSEUDO
CD                             DENSITY UNITY FOR EACH ZONE, FLUX WEIGHTED
CD                          2- PRODUCE ONE-TO-ONE NUCLIDE DATA ONLY FOR THE
CD                             ONES HAVING NON-ZERO CONCENTRATIONS WITH FLUX
CD                             WEIGHTING USING FILE -RZFLUX-
CD                          3- SAME AS 2 EXCEPT FLUX, ADJOINT WEIGHTING
CD                             REQUIRING FILE -PERTUB-
CD     IX(51)          OPTION TO GENERATE A DISTRIBUTED NEUTRON SOURCE FILE
CD                          -FIXSRC- USING FLUX FROM -RTFLUX-
CD                          1- TOTAL PRODUCTIONS FROM FISSION MULTIPLIED BY
CD                             XX(3) NORMALIZED TO A TOTAL OF XX(3)*XX(4)
CD                             IF XX(4) IS NON ZERO, XX(3) SET TO UNITY IF 0
CD                          2- TOTAL DELAYED NEUTRON SOURCE USING FILE
CD                             -DLAYXS-
CD                          3- ASYMPTOTIC DELAYED NEUTRON SOURCE USING THE
CD                             FAMILY OF LONGEST HALF LIFE (ASSUMES DISTINCT
CD                             ONE APPLIES) USING FILE -DLAYXS-
CD     IX(52)          OPTION TO GENERATE A ZONE-GROUP DISTRIBUTED SOURCE
CD                          FILE -FIXSRC- USING ZONE AVERAGE FLUX FILE
CD                          -RZFLUX- (SEE OPTIONS IMMEDIATELY ABOVE)
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          CICSURE
C
CL     BLANK1, (XX(I),I=1,100), (IX(I),I=1,100)
C
C
CD     BLANK1          END OF FILE IDENTIFIER (6H      ) OR (6HBLANK )
C
C-----------------------------------------------------------------------

CEOF
```

(CONT)

```
C*****************************************************************************
CN          DATE 1-1-76 (REFERENCE TO 11-26-74)
C
CF         PERTUB
CE         PERTURBATION DATA - REGULAR AND ADJOINT FLUX INTEGRALS
C
C*********************************************************************


C-------------------------------------------------------------------
CR         FILE IDENTIFICATION
C
CL    HNAME,(HUSE(I),I=1,2),IVERS
C
CW          3*MULT + 1
C
CD    HNAME              HOLLERITH FILE NAME - PERTUB - (A6)
CD    HUSE               HOLLERITH USER IDENTIFICATION - (A6)
CD    IVERS              FILE VERSION NUMBER
C
CN    MULT          1 FOR LONG WORD, 2 FOR SHORT WORD MACHINES
C
C-------------------------------------------------------------------


C-------------------------------------------------------------------
CR          FILE REFERENCE INFORMATION
C
CL    BIGDAD,XK,CR,X1,NZONE,NGROUP,IND,N1,N2,N3,N4
C
CW    11
C
CD    BIGDAD             BIG-DADDY NORMALIZATION FACTOR
CD                          INTEGRAL  ADJOINT*CHI*FORWARD*NUSIGF/K
CD    XK                 MULTIPLICATION FACTOR (K-EFF)
CD    CR                 PRIMITIVE FISSILE CONVERSION RATIO
CD    X1                 ABSORPTION RATE IN FISSILE NUCLIDES
CD    NZONE              NUMBER OF GEOMETRIC ZONES
CD    NGROUP             NUMBER OF NEUTRON ENERGY GROUPS
CD    IND                OPTION FOR INCLUDING TRANSPORT INTEGRALS
CD    N1                 FLAG ON PROBLEM TYPES -
CD                         0- MEANING NO PROBLEMS WERE SOLVED, OR THEY
CD                            WERE EIGENVALUE PROBLEMS
CD                         1  IS ADDED TO THIS IF A FIXED SOURCE FORWARD
CD                            PROBLEM WAS SOLVED
CD                        10  IS ADDED TO THIS IF A FIXED SOURCE ADJOINT
CD                            PROBLEM WAS SOLVED
C     N2                 RESERVED FOR FUTURE USE
C     N3                 RESERVED FOR FUTURE USE
C     N4                 RESERVED FOR FUTURE USE
```

(CONT)

```
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
CR          INTEGRALS FOR PRODUCTION MACRO
C
CL     ((T(M,K),M=1,NZONE),K=1,NGROUP)
C
CW     NZONE*NGROUP
C
CD     T                    FLUX(K)*CHI(KK)*ADJOINT(KK), INTEGRAL OVER KK
CD                             AND VOLUME, DIVIDED BY THE MULTIPLICATION
CD                              FACTOR, VOLUME INTEGRALS
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR         FLUX, ADJOINT VOLUME INTEGRALS
C
CL     ((S(M,KK),M=1,NZONE),KK=1,NGROUP)
C
CW     NZONE*NGROUP, NGROUP RECORDS
C
CD     S                    FLUX(KK)*ADJOINT(K)  VOLUME INTEGRALS
CD                                (INTO GROUP K)
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          INTEGRALS FOR TRANSPORT
C
CC          PRESENT ONLY IF IND.GT.0
C
CL     ((D(M,K),M=1,NZONE),K=1,NGROUP)
C
CW     NZONE*NGROUP
C
CD     D                    FLUX(K)*ADJOINT(K)  VOLUME INTEGRALS
C-----------------------------------------------------------------------

CEOF

C***********************************************************************
CN          DATE 1-1-76 (REFERENCE TO 11-26-74)
C
CF          RSTRTR
C
CE          CODE-BLOCK-DEPENDENT RESTART DATA SAVED FOR RECOVERY
C
C***********************************************************************
```

(CONT)

```
C-------------------------------------------------------------------
CR          FILE IDENTIFICATION
C
CL     HNAME,(HUSE(I),I=1,2),IVERS
C
CW     3*MULT + 1
C
CD     HNAME               HOLLERITH FILE NAME - RSTRTR - (A6)
CD     HUSE(I)             HOLLERITH USER IDENTIFICATION(2A6)
CD     IVERS               FILE VERSION NUMBER
CD                           VERSION 1 RESERVED FOR VENTURE
C
CN     MULT           1 FOR LONG WORD, 2 FOR SHORT WORD MACHINES
C
C-------------------------------------------------------------------


C-------------------------------------------------------------------
CR          FILE REFERENCE INFORMATION
C
CL     NFI1,NFI2,NFI3,N1,N2,N3,N4,N5,NR1,NR2,L2
C
CW     11
C
CD     NFI1 - NFI3         FILE IDENTIFICATION FLAGS
CD     N1 - N5             RESERVED
CD     NR1                 NUMBER OF RECORDS OF TYPE 1 DATA
CD     NR2                 NUMBER OF RECORDS OF TYPE 2 DATA
CD     L2                  LENGTH OF ALL RECORDS OF TYPE 2 DATA
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          RECORD LENGTHS OF TYPE 1 DATA
C
CL     (NWIR(J),J=1,NR1)
C
CW     NR1
C
CD     NWIR(J)             NUMBER OF WORDS IN TYPE 1 DATA RECORD RECORD J
C
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          RESTART DATA RECORDS, TYPE 1
C
CL     (DARS(I),I=1,M)
C
CW     M, WHICH IS NWIR(J) FOR RECORD SEQUENCE J , NR1 RECCRDS
C
CD     DARS(I)             CODE DEPENDENT RECOVERY DATA ARRAY TYPE 1
```

(CONT)

```
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -


C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
CR          RESTART DATA RECORDS, TYPE 2
C
CL     (DARR(I),I=1,L2)
C
CW          L2, NR2 RECORDS
C
CD     DARR(I)            CODE DEPENDENT RECOVERY DATA ARRAY TYPE 2
C
C- - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -

CEOF

C***********************************************************************
CN          DATE 1-1-76 (REFERENCE TO 11-26-74)
C
CF          FISSOR
C
CE          FISSION SOURCE BY INTERVAL AND DISTRIBUTION FUNCTION
C
C***********************************************************************

C-----------------------------------------------------------------------
CR          FILE IDENTIFICATION
C
CL     HNAME,(HUSE(I),I=1,2),IVERS
CW          3*MULT + 1
C
CD     HNAME               HOLLERITH FILE NAME - FISSOR - (A6)
CD     HUSE                HOLLERITH USER IDENTIFICATION (A6)
CD     IVERS               FILE VERSION NUMBER
C
CN     MULT           1 FOR LONG WORD, 2 FOR SHORT WORD MACHINES
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          FILE REFERENCE INFORMATION
C
CL     TIME, POWER, KEFF, IM, JM, KM, NCY, NG, NZ
C
CW     9
C
CD     TIME                REFERENCE REAL TIME, DAYS
CD     POWER               POWER LEVEL FOR ACTUAL NEUTRONICS PROBLEM,
CD                              WATTS THERMAL
CD     KEFF                MULTIPLICATION FACTOR
CD     IM                  NUMBER OF FIRST DIMENSION FINE INTERVALS
CD     JM                  NUMBER OF SECOND DIMENSION FINE INTERVALS
CD     KM                  NUMBER OF THIRD DIMENSION FINE INTERVALS
```

(CONT)

```
CD     NCY                REFERENCE COUNT (CYCLE NUMBER)
CD     NG                 NUMBER OF ENERGY GROUPS
CD     NZ                 NUMBER OF ZONES
C
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR           FISSION SOURCE DISTRIBUTION FUNCTION
C
CL           ((CHIM(N,K),N=1,NZ),K=1,NG)
C
CW           NG*NZ
C
CD           CHIM(N,K)    SOURCE OF NEUTRONS IN GROUP K, ZONE N
C
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR           FISSION SOURCE VALUES
C
CL     ((PFS(I,J),I=1,IM),J=1,JM)
C
CW           IM*JM, KM RECORDS
C
C      PFS                FISSION SOURCE BY INTERVAL, NEUTRONS/SEC/CC
C
C-----------------------------------------------------------------------

CEOF


C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C
C
C         THE FOLLOWING DOCUMENTS HOW A SPECIAL FILE IS WRITTEN IN BCD
C         FOR TRANSMISSION OF THE MAIN RESULTS FROM A neutronics problem
C         TO ANOTHER INSTALLATION IN A SINGLE FILE, COMPLETE WITH THE
C         ESSENTIAL DOCUMENTING INFORMATION
C
C***************** DEFINITIONS ****************************************
C      IGOM          GEOMETRY
C      NZONE         NUMBER OF ZONES
C      NREG          NUMBER OF REGIONS
C      NZCL          NUMBER OF ZONE CLASSIFICATIONS
C      NCINTI        NUMBER OF FIRST DIMENSION COARSE MESH INTERVALS
C      NCINTJ        NUMBER OF SECOND DIMENSION COARSE MESH INTERVALS
C      NCINTK        NUMBER OF THIRD DIMENSION COARSE MESH INTERVALS
C      NINTI,IM      NUMBER OF FIRST DIMENSION FINE MESH INTERVALS
C      NINTJ,JM      NUMBER OF SECOND DIMENSION FINE MESH INTERVALS
C      NINTK,KM      NUMBER OF THIRD DIMENSION FINE MESH INTERVALS
C      IMBL          FIRST BOUNDARY INDICATOR ON FIRST DIMENSION
C      IMBR          LAST BOUNDARY INDICATOR ON FIRST DIMENSION
C      JMBT          FIRST BOUNDARY INDICATOR ON SECOND DIMENSION
C      JMBB          LAST BOUNDARY INDICATOR ON SECOND DIMENSION
C      KMBF          FIRST BOUNDARY INDICATOR ON THIRD DIMENSION
C      KMBR          LAST BOUNDARY INDICATOR ON THIRD DIMENSION
```

(CONT)

```
C     NBS          NUMBER OF BUCKLING SPECIFICATIONS
C     NBCS         NUMBER OF CONSTANTS FOR EXTERNAL BOUNDARIES
C     NIBCS        NUMBER OF CONSTANTS FOR INTERNAL BOUNDARIES
C     NZWBB        NUMBER OF ZONES WHICH ARE BLACK ABSORBERS
C     NTRIAG       TRIAGONAL GEOMETRY OPTION
C     NRASS        REGION ASSIGNMENT OPTION
C     NGOP         NOT USED
C     XMESH        COARSE MESH BOUNDARIES, FIRST DIMENSION
C     YMESH        COARSE MESH BOUNDARIES, SECOND DIMENSION
C     ZMESH        COARSE MESH BOUNDARIES, THIRD DIMENSION
C     IFINTS       NUMBER OF FINE MESH INTERVALS PER COARSE MESH
C                    INTERVAL, FIRST DIMENSION
C     JFINTS       NUMBER OF FINE MESH INTERVALS PER COARSE MESH
C                    INTERVAL, SECOND DIMENSION
C     KFINTS       NUMBER OF FINE MESH INTERVALS PER COARSE MESH
C                    INTERVAL, THIRD DIMENSION
C     VCLR         REGION VOLUMES
C     BSQ          BUCKLING VALUES
C     BNDC         BOUNDARY CONSTANTS
C     BNCI         INTERNAL BLACK BOUNDARY CONSTANTS
C     NZHBB        ZONE NUMBERS WITH BLACK ABSORBER CONDITIONS
C     NZC          ZONE CLASSIFICATIONS
C     NZNR         ZONE NUMBER ASSIGNED TO EACH REGION
C     MR           REGION ASSIGNMENTS TO MESH INTERVALS
C                    IF NRASS EQ 0  COARSE MESH
C                    IF NRASS EQ 1  FINE MESH (ALWAYS THIS OPTION)
C     TIME         REFERENCE REAL TIME
C     POWER        POWER LEVEL
C     VOL          VOLUME OVER WHICH POWER WAS DETERMINED
C     NCY          REFERENCE COUNT (CYCLE NUMBER)
C     PWR          POWER DENSITY
C     NDIM         NUMBER OF DIMENSIONS
C     NGROUP       NUMBER OF ENERGY GROUPS
C     ITER         OUTER ITERATION NUMBER AT WHICH FLUX WAS WRITTEN
C     EFFK         EFFECTIVE MULTIPLICATION FACTOR
C     FREG         REGULAR TOTAL FLUX
C*********************************************************************
C
C*********************************************************************
C
      READ(ISAV,1001)    (TITLE(I),I=1,24)
C
C*********************************************************************
C
C     START INTERFACE GEODST
C
      READ(ISAV,1002)    IGOM,NZONE,NREG,NZCL,NCINTI,NCINTJ,NCINTK,
     *                   NINTI,NINTJ,NINTK,IMBL,IMBR,JMBT,JMBB,KMBF,
     *                   KMBR,NBS,NBCS,NIBCS,NZWBB,NTRIAG,NRASS,
     *                   (NGOP(I),I=1,5)
      NCBNDI = NCINTI + 1
      READ(ISAV,1003)    (XMESH(I),I=1,NCBNDI)
      NCBNDJ = NCINTJ + 1
      READ(ISAV,1003)    (YMESH(J),J=1,NCBNDJ)
```

(CONT)

```
      NCBNDK = NCINTK + 1
      READ(ISAV,1003)    (ZMESH(K),K=1,NCBNDK)
      READ(ISAV,1002)    (IFINTS(I),I=1,NCINTI)
      READ(ISAV,1002)    (JFINTS(J),J=1,NCINTJ)
      READ(ISAV,1002)    (KFINTS(K),K=1,NCINTK)
      READ(ISAV,1003)    (VOLR(L),L=1,NREG)
      READ(ISAV,1003)    (BSQ(N),N=1,NBS)
      READ(ISAV,1003)    (BNDC(N),N=1,NBCS)
      READ(ISAV,1003)    (BNCI(N),N=1,NIBCS)
      IF(NZWBB.LE.0) GO TO 100
      READ(ISAV,1002)    (NZHBB(N),N=1,NZWBB)
  100 CONTINUE
      READ(ISAV,1002)    (NZC(M),M=1,NZONE)
      READ(ISAV,1002)    (NZNR(L),L=1,NREG)
      IF(NRASS.GT.0) GO TO 101
      II = NCINTI
      JJ = NCINTJ
      KK = NCINTK
      GC TO 102
  101 CONTINUE
      II = NINTI
      JJ = NINTJ
      KK = NINTK
  102 CONTINUE
      DC 103 K=1,KK
      DO 104 J=1,JJ
      READ(ISAV,1002)    (MR(I),I=1,II)
  104 CONTINUE
  103 CONTINUE
C     END INTERFACE GEODST
C
C*********************************************************************
C
C     START INTERFACE PWDINT
C
      READ(ISAV,1004)    TIME,POWER,VOL,IM,JM,KM,NCY
C     IM = NINTI
C     JM = NINTJ
C     KM = NINTK
      DO 105 K=1,KM
      DC 106 J=1,JM
      READ(ISAV,1003)    (PWR(I),I=1,IM)
  106 CONTINUE
  105 CONTINUE
C
C     END INTERFACE PWDINT
C
C*********************************************************************
C
C     START INTERFACE RTFLUX
C
      READ(ISAV,1005)    NDIM,NGROUP,NINTI,NINTJ,NINTK,ITER,EFFK,POWER
      DC 107 K=1,NINTK
      DO 108 N=1,NGROUP
```

(CONT)

```
      DO 109 J=1,NINTJ
      READ(ISAV,1003)    (FREG(I),I=1,NINTI)
  109 CONTINUE
  108 CONTINUE
  107 CONTINUE
C
C     END INTERFACE RTFLUX
C
C*********************************************************************
C
 1001 FORMAT(12A6)
 1002 FORMAT(12I6)
 1003 FORMAT(6E12.5)
 1004 FORMAT(3E12.5,4I6)
 1005 FORMAT(6I6,2E12.5)
C
C*********************************************************************
CEND OF THE FILE
C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C*C
```

SEARCH File Additions

The specification NRCH(1) > 0 is used to indicate that macroscopic cross sections are to be recalculated during a direct search. Option NRCH(2) indicates secondary search specifications (reference set) to be used if the specified constraints on the search eigenvalue are not satisfied using the primary search data.

FIXSCR File Additions

In the local implementation, a fixed source may be given by zone and energy. By setting IDIST = 2 and NDCOMP = NZONE (in the 1D record), the input processor will read a 10D record ((ZSOR (L,N),L=1, NDCOMP), N = 1, NGROUP), NZONE being the number of zones and NGROUP the number of groups.

END OF SECTION

Section 205: Overlay of Blocks of Program

For effective use of the computer memory, groups of subroutines must be brought from auxiliary storage when needed and laid over others no longer needed. Shown in Fig. 205-1 is a listing of the cards which are recommended for execution on an IBM machine to provide overlay instructions to the loader. The main program resides in memory along with any subroutines (and label common) not assigned to an overlay level. Control to the lowest level must be resident for return through the calling routines without input of program. Thus the specifications identify groups of subroutines along any access sequence, control passing to level D, then level E, etc. Blocks of program assigned ("inserted" at) the same level share storage; the storage requirement for program is the sum of the maximum requirements at each level.

FIGURE 205-1. PROGRAM OVERLAY STRUCTURE

THE FOLLOWING LISTING SHOWS THE COMMUNICATION THROUGH THE ROUTINES WITH TWO LEVELS OF OVERLAY, D AND E. IN ADDITION, THE FOLLOWING ROUTINES (AND LABEL COMMON BLOCKS) ARE IN THE ROOT SEGMENT.

MAIN,DRIV,DIFF,SKER,FERR,STOR,NROD,DOPC,SEEK,RITE,CRIT,TIMER,DEFILE
CLOSDA

```
OVERLAY LEVELD
INSERT VENT,IONO,CORE,CORI,CORP,GNAM,CORD,CORB,DDSP,DASU,JPRT
OVERLAY LEVELD
INSERT GETCOR,FRECOR
OVERLAY LEVELD
INSERT MAC1,MAC2,MAC3,MAC4,MAC5,MAC6,MACA,MACB,CHDM,SCAL
OVERLAY LEVELD
INSERT CON1,MSH0,NRCF,MSH1,CON2,CON3,CKCT,CON4,CON5,CON7,CON9,BNDY
INSERT MSH3,GEOQ
OVERLAY LEVELD
INSERT PHIA,PHI1,PHI2,PHI3,PHI4,PHI5,PHI6,PBND,PC2D,PC3D,EDBN,SDBN
INSERT PHI7,TOIP,QDBN,RDBN,GRXP,PAN1,PAN2
OVERLAY LEVELD
INSERT ORLX,ORIA,MUCK,ORLB,ORLC,ORLD,ORLE,ORLF,LAXR,LAXP,BATG,LUCK
INSERT ORLR,CCN6,RCOV
OVERLAY LEVELD
INSERT ADN1,ADN2,ADN3,DCID,DSDF,DIMS,AJDS,DIM1,DIM2,CMES,CHVL,DIM3
INSERT ZVRV,CRGV,FIRD,FLMH
OVERLAY LEVELD
INSERT COMC,LCAL,FLXR,FXSR,BSQV,AJNT,REV1,PROS,ZIO3
INSERT SAV1,SAV2,SAV3,SAV4,SAV5,SAV6,SAV7,FEFS
OVERLAY LEVELD
INSERT OUTR,BALC,ZINS,CHBF,CHEV,RDAB,XTRP,JUSB,ATED,FFGG,RDUE,RELX
INSERT FSOR,SSOR,PSOR,FLUX,LTRG,BHAV,OELX,NEWB
OVERLAY LEVELE
INSERT MUEX,ETR1,ETR2,SGDA
OVERLAY LEVELE
INSERT DOIN,BBES,WRES,PREC
OVERLAY LEVELE
INSERT FOU1,SCU1,POU1,INR1,LOU1,LEK1
OVERLAY LEVELE
INSERT FOU2,SCU2,POU2,INR2,LOU2,LEK2
OVERLAY LEVELE
INSERT FOU3,SCU3,POU3,INR3,LOU3,LEK3
OVERLAY LEVELE
INSERT FOU4,SOU4,POU4,INR4,LOU4,LEK4,QDUE,QELX,SOUX,J1C4
OVERLAY LEVELE
INSERT FOU5,SCU5,POU5,INR5,LOU5,LEK5,J1C5
OVERLAY LEVELE
INSERT FOU6,SOU6,INR6,DELX
OVERLAY LEVELE
INSERT FOUX,SCUY,POUX,INRX,LOUX,LEKX,SOUZ,J1CX
OVERLAY LEVELD
INSERT EDIT,POUT,NBAL,SOBL,FISS,FLXW,BSQS,PNDN,PTVL,PTZF,JINT
OVERLAY LEVELD
INSERT PERO,RTUB,MRPT,QOUT,BBB1,BBB2,EASU
OVERLAY LEVELE
INSERT PERT,TUFY,LIFE,DAFA,MAPS,PMAP
OVERLAY LEVELE
INSERT JERT,JUFY,JIFE,JAFA,JAPS,JMAP,JGET
```

END OF SECTION 205

Section 220: Conversion to Other Computers

The reference code is designed for a large-memory, short-word, IBM 360 model 360 or 370 machine. We anticipate another version of the code being made available for long-word machines, which should be obtained rather than attempt conversion. This discussion addresses aspects of the programming which must receive attention in converting between machines. Comment lines within the source deck identify specific locations in the source language where special action is required.

On an IBM machine, much of the calculation is done in double precision and certain data carried as long words. On long-word machines, this data should be carried as regular length and the associated double precision operations changed to single precision. This change is essential to minimize storage requirements. Alphanumeric characters are carried in the guise of real numbers (Hollerith) as A(6) requiring long-word storage on an IBM machine.

As a convenience for conversion, a multiplier is carried through the routines, MULT or NDP or LX(39), which must be 2 for an IBM machine and 1 for long-word machines. This multiplier adjusts the lengths of words for short-word storage and manipulations avoiding extensive reprogramming upon conversion.

The following basic changes are required for use on a long-word machine:

1. Remove all REAL*8 statements.
2. Supply single precision library functions, e.g., SQRT and EXP instead of DSQRT and DEXP.

3. Change all references to "Double Precision," as in function definition statements.
4. Change LX(39) to 1 from 2.
5. Change the apostrophes which delimit alphanumeric strings in FORMAT and DATA statements.
6. Replace the subroutine TIMER to provide information from the local system.

   ICLOCK -- gives cpu time

   ITTIME -- gives clock time

   MODEL -- gives computer model

   IDAY -- gives alphanumeric: Month-Day-Year

   ISTIME -- gives cpu time remaining

   JOBNUM -- gives alphanumeric: Job number

   IOLEFT -- gives the number of I/O's remaining

   TIME -- gives alphanumeric: time of day
7. Satisfy the data access, transfer requirements including the dynamic opening of the files with parameters which are problem dependent and defaulting the files to be resident by replacing the data handling service routines.
8. Provide local capability to allocate memory at run time, or fix the allocations for container arrays and communication.
9. Provide the necessary overlay structure.
10. The assembly language routines can only be used on compatible IBM machines (otherwise use the Fortran source decks).
11. Correct any discrepancies missed by the IBM compiler (and please report this information back to us).

Local system routines would be needed to satisfy items 6, 7, and 8, unless those supplied are compatible.

The code is used locally as a module of a computation system. Effecting stand alone capability should not be hard using those modules needed including input data processing capability. It should be most attractive to implement an equivalent modular system, either one-to-one with that in use at ORNL, or adapt the modules into another system.

In converting this code, consideration should be given to data storage and transfer requirements. If large problems are to be solved, even a large extended core cannot contain a set of the flux values, so they should be carried on disc. Some of the data is used frequently, so it needs to be carried in even a small memory; suggestions for partitioning the data are given in the source program on comment lines.

END OF SECTION

Section 225: The Data Handling Strategy

Utilization of a specific computer facility can be improved by carefully tailoring the procedure of calculation. Of critical importance in solving large problems are the details of transferring data to and from memory using auxiliary storage within any hierarchy. The available fast memory and slow memory must be allocated carefully, and judicious choices must be made between alternatives in blocking the data and transferring it between the individual storage devices. Modifications to the procedures employed in this code may be found desirable. However, the capability of a particular facility in regard to rates of data transfer and storage must be well understood, as well as the strategy employed in this code, if a modification will effect improvement. A description is given in this section of the strategy used in handling data.

Consider an internal point for one energy group in a three-dimensional multigroup problem. It is located on a row of points, several of these rows make up a plane of points, and the third dimension involves a series of planes. The points are carefully arranged so that in the usual orthogonal coordinate systems, each internal point has six nearest neighbors, two on the row, two on a column in the plane, and two in the adjacent planes. Space coupling yields equation constants relating the flux at the reference point with values at nearest neighbor locations. Given the pointwise fission and inscattering source values, and removal terms for absorption and outscattering, this space problem is partially resolved by inner iteration, recalculation of the individual flux values by applying the equations repeatedly over the mesh in an ordered fashion.

During each outer iteration the fission source is recalculated, and for the space problem at each energy group, the scattering source is recalculated. Thus, at any space point location, fission or scattering at any energy may produce a source at any other energy. A full scattering matrix is allowed which permits scattering from any group to any other group; however, often there is only downscatter. Thus, the calculation proceeds from the highest energy downward. Source neutrons may be produced by fission at any energy, but these are summed to give a single space array of the total fission source with distribution of this into the individual groups at each point in space.

In one of the modes of data handling, the flux values are stored on a direct access device with data for each plane stored in a direct access record, ordered by increasing plane number and then by increasing energy. Thus, the data is carried in the order needed for the inner iteration process at one energy. Then for the source calculation, they may be accessed one plane at a time over energy groups by skipping down through the file. The individual records may be accessed directly with a single repositioning of the disc head using the capability of the operating system to account for record access points. Upon reading or writing flux values, they are processed sequentially in the forward sense as much as possible to minimize the amount of disc head movement.

With one of the calculational procedures, one plane of flux data must be transferred into memory and the next operation involves writing out another plane of newly calculated flux data, not on adjacent planes. To realize efficient data handling, the last iterate and the present iterate flux values are carried in different files. This permits sequential

reading and writing. A third file is also carried because the outer iteration acceleration schemes need three successive iterate sets of the fluxes, and the calculation proceeds by alternating between the three direct access flux files.

The equation constants for space coupling and total loss are stored on disc as needed, initially calculated from nuclide concentrations and microscopic cross sections. This is a direct access file which permits efficient data access during iteration for whatever mode of data handling is selected.

The macroscopic scattering cross sections are blocked for all compositions and energy groups by inscattering group. Thus, the inscattering source calculation is done by sequential processing of this data, one record read for each energy group each outer iteration.

The primary data handling modes in the code are described below in the order of increasing amount of data transfer required. At the time this is written there are parallel routines to implement seven different procedures. The important ones are the space stored, the multirow stored and the multiplane stored mode with provision for multilevel storage transfers. The all-stored mode is little needed, especially with the capability to default key scratch files to memory and the ability to store the full flux file in memory when space allows in the space stored mode. The row-stored mode for three-dimensional problems is so hopelessly data transfer bound as to be generally an ineffective computer application. This modification will require a major restructuring of the code to realize all the gains desired regarding storage use and flow of a calculation.

All Stored Mode

For small problems, the equation constants, one set of flux values, and the necessary source values are stored in the computer memory. The calculation proceeds with very little data transfer. Special procedures are used for one-dimensional problems.

Space Stored Mode

For problems of moderate size, the equation constants, the flux values, and the necessary source values are stored in the computer memory for the space problem at one energy. Inner iteration is done with minimum data transfer, but the scattering data and flux values must be read for the source calculation. When the assigned memory space allows, a later version of the code may store all of the flux values in this mode.

Multirow Stored Mode

For two-dimensional calculations, in this mode the space problem at one energy is further partitioned to reduce the memory requirement. Data for several rows of fluxes are stored and inner iteration proceeds with the minimum amount of data transfer for a given problem using the least amount of memory necessary. This mode of data handling is a subset of that described in more detail below.

Multiplane Stored Mode and Multilevel Data Transfer Mode

In these modes, data for several planes of a three-dimensional problem are stored in fast memory or slow memory. Consider the array of mesh points normal to rows for an arbitrary number of columns and planes:

Column	1	2	3	4	5
Plane					
1	.	.	.	.	.
2	.	.	.	.	.
3	.	.	.	.	.
4	.	.	.	.	.
5	.	.	.	.	.
6	.	.	.	.	.

Each dot represents a row of points for which new inner iteration iterate estimates of the flux values will be obtained simultaneously. The calculation proceeds in such a way that the latest values are always used in the calculation in the normal ordered sense. That is, using the first subscript to refer to column and the second to plane, after fluxes for row $a_{1,1}$ are obtained, fluxes for rows $a_{1,2}$ and $a_{2,1}$ may be calculated. Considering that the calculation proceeds in order across the columns on each plane using the latest values of the fluxes obtained for the plane above and the column to the left, the process may be described as follows:

Plane	Iteration
1	1
2	1
1	2
3	1
2	2
1	3
4	1
3	2

Plane	Iteration
2	3
1	4

The procedure is as follows after it develops to the stage where n planes of data are stored:

Plane	Iteration
m	1
m-1	2
m-2	3
m-3	4
.	.
.	.
.	.
m-n-1	n-2
m-n	n-1
m-n+1	n

Completion of the procedure is as follows, where M is the total number of planes:

Plane	Iteration
.	.
.	.
M	n-3
M-1	n-2
M-2	n-1
M-3	n
M	n-2

Plane	Iteration
M-1	n-1
M-2	n
M	n-1
M-1	n
M	n

Storing the equation constants and source values for n planes and the flux values for n+2 planes, n inner iterations are done each full sweep with one access of equation constants, one access of old flux values, and one transfer of new flux values for each plane of the problem. If more inner iterations are done than the available storage allows in one sweep, the process is repeated. The amount of data transfer is minimized relative to computation with use of the minimum amount of memory for that problem which is too large to be handled in the more efficient modes above. Equation constants and also flux values are each separately blocked into one record for each plane. We may block more than one plane of flux values in one record when the amount of memory assigned allows this, and probably also the source, in an advanced version.

In the "multilevel data transfer" mode, data is moved from slow memory into fast memory in small blocks as needed.

One Row Stored Mode

To handle the largest possible problem in the minimum amount of memory, and yet solve for new values of the fluxes along a row, this mode of data handling treats only one row at a time. It applies only to the three-dimensional problem (the space stored mode satisfies

one-dimensional problem requirements and the multirow stored mode satisfies two-dimensional problem requirements). Storage is allocated for the necessary five rows of flux values and equation coefficients associated with one row. The calculation proceeds across the space mesh each inner iteration. Calculation on local computers in this mode show it to be very inefficient in total time due to the extreme data transfer penalty.

Defaulting Files to Memory

When the allocated memory space allows, individual data files are selectively defaulted to reside in memory as most effective in reducing data transfer, using the capability of the data transfer service routines.

Changing File Structure

The two places in this code where data transfer is a severe burden are the problem iteration and calculation of the regular, adjoint flux integrals. The code closes out the direct access files containing the flux values prior to performing the perturbation integrals and reopens them, often with a different blocking (changed record lengths). Such action of closing and reopening the same file may not be accomplished simply with some computer systems using certain modes of access. In this code the mode of data access is changed when necessary to perform the task with the local implementation of the data transfer service routines.

Input/Output Operations

The number of data Input/Output operations is approximated for three-dimensional problems by the following equation:

Let I = the average number of inner iterations in each group,

L = the number of planes treated simultaneously $\leq I$,

N = the number of outer iterations,

G = the number of groups,

B = the average actual inscattering bandwidth in groups,

P = the number of planes,

R = the number of rows,

Θ = the number of data Input/Output operations, disc-memory;

$$\Theta \simeq AG\left[500 + (N+2)\begin{cases}[2] & \text{all stored mode}\\ [8+B] & \text{space stored}\\ 4 + P\left[4\left(\frac{I+1}{L}\right) + B\right] & \text{multiplane stored}\\ 4 + PR[4I + 4 + B] & \text{one row stored}\end{cases}\right]$$

Where A is the average physical block size of the records, 1 for small problems but increasing with problem size. There is a direct dependence on the scattering band width not shown and Chebyshev acceleration adds 3 inside the square brackets. Typically $N \simeq 3PR/I$.

Our attempts to seek near optimum selection of the mode of data handling as dependent on problem size and local charging algorithms have not been successful. On the local computers it is often desirable to use a large amount of memory to minimize data input/output provided job turnaround is satisfactory.

END OF SECTION

APPLICATION INFORMATION

In the following sections, application information is supplied which is directed to the needs of the program users. They are referred to the introductory section of this report for a broad coverage of the function of this neutronics code block, and to the later sections for the computation algorithms. A user flow chart is presented in Figure 001-1 on page 001-3. Specific program considerations are given in Section 401. The discussion (disclaimer) on input data is in 403, error checking is covered in 405, and restart and recovery in Section 410. Section 440 addresses edited results and 450 the selected sample problems.

END OF SECTION

Section 401: Program Considerations

Application of this code will generally be more reliable the more intimately familiar the user is with its contents. In this section, certain specific aspects are addressed.

1) Major program options have been covered in Section 204. Generally, these provide unique functions with minimum interaction. Automated selection between procedures is provided as default, but reasonable care must be taken to obtain desired edits without excess printing and to control the generation of interface data files.

2) There are a few constraints on the range of values of the variables:

   a) Data used together cannot vary by more than perhaps $10^{\pm 6}$ and carry significance (atom density times cross section for the contributions to a macroscopic cross section from two or more nuclides),

   b) Data outside of the range of $10^{\pm 40}$ can be expected to produce chaos (power level for example), and

   c) Large step changes in the mesh spacing, say by a factor of 100, can cause difficulty in converging the iterative process to effect an acceptable solution.

3) All major data arrays are variably dimensioned and storage allocation is done dynamically. Problems have been solved which contained over 1000 points on a line and over 100 energy groups have been treated.

4) The larger the problem measured in terms of space-energy points, the more storage required or the more data which must be moved from auxiliary storage during the calculation. Several data handling modes are provided by parallel coding which require increasingly

less core space and more data handling. Automatic selection of the mode of data handling is done to effect efficient computer use. Actual storage requirements are a complicated function of the variables (the nature of the problem and its size) and the mode of data handling; these requirements are edited the first access of this neutronics code to provide information; this data could be collected as background by a user for reference.

5) The constants to which values are assigned within the code are generally limited to those covered by equations in the 700 series of Sections. Of course constants like pi are assigned values to machine significance.

6) It is assumed that dimensions are in centimeters, nuclide concentrations are in atoms/barn-cm, and microscopic cross sections are in barns/atom. Quite generally the product of nuclide concentration and microscopic cross section must yield a macroscopic value having units of cm^{-1} for consistency.

7) Man-machine interaction during execution is not allowed.

8) Microfiche output is now available locally and is recommended for the bulk of the printout.

9) The programming has been done in a way to avoid underflows, overflows, and divide by zero. We recommend that the operating system be allowed to detect such occurrences and terminate a calculation. Should such an event occur, a cause should be identified in the data supplied or traced to a deficiency in the program and rectified; it is probably due to inadequate data or possibly inconsistent instructions.

10) The use of special implementations of the computer system data transfer routines can indeed improve computer utilization, but some caution is in order regarding the user burden when the use has strange requirements and mysterious input/output errors may cause serious loss in productivity.

11) Except for nuclide concentration searches, the microscopic cross sections and nuclide concentrations are accessed only once; all subsequent calculations are done with the macroscopic cross sections calculated initially, including the estimate of the conversion ratio and the perturbation integrals and associated results.

END OF SECTION

Section 403: Input Data

The VENTURE code block does not read data from cards. All data for a calculation must be provided through the interface files. To supply the required data, a separate data processor must be used. The agreement reached in the code coordination effort was that all input data would be processed by a freeform format input data processor. An input processor developed at LASL[a] is in service as revised locally. Certain special input processors have been implemented and are in use locally which read data in a fixed-form format; these are included in the VENTURE code package. A separate document accompanying this code describes the punched card input required by these processors.[b]

END OF SECTION

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[a] G. E. Bosler et al., "LASIP-111, A Generalized Processor for Standard Interface Files," ERDA Report, Los Alamos Scientific Laboratory, LA-6280-MS (April 1976).

[b] D. R. Vondy et al., "Input Data Requirements for Special Processors in the Computation System Containing the VENTURE Neutronics Code," ERDA Report, ORNL-5229 (1976).

Section 405: Error Checking

An error discovered in the process of calculation is normally fatal and its cause is identified by an error message. Also, certain warning messages are printed, as to indicate lack of convergence if the maximum number of iterations or the allowed time is exceeded.

The fatal errors are one of the following types: those encountered in processing interface data files (error number 666), data transfer errors (error number 444), other interpreted errors (error number 555), and system detected errors. Hopefully the information printed will adequately describe the cause allowing corrective action to be taken.

For arithmetic operations where necessary, checks are made for overflows, underflows, and divide by zero. In a normal run, these types of errors should not occur; if one does occur, it is deemed fatal, and the cause should be traced and corrective action taken.

Input data processors contain a reasonable amount of checking to identify discrepancies and cause abort before calculations are done; still such a wide range of data is allowed that effort to confirm that correct data was supplied will be a good and usually necessary investment. For example, if a nuclide is assigned a concentration which is multiplied by the wrong power of ten, the wrong problem will be solved and incorrect interpretation of the results is probable.

END OF SECTION

Section 407: Implied Capability and Limited Implementation

Most of the interface data files used by the VENTURE code are formatted in accordance with standard definitions drawn up in an interinstallation effort. We have attempted to keep the coding up to date with the specifications through the period when these were being modified to satisfy requirements. We believe this implementation is a reasonable one in that the records are properly read and written within certain imposed restrictions and interpretations, at least compatible with the locally implemented modules which process input data. Still certain of these specifications imply capability which is rather general and only a subset of possible alternatives has been implemented in some instances. This section addresses this subject to identify what is actually available for application. The qualifications are given for each of the files for which restrictions apply.

Files ISOTXS and GRUPXS

The fission-source data by nuclide may be in the form of $\nu\sigma_f(g)\ \chi\ (g \rightarrow g')$. The macroscopic data is recast into the separable form $\nu\Sigma_f(g)$, $\chi(g)$ without carrying the full group to group dependence. Both the production term ($\nu\Sigma_f$) and the distribution function (χ) are made zone dependent. The P_1 data must contain the Legendre coefficient.

Only simple blocking of the scattering data is assumed, not certain possibilities which could lead to only partially filled data blocks.

File GEODST

At the time this is written, 30° and 90° triangular and (Θ-R-α) geometries have not been implemented. The user is cautioned to refer to the figures in Section 702 for actual orientations implemented; no other

options are available. Thus hexagonal geometry is treated as shown in the figure with the X and Y coordinates at 60° and limitations of the implementation usually require full core treatment when hexagonal assemblies are involved because usual symmetry conditions cannot be represented directly. The repeating (periodic) boundary with the opposite face is allowed only for the first boundary condition (IMBL), no others. The rotational symmetry condition (repeating, periodic, with the next adjacent face or along the face) is allowed only for the right boundary of the first dimension (IMBR) causing the point of rotation to be remote from the origin. No option which causes the geometry to be reduced to a triangle has been implemented; a triangular flux array would impact many of the interfacing data files, and a resolution of the difficulty has not been addressed. To blank out a volume of a problem, a material can be assigned to it along with the internal black absorber condition which applies the nonreturn boundary condition at the internal surfaces of this material.

File Search

The direct criticality search procedure is implemented for NMAXNP = 0. In this calculation, changes in macroscopic scattering and transport properties are ignored causing the result obtained to have some uncertainty due to this approximation, although automatic recalculation of the macroscopic cross sections is done to move toward a consistent solution. If NRCH (2) is >0, a secondary search will be done when constraints are not satisfied unless overridden by IX (11) in the DTNINS record in the CONTRL file; it is possible for the data to present a never-ending calculation, so care must be exercised in specifying more

than one set of search data, the instructions for their use, and the constraints for acceptable solutions.

END OF SECTION

Section 410: Restart and Recovery Procedures

A simple scheme is used to save the data required for restart and to access it for a subsequent calculation. On user request, a restart data file (RSTRTR described in Section 204) is generated periodically and also after a successful exit is made from the iteration procedure. Thus continuation is allowed only from some well-defined state of the calculation. A successful completion can occur only if (1) the convergence criteria specified are satisfied, (2) the limiting number of outer iterations is reached, or (3) automated procedure for assessing processor time or data transfers causes termination of the iterative process before system termination. The data is saved periodically on a cycle of processor time when so specified in the CONTRL file record.

The restart procedure is designed to effect the continuation of the iterative process terminated at some point in a previous computer run. The general procedure consists of recalculation of cross sections and equation constants from the data in the normal user input for the new computer run. Then the data saved from the prior run is accessed and the calculation continued. Certain initialization procedures are bypassed, as of the flux and the acceleration parameters. Some changes in the input data are allowed, some will be ignored, and others will cause abort; generally, no change is admissible which would cause changes in the locations of data in memory.

The data saved for restart consists of one iterate set of flux values and the principal data used in the iterative procedure. This data is sufficient for continuing the iteration, but not always sufficient to duplicate the process; acceleration schemes requiring

more than one iterate flux set will establish only after the necessary information has been accumulated.

For a usual restart, the following are necessary (see file CONTRL in Section 204):

1. The special restart data file must be available from a previous computer run (normally on tape for short-term storage).
2. Restart must be specified in the user input control data.
3. The number of outer iterations will often have to be increased to allow the desired convergence level to be satisfied.
4. Complete data file requirements must be satisfied normally requiring a full user input data deck (the same as for the original run), except that when such interface data files as GRUPXS have been generated and saved by other code blocks, they need not be regenerated.

Input data which cannot be changed because the data storage locations would be altered include the following; note that the saved iterate flux values will be used for the restart:

1. Number of dimensions and energy groups.
2. Number of mesh points along each coordinate and the number of material composition zones.
3. Mode of data handling during the iterative process, and normally the number of inner iterations which alters the use of data storage.
4. Basic problem type should not be changed (as from P_1 to P_0, usual eigenvalue problem to search or adjoint or fixed source).

Generally the previous procedure will be continued. Thus, the overrelaxation coefficients will be saved and used. However, such basic

control options as of use or not of Chebyshev acceleration on outer iterations may be changed.

Although it might be better to start the problem over, the following are allowed changes for restart:

1. Nuclide assignments and concentrations.
2. Microscopic cross sections.
3. The geometry (if both are orthogonal, not if one is hexagonal or triagonal), usually not desirable.
4. Boundary conditions excluding any change in the mesh-point assignments of internal black absorber.
5. The mesh point spacing and the assignment of points to regions and regions to zones.

Thus if a modest change is desired in any of the above data, it may be made.

Note also that any problem may be started from an existing data file of the flux values, RTFLUX, provided that the data in this file maps properly in space and energy. Remapping is allowed; when done, it is assumed that a regular expansion of the mesh points was made and a simple linear interpolation of flux values is done. This allows a many-point problem to be initialized from a coarse solution, and/or fewer groups to be treated.

Automatic initialization of successive neutronics problems is provided for by the control module in the system using the point flux values and information about the acceleration data.

END OF SECTION

Section 440: Edited Results

This discussion about the printout of data follows the editing order. All edits are preceded by brief headings for documentation. Major edits are under user control. The use of microfiche is recommended locally for primary edits.

Problem Documentation

Information is first edited which documents the neutronics problem and use of the computer and the program to solve it. Certain details can not be edited, a task assigned elsewhere, as to an input data processor or a file editor:

1. Zone (material) assignments to mesh points,
2. Nuclide concentrations and referencing data to effect concentration, microscopic cross section association,
3. Microscopic cross sections, and
4. The contents of certain data files which may be used.

The problem documentation information edited is:

1. Reference time obtained from the nuclide concentration file ZNATDN.
2. Certain problem documenting information including the type, independent variables and meshpoint locations.
3. Memory requirements with alternatives.
4. Data file space requirements.
5. Selected mode of data handling.
6. Microscopic group-ordered cross section file title.
7. Macroscopic cross sections on option.
8. Information about initialization and selection of acceleration procedures and parameters.

Iterative Results

Each outer iteration, information is extracted about the iterative process and is edited unless overridden by user option:

1. The calculation mode: normal, Chebyshev acceleration, single or double error mode or forced extrapolation.
2. Assessment of inner and outer iteration convergence.
3. The maximum relative flux change from one outer iteration to the next.
4. Estimates of the eigenvalue of the dominant outer iteration error vector.
5. The outer iteration acceleration factors including estimates of the parameters for extrapolation.
6. The total fission source.
7. The estimate of the eigenvalue of the problem (the multiplication factor or the search problem eigenvalue or the rebalancing factor for fixed source problems), determined from an overall neutron balance or other formulation in use.

In addition, information about the inner iteration behavior may be obtained as a higher level of edit.

Summary

When iteration on the neutronics problem is terminated, certain information is printed:

1. Estimate of the absolute relative flux error (associated with termination of the iteration process).
2. Reliability estimates of the multiplication factor.
3. Iteration parameters in use.

4. Gross neutron balance information (leakage, losses, productions, and power level normalization).
5. Processor and clock times used.
6. Fraction neutron loss to the search parameter for certain criticality search problems.
7. The peak first group flux in each zone and the flux spectrum where the peak first group flux occurs.
8. Peak power density, and peaks by zone.
9. Primitive conversion ratio and fissile consumption rate given the required data.
10. Energy spectrum and space map by zone of the adjoint flux when available.

Results from the Calculation

Edits of the following are available to the analyst on option:

1. Neutron balance data by energy group and zone.
2. Neutron balance by energy group.
3. Average flux by zone and group, regular and adjoint.
4. Point neutron flux values.
5. Power density map over space.
6. Power density traverses through the peak.
7. Neutron density map over space (given group velocity data).
8. Neutron density traverses through the peak.
9. Adjoint neutron flux values when calculated.
10. Calculated axial buckling values by traversed zone and group when requested on one or two planes.
11. Certain perturbation information given solutions for both a regular problem and an adjoint problem (neutron lifetime given group velocity

data) at the macroscopic cross section level (microscopic data is not reaccessed) including the estimates for 100% changes in the macroscopic cross sections and a simple assessment of uncertainty in k assuming equal relative uncertainties in the individual macroscopic cross sections.

Other Results

Other results may be produced by other modules in the system, such as integrated reaction rates and interpretation (fuel conversion ratio, etc.) by the reaction rate module.

END OF SECTION

Section 450: Sample Problems

A separate report is to be issued covering a number of sample problems since a few are inadequate to check conversion to another computer type than used in the development.

Three sample problems are presented here. The first two were taken from the set of problems for which reliable answers are known and were reported in ORNL-TM-3793, "Job Stream of Cases for the Computer Code CITATION." Thus, the descriptions for these problems in the form of input data for this older code are available as well as the results. A third problem involves both a nuclide search and a dimension search for a fast reactor.

Table 450-1 shows a list of the input for these problems as three "stacked" cases. An input data deck begins with the necessary job control instructions. These cause access of the catalog procedure and include override values of the parameters for allocation of data files to auxiliary storage, and supplemental information about files, as needed. The data set containing the codes is defined causing the driver routine to be placed in memory, where it remains resident, and is entered. The input instructions define a control module which is accessed by the driver to perform its initial role which requires input data instructions including a title, the space allocation for data arrays, and the calculational path through the code modules. Each block of input data used independently by a module contains a header card and is terminated by an END card. The input data are processed by the input processor.[a] Table 450-2 displays

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[a]Primary system documentation and input processor requirements are covered in ORNL-5158.

input data for two of the cases in the form required by the special processors[a] but not used for the edits reported herein.

Table 450-3 displays selected printout from the computer run. Since this code is active and undergoing continuing development, the output shown may not agree one-to-one with that produced by a specific version; however, the end results should be in very close agreement.

VENTURE Sample Problem 1

"Periodic Boundary in Theta-R Geometry, Case A4 with Black Absorber 24X20X3 Group, 1440 Points Stream of CITATION Cases ORNL 72"

This is an eigenvalue problem in ΘR geometry which is a 180° segment. Due to symmetry conditions, the problem can be solved with reflecting boundaries by reorientation (see Case A1 in the reference report). As oriented, the repeating, periodic boundary condition is required to account for net leakage across the surface, testing this option. The number of internal mesh intervals is shown along coordinates for each coarse interval and the spacing in centimeters. Note that the first coordinate in the user input specifications is Θ, not R. The "surface" at the start of columns does not exist (ΘR vanishes as $R \to 0$), but seems to in general purpose instructions.

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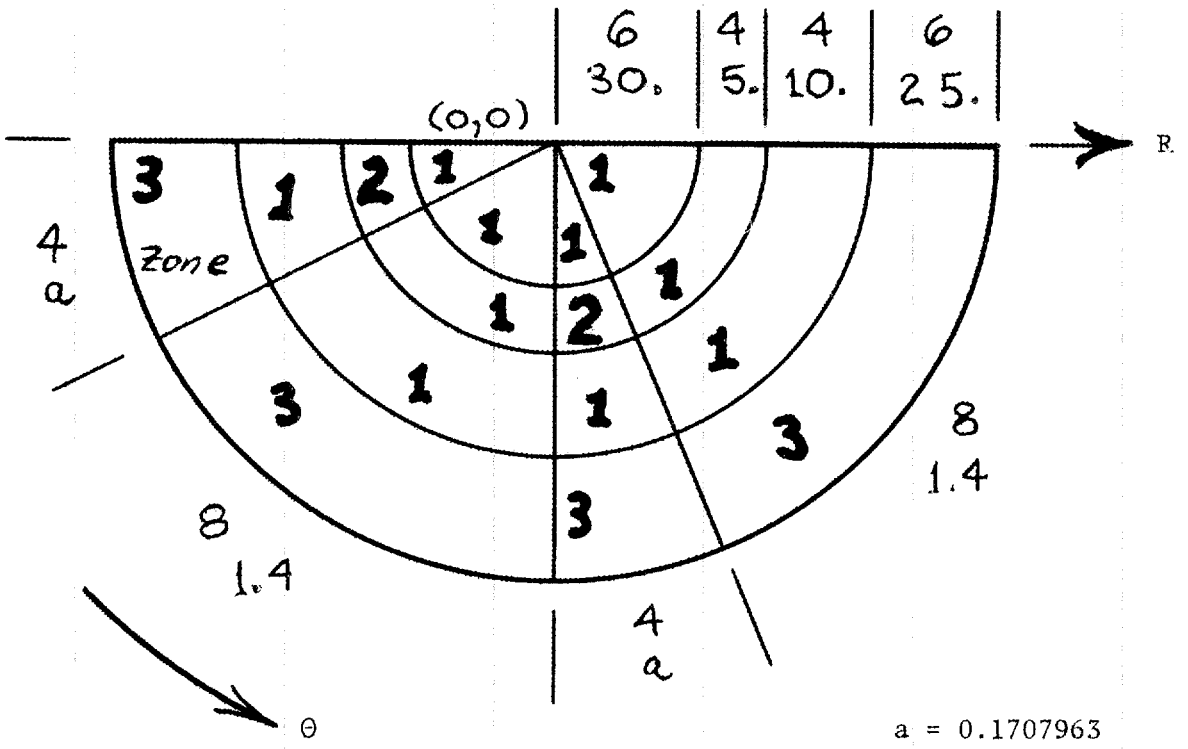
[a]Input requirements for special processors are given in ORNL-5229.



COARSE MESH SKETCH OF VENTURE SAMPLE PROBLEM 1.[a]

The macroscopic cross sections are provided in pseudo microscopic form to generate an ISOTXS cross-section file. The normal neutron flux eigenvalue problem was solved and then the adjoint problem using k_{eff} from the normal problem. The problem was solved with all data stored in the computer memory which minimizes input/output of data between memory and disc. The default procedure for such small problems contained in memory is one inner iteration at each group.

VENTURE Sample Problem 2

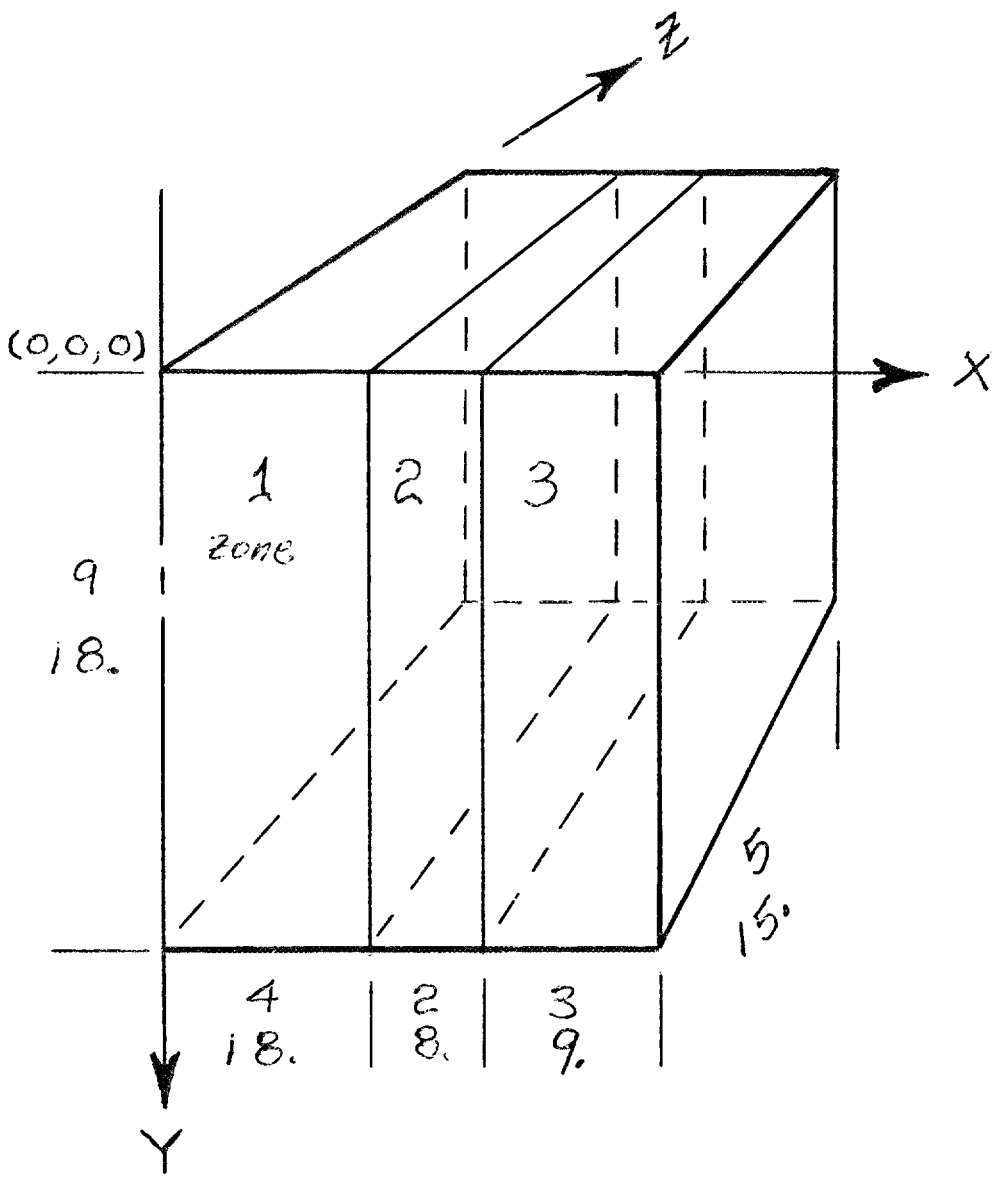
"3-D (X,Y,Z) Buckling Search (Old Whirlaway Case)

9x9x5x2 Group, 810 Points Stream of CITATION Cases ORNL 72"

This problem treats one-quarter of a reactor and involves three zones of different compositions. Again macroscopic cross sections are presented

[a]Origional erroneous material assignments have been corrected.

as pseudo microscopic, but here in the group-ordered file GRUPXS requiring no processing prior to use in the VENTURE code block. The problem is artificial in that the solution requested is the eigenvalue of a buckling search, not usually directly applicable to a three-dimensional problem. However there is simply a neutron loss rate equal to $DB_{\perp}^2 \phi$ over the problem. The eigenvalue problem was solved in the multiplane stored mode of data handling and also the following adjoint problem. Perturbation calculations are also done and space point importance maps are printed.



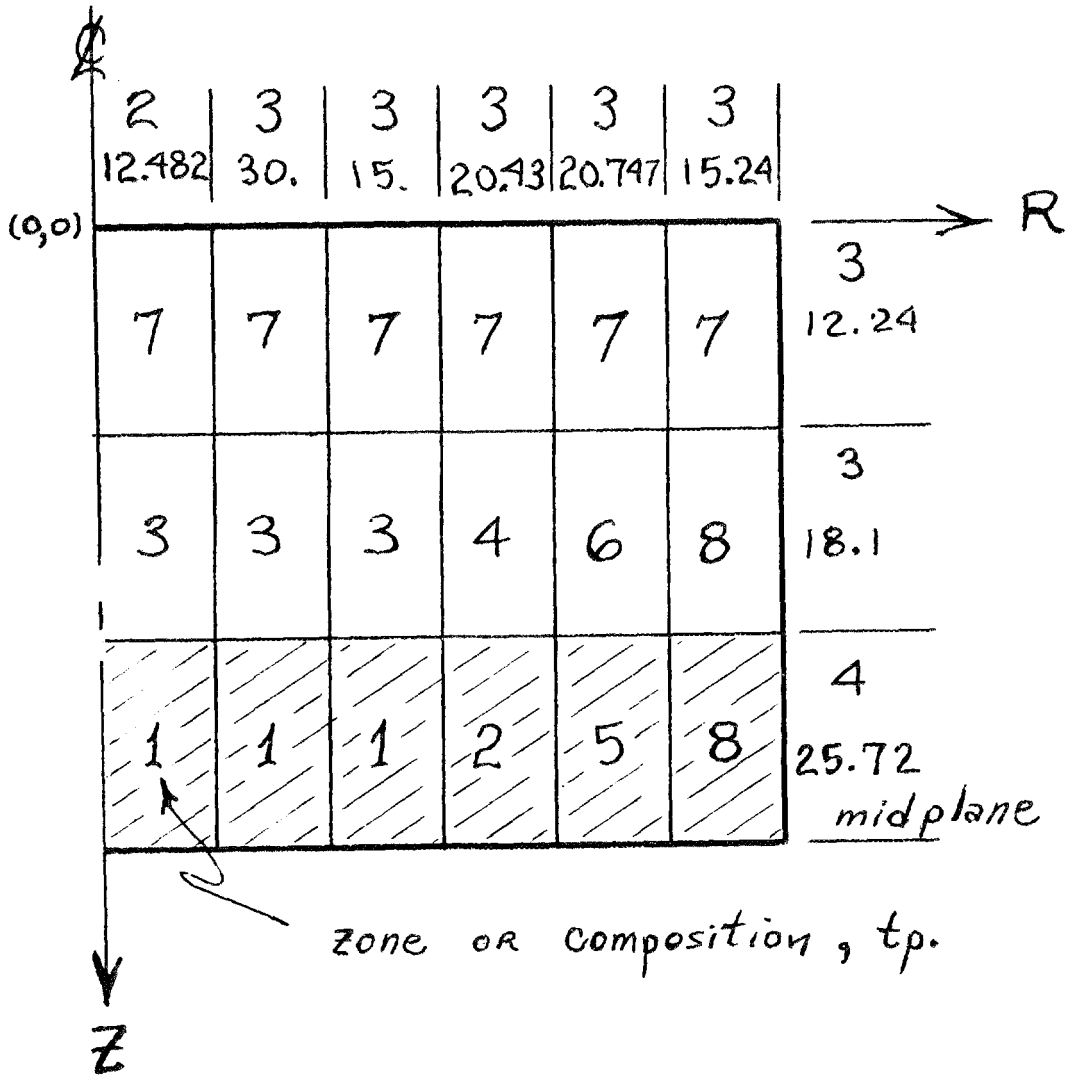
COARSE MESH SKETCH OF VENTURE SAMPLE PROBLEM 2.

VENTURE Sample Problem 3

"2-D 17 x 10 - 5 GROUP SEARCH PROBLEM

PRIMARY SEARCH = NUCLIDE (DIRECT) - SECONDARY SEARCH = DIMENSION"

This problem treats two-dimensional (R,Z) geometry. The input instructions for the problem first instruct the code to do a direct nuclide criticality search for a multiplication factor of 1.01 by adding a mixture of heavy metal (^{238}U, ^{239}Pu, ^{240}Pu). The solution is found to be 19% addition of material, exceeding the amount of material allowed to attain the desired multiplication factor. The input instructions further specify that all of the available material (100%) should be added and that a secondary search be done to attain the desired state. This second search is a dimension search in which the widths and heights of specific coarse mesh intervals, the shaded area shown in the sketch, are to be adjusted. The requirements for the desired state are determined and the adjoint problem is solved and perturbation calculation done. In addition, nuclide reaction rates are produced and printed. The geometric description of the problem is shown on the next page.



COARSE MESH SKETCH OF VENTURE SAMPLE PROBLEM 3.

Reference Test Problems

To support conversion of the VENTURE and related codes to other computers, a set of reference test problems has been selected. Input data for these problems and results are included in the code distribution package.[a]

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[a]ORNL/TM-5887

Table 450-1. Input Data for Sample Problems in the Input Processor Format

```
//USERID   JOB (CHARG),'ADRES-NAME COL 25-44',
// MSGLEVEL=(1,1)
//*CLASS   CPU95=03M,REGION=0350K,IO=025,LINES=19,CARDS=00
//STEP EXEC BCIDVENT,
// NB1=1,NB2=1,B1=3520,B2=15360,NX=2,NS=50,N1=100,
// N2=4,N3=13,N4=1,N5=6,N6=10,N7=1,N8=1,N9=2,N10=2,N11=3,N12=5,N13=2,
// N14=1,N15=10,N16=4,
// GOSIZE=350K
//GO.SYSIN DD *
=CONTROL1
*****************VENTURE RUN - SAMPLE PROBLEMS*********************
018000                                                          1
  1  6  7  1  7  1  6  7  9  0
END
 INPUT PROCESSOR DATA.
0V CONTRL
1D PROINS  /
* PERIODIC BOUNDARY IN THETA-R GEOMETRY, CASE A4 WITH BLACK ABSORBER   *
* 24X20X3 GROUP, 1440 POINTS  FWRD. + ADJ.                             *
*GWCRUN* *GWCRUN*  0.0 74R 0 100R
1D DVRINS  0.0 100R  18000  0 99R
1D XCPINS  0.0 100R  0 0 0 1 0 18R  1 1  0 76R
1D DTNINS  0.0 3R  1.0 3R  0.0 1.6 0.0 0.0 1.0-6 5.0-5  0.0 88R
   0 3R 1 0 1 0 13R 50 0 8R 1 1 1 1 1 0 67R
1D *      *  0.0 100R 0 100R
0V ISOTXS
1D  3  3  0  1  0  1  1  1
2D  /
*CITATION MACROS TO MICROS                                            *
*ZONE1* *ZONE2* *ZONE3*  0.6 0.4 0.0  0.0 3R 0.0 4R  0 3 6
4D (*ZONE1*) 3R  0.0 1.0 0.0 4R 0 1 1 0 5R 1 1 0
  0  1  1 2 2  1 1 1
5D  1.987677-1  3.833180-1  9.962149-1  0.0 3R
    0.0  2.864-2  1.132-1   0.0  8.0-14 1.0-12
    0.0  9.4375+10  1.088+11  0.6  0.4  0.0
7D  0.0  0.0  4.378-2  0.0  4.295-2
4D (*ZONE2*)  3R  0.0 6R 0 8R  1  1  0
  0  1  1 2 2  1 1 1
5D  1.8205-1  2.745745-1  3.333333-1  0.0 3R
    1.3-2  8.0-3  0.0
7D  0.0  0.0  4.3-3  0.0  2.5-3
4D (*ZONE3*) 3R  0.0 6R  0 8R 1 1 0
  0  1  1 2 2  1 1 1
5D  2.438430-1  3.261580-1  5.048977-1  0.0 3R
    0.0  2.9-3  7.16-3
7D  0.0  0.0  2.016-2  0.0  1.392-2
0V GEODST
1D /
  8  3 16  1  4  4  1 24 20  1  3  3  1  2  1  1  /
  1  6  3  1  0  1  0 5R  /
3D /
```

(CONT)

```
        0.0  1.707963-1    1.570796    1.741593    3.141593
        0.0   30.0  35.0  45.0  70.0
  4  8  4  8  /
  6  4  4  6  /
5D  /
  7.685832+1        6.3+2  7.685832+1        6.3+2  2.775439+1      2.275+2
  2.775439+1      2.275+2  6.831851+1        5.6+2  6.831851+1        5.6+2
  2.455197+2     2.0125+3  2.455197+2     2.0125+3
       1.0-3 /
  0.0 3R 0.4692  0.0 2R   0.0 2R  0.4692 /
  2       1 1 1 /
  1 4R  2  1  2  1 5R  3  4R
7D  /
 (1 4R  2 8R  3 4R  4 8R) 6R  /
 (5 4R  6 8R  7 4R  8 8R) 4R  /
 (9 4R 10 8R 11 4R 12 8R) 4R  /
(13 4R 14 8R 15 4R 16 8R) 6R  /
0V NDXSRF
1D /
  3  1  3  3  3  0
2D /
  (*ZONE1* *ZONE2* *ZONE3*) 2R  0.0 6R  0  3R  3  0  0  0
  (1 2 3) 2R
3D /
  3.125352+3  5.550879+1  4.516035+3  1.0 3R  1 3R
0V ZNATDN
1D /
  0.0  0  3  3  1
2D /
  1.0 0.0 0.0 0.0 1.0 0.0 0.0 0.0 1.0
    STOP
END
 INPUT PROCESSOR DATA.
0V CONTRL
1D PROINS /
* 3-D (X,Y,Z) BUCKLING SEARCH (OLD WHIRLAWAY CASE) - 9X9X5X2            *
* RUNNING IN THE PLANE STORED MODE - 4 PLANES STORED                    *
*      * *      *  0.0 74R  0 100R
1D DVRINS  0.0 100R  18000  0 99R
1D XCPINS  0.0 100R  0 23R  1  0 76R
1D DTNINS  0.0  1.0  0.0  10.0  1.0 2R  0.09  0.0 3R  1.0-6  5.0-5
  0.0 88R
  0 3R  1  4  1  0 13R  50  0 8R  1 5R  0  1  0  1 6R  0 2R 5 1 1 0 3R
  1  0  1  1  0 2R  0  1  2  0  2  4  0 38R
1D *      *  0.0 100R  0 100R
0V GRUPXS
1D /
  2  3  0  1  0  1  18  0  0  0  1  1  0  0
2D /
* GRUPXS CROSS SECTIONS FOR VENTURE SAMPLE PROBLEM                      *
  (*ZONE1* *ZONE2* *ZONE3*)
  1.0  0.0  0.0 2R  0.0 3R
4D /
  (*      *) 3R  (*CITNXS*) 3R  (*      *) 3R /
```

(CONT)

```
  0.0 3R  6.25-11 2.5-11 0.0  0.0 3R  0.0 3R  0.0 3R  0.0 3R  0.0 3R /
  0 3R  0  1  1 2R  0  0 7R
5D /
  2.222222-1  1.960784-1  2.777778-1 /
  0.0 3R /
  4.0-4  5.0-4  5.2-4 /
  8.0-4  2.0-4  0.0 /
  5.0  2.0  0.0/
  1.0 2R  0.0 /
5D /
  2.777778-1  2.949854-1  3.831418-1 /
  0.0 3R /
  1.55-3  3.8-3  8.0-3 /
  3.15-3  2.5-3  0.0 /
  20.0  10.0  0.0 /
  0.0 3R
7D /
  1 3R  1 3R
8D /
  0.0 3R
7D /
  2 3R  1 3R
8D /
  0.0  3.3-3  0.0  5.2-3  0.0  6.7-3
0V GEODST
1D /
  14  3  3  1  3  1  1  9  9  5  1  0  0  1  0  0  1  6  1  0  0  1
  0 5R /
4D /
  0.0  8.0  16.0  25.0
  0.0  18.0
  0.0  15.0
  4  2  3 /
  9 /
  5 /
5D /
  2160.0  2160.0  2430.0 /
  0.0109045 /
  0.0  1.0+30  1.0+30  0.0  1.0+30  1.0+30 /
  0.4692 /
  1 3R /
  1  2  3 /
7D /
 (1 4R  2 2R  3 3R) 9R /
7D /
 (1 4R  2 2R  3 3R) 9R /
7D /
 (1 4R  2 2R  3 3R) 9R /
7D /
 (1 4R  2 2R  3 3R) 9R /
7D /
 (1 4R  2 2R  3 3R) 9R /
0V NDXSRF
1D /
```

(CONT)

```
  3  1  3  3  3  0
2D /
  (*ZONE1* *ZONE2* *ZONE3*) 2R  0.0 6R  0 3R  3  0  0  0
  (1  2  3) 2R
3D /
  2160.0  2160.0  2430.0 /
  1.0  1.0  1.0 /
  1  1  1
0V ZNATDN
1D /
  0.0  0  3  3  1
2D /
  1.0  0.0 2R /
  0.0  1.0  0.0 /
  0.0  0.0  1.0
STOP
END
 INPUT PROCESSOR DATA.
 0V CONTRL
1D PROINS /
* 2-D  17X10 - 5 GROUP SEARCH PROBLEM                                    *
* PRIMARY SEARCH = NUCLIDE(DIRECT) - SECONDARY SEARCH = DIMENSION        *
*      * *      *  0.0 74R  0 100R
1D DVRINS  0.0 100R  18000  0 99R
1D XCPINS  0.0 100R  0 3R  1  0 18R  1  1  0 76R
1D DTNINS /
0.0 3R  2345.0  1.0  0.5  0.0 4R  1.0E-6  5.0E-5  0.0 88R /
 0 3R  1 3R  0 3R  7  0 9R  35  0 8R  1  1  0  1  1  0  1  0  0  1 5R
  0  0  5  1  1  0 3R  1  0  1  1  0 3R  1  2  0 41R
1D RRTINS  0.0 100R  0 5R  1  0  0  0  1  1  1  0  1  0 86R
1D *      *  0.0 100R  0 100R
0V ISOTXS
1D /
 5 15 0 4 0 1 1 1
2D /
* 5 GROUP LMFBR CROSS SECTION SET.                                       *
  *O-16  * *NA-23 * *CR-N  * *MN-55 * *FE-N  * *NI-N  * *MO-N  *
  *TA-181* *U-235 * *U-238 * *PU-239* *PU-240* *PU-241* *PU-242*
  *SSFP  *
 0.755037 0.238025 0.006938  0.0 2R /
 2579.927 891.3213 324.5034 109.3773 41.77161 /
 1.49182E+7 8.2085E+5 6.73795E+4 9118.816 748.5188 1.0E-4 /
 0 3 6 9 12 15 18 21 24 27 30 33 36 39 42
4D /
  *O-16  * *CITNXS* *O-16  * /
 15.86200 0.0 5R /
 0 0 0  0 5R 1 1 0 0 1 /
  1  2  3  2  2 /
 1 5R
5D /
 2.001419E+00 3.538190E+00 3.530899E+00 3.586479E+00 3.802440E+00
 0.0 0.0 0.0 0.0 0.0
 6.058659E-03 0.0 0.0 0.0 4.388488E-16
7D /
```

(CONT)

```
 2.166470E+00 3.647599E+00 4.272870E-01 3.463120E+00 1.759329E-01
 1.122229E-07 3.562880E+00 1.304229E-01 3.677589E+00 8.492589E-02
4D /
  *NA-23 * *CITNXS* *NA-23 * /
 22.78600 0.0 5R /
 6 1 1  0 5R 1 1 0 0 1 /
  1  2  3  2  2 /
 1 5R
5D /
 2.036969E+00 3.538750E+00 4.970710E+00 1.154060E+01 3.192539E+00
 0.0 0.0 0.0 0.0 0.0
 1.786468E-03 5.146489E-04 1.094200E-03 1.207110E-02 5.816218E-03
 1.541630E-06 0.0 0.0 0.0 0.0
 2.000000E+00 0.0 0.0 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 2.622210E+00 3.743600E+00 4.186479E-01 4.857280E+00 1.324430E-01
 1.452600E-04 1.609309E+01 1.414840E-01 3.054230E+00 5.449740E-02
4D /
  *CR-N  * *CITNXS* *CR-N  * /
 52.01000 0.0 5R /
 5 0 0  0 5R 1 1 0 0 1 /
  1  2  3  4  5 /
 1 5R
5D /
 1.895960E+00 2.847699E+00 4.099540E+00 1.258560E+01 4.485060E+00
 0.0 0.0 0.0 0.0 0.0
 3.482590E-03 4.594687E-03 7.548548E-03 1.374699E-01 1.257820E-01
7D /
 2.654610E+00 3.672379E+00 2.405180E-01 4.268359E+00 3.898390E-02
 6.128579E-03 1.243190E+01 1.094289E-01 0.0 4.783079E-04
 4.296340E+00 3.122900E-02 0.0 0.0 2.785960E-05
4D /
  *MN-55 * *CITNXS* *MN-55 * /
 54.46600 0.0 5R /
 5 1 1  0 5R 1 1 0 0 1 /
  1  2  3  4  2 /
 1 5R
5D /
 2.591649E+00 5.235530E+00 1.456410E+01 6.231160E+01 1.002660E+02
 0.0 0.0 0.0 0.0 0.0
 4.334409E-03 1.134890E-02 5.448210E-02 3.652869E-01 3.209069E+00
 1.073100E-04 0.0 0.0 0.0 0.0
 2.000000E+00 0.0 0.0 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 2.974719E+00 5.436890E+00 4.263680E-01 1.396750E+01 1.851780E-01
 1.911900E-02 7.817009E+01 4.328420E-01 5.918168E-03 5.526468E-04
 1.468200E+02 1.011980E-01
4D /
  *FE-N  * *CITNXS* *FE-N  * /
 55.84500 0.0 5R /
 5 0 0  0 5R 1 1 0 0 1 /
  1  2  3  4  2 /
```

(CONT)

```
 1 5R
5D /
 2.168090E+00 3.482690E+00 6.566119E+00 9.031090E+00 1.055570E+01
 0.0 0.0 0.0 0.0 0.0
 2.519850E-03 5.252499E-03 1.946380E-02 5.074910E-02 2.056830E-02
7D /
 2.565539E+00 3.926530E+00 3.419320E-01 7.636379E+00 3.941110E-02
 1.161280E-02 8.834049E+00 8.631974E-02 0.0 5.354248E-04
 1.047090E+01 6.575638E-02
4D /
  *NI-N  * *CITNXS* *NI-N  * /
 58.70500 0.0 5R /
 5 0 0  0 5R 1 1 0 0 1 /
  1  2  3  4  5 /
 1 5R
5D /
 2.299829E+00 4.373010E+00 1.716609E+01 1.579460E+01 1.633490E+01
 0.0 0.0 0.0 0.0 0.0
 7.411516E-02 9.023577E-03 1.714480E-02 1.964660E-02 3.636980E-02
7D /
 2.735749E+00 4.621889E+00 2.409970E-01 1.836949E+01 1.592640E-01
 5.383287E-03 1.589590E+01 9.364969E-02 0.0 5.395960E-04
 1.617560E+01 9.805179E-02 0.0 0.0 4.569250E-06
4D /
  *MO-N  * *CITNXS* *MO-N  * /
 95.06600 0.0 5R /
 5 1 1  0 5R 1 1 0 0 1 /
  1  2  3  3  4 /
 1 5R
5D /
 3.663779E+00 7.085640E+00 7.328959E+00 7.271429E+00 1.323520E+01
 0.0 0.0 0.0 0.0 0.0
 2.366135E-02 6.210750E-02 2.112700E-01 1.518339E+00 3.248449E+00
 1.485650E-03 0.0 0.0 0.0 0.0
 2.000000E+00 0.0 0.0 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.577000E+00 8.479199E+00 8.577590E-01 7.315180E+00 7.333905E-02
 1.588170E-02 5.658710E+00 3.783630E-02 8.116618E-04 9.642159E+00
 2.030290E-02 0.0 2.710729E-05
4D /
  *TA-181* *CITNXS* *TA-181* /
 179.3900 0.0 5R /
 7 1 1  0 5R 1 1 0 0 1 /
  1  2  3  3  2 /
 1 5R
5D /
 4.137730E+00 6.666160E+00 1.075010E+01 1.687169E+01 2.470959E+01
 0.0 0.0 0.0 0.0 0.0
 7.648069E-02 2.887599E-01 8.258290E-01 3.224420E+00 6.866340E+00
 3.773690E-03 0.0 0.0 0.0 0.0
 2.000000E+00 0.0 0.0 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
```

(CONT)

```
 5.053289E+00 7.277980E+00 1.300570E+00 1.042640E+01 1.379640E-01
 2.069130E-02 1.451040E+01 7.560796E-02 1.500330E-03 2.003560E+01
 3.956910E-02
4D /
  *U-235 * *CITNXS* *U-235 * /
 233.0250 3.148100E-11  0.0 4R /
 1 1 1  0 5R 1 1 0 0 1 /
  1  2  3  3  3 /
 1 5R
5D /
 4.760500E+00 8.222549E+00 1.359530E+01 1.914319E+01 3.180229E+01
 0.0 0.0 0.0 0.0 0.0
 6.753063E-02 2.953396E-01 8.323002E-01 2.340739E+00 6.114193E+00
 1.276409E+00 1.422770E+00 2.397539E+00 5.349660E+00 1.433350E+01
 2.667859E+00 2.457879E+00 2.433379E+00 2.430380E+00 2.430070E+00
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.856970E+00 7.983669E+00 7.749810E-01 1.061980E+01 1.128620E-01
 6.262079E-03 1.135630E+01 3.006150E-02 6.019380E-04 1.172910E+01
 1.911250E-02 2.076550E-05
4D /
  *U-238 * *CITNXS* *U-238 * /
 236.0060 3.162500E-11  0.0 4R /
 2 1 1  0 5R 1 1 0 0 1 /
  1  2  3  4  3 /
 1 5R
5D /
 4.846760E+00 8.571039E+00 1.344970E+01 1.768149E+01 1.890230E+01
 0.0 0.0 0.0 0.0 0.0
 8.457595E-02 1.702173E-01 4.804530E-01 9.735650E-01 1.381539E+00
 3.346020E-01 2.376520E-04 0.0 0.0 0.0
 2.786519E+00 2.466439E+00 0.0 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.988910E+00 1.002520E+01 1.818430E+00 1.325670E+01 1.357570E-01
 4.470190E-02 1.698059E+01 4.110790E-02 5.152000E-04 2.062660E-04
 1.838379E+01 1.897440E-02 3.887150E-04
4D /
  *PU-239* *CITNXS* *PU-239* /
 236.9990 3.258600E-11  0.0 4R /
 1 1 1  0 5R 1 1 0 0 1 /
  1  2  3  3  2 /
 1 5R
5D /
 4.954309E+00 8.718180E+00 1.417930E+01 1.948119E+01 3.271959E+01
 0.0 0.0 0.0 0.0 0.0
 1.869965E-02 1.703405E-01 5.475597E-01 1.758830E+00 5.105810E+00
 1.883070E+00 1.544629E+00 1.793650E+00 3.520470E+00 9.376289E+00
 3.159670E+00 2.908930E+00 2.874129E+00 2.870489E+00 2.870060E+00
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.755099E+00 8.660600E+00 6.977440E-01 1.152080E+01 5.938330E-02
 1.403850E-02 1.228110E+01 5.996540E-02 1.393650E-04 1.321710E+01
 2.247640E-02
```

(CONT)

```
4D /
 *PU-240* *CITNXS* *PU-240* /
 237.9900 3.282700E-11  0.0 4R /
 2 1 1  0 5R 1 1 0 0 1 /
  1  2  3  4  3 /
 1 5R
5D /
 5.054469E+00 8.604670E+00 1.371420E+01 1.888170E+01 2.418489E+01
 0.0 0.0 0.0 0.0 0.0
 9.490967E-02 2.099380E-01 5.826710E-01 1.765706E+00 5.535801E+00
 1.543460E+00 2.327840E-01 1.008230E-01 8.248240E-02 5.786900E-02
 3.146529E+00 2.935940E+00 2.874260E+00 2.870649E+00 2.870070E+00
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.944110E+00 1.004100E+01 9.152250E-01 1.332420E+01 9.741586E-02
 1.617920E-02 1.696700E+01 3.657120E-02 4.508259E-05 1.091320E-04
 1.921140E+01 3.237760E-02 1.642760E-05
4D /
 *PU-241* *CITNXS* *PU-241* /
 238.9780 3.305100E-11  0.0 4R /
 1 1 1  0 5R 1 1 0 0 1 /
  1  2  3  4  3 /
 1 5R
5D /
 5.104230E+00 8.643849E+00 1.269630E+01 1.976459E+01 3.767090E+01
 0.0 0.0 0.0 0.0 0.0
 2.668953E-02 2.172995E-01 6.064100E-01 1.668990E+00 5.614212E+00
 1.703650E+00 1.869960E+00 3.036860E+00 6.653950E+00 1.995859E+01
 3.256940E+00 3.005619E+00 2.973280E+00 2.969489E+00 2.969060E+00
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 4.529670E+00 7.873819E+00 1.165449E+00 9.113990E+00 3.188040E-01
 7.122946E-02 1.127190E+01 4.141530E-02 5.656999E-03 2.550660E-04
 1.2999C0E+01 2.077500E-02 1.391030E-03
4D /
 *PU-242* *CITNXS* *PU-242* /
 240.1450 3.276200E-11  0.0 4R /
 3 1 1  0 5R 1 1 0 0 1 /
  1  2  3  2  3 /
 1 5R
5D /
 4.493779E+00 7.721160E+00 1.416950E+01 2.093379E+01 2.866119E+01
 0.0 0.0 0.0 0.0 0.0
 4.164982E-02 1.358470E-01 4.516167E-01 1.535060E+00 5.900109E+00
 1.453540E+00 1.398230E-01 4.632320E-02 0.0 0.0
 3.1228C0E+00 2.885630E+00 2.812289E+00 0.0 0.0
 7.550370E-01 2.380250E-01 6.937999E-03 0.0 0.0
7D /
 5.051700E+00 9.356939E+00 6.037650E-01 1.433580E+01 1.291580E-01
 1.092240E-02 1.935210E+01 4.589510E-02 2.431760E+01 3.522350E-02
 6.624369E-05
4D /
 *SSFP  * *CITNXS* *SSFP  * /
 161.0000 0.0 5R /
```

(CONT)

```
 4 0 0  0 5R 1 1 0 0 1 /
  1  1  1  1  1 /
 1 5R
5D /
 3.563750E-02 1.371830E-01 3.716339E-01 9.294800E-01 3.085389E+00
 0.0 0.0 0.0 0.0 0.0
 3.680390E-02 1.409680E-01 3.771360E-01 9.283320E-01 3.130919E+00
7D /
 0.0 0.0 0.0 0.0 0.0
0V GEODST
1D /
 7 8 18 1 6 3 1 17 10 1 1 2 2 1 2 2 1 6 1 0 0 1 0 5R
3D /
0.0 12.482 42.482 57.482 77.912 98.659 113.899 /
 0.0 12.24 30.34 56.06 /
 2 3 5R /
 3 3 4
5D /
 5991.004 63406.07 57658.88 106365.1 140865.9 124564.3 8859.246
 93762.25 85263.5 157288.2 208306.6 184200.5 12588.94 133235.6
 121159.0 223505.7 296002.6 261747.9 /
 0.0 /
 0.0 0.4692 2R  0.0  0.4692 2R /
 0.4692 /
 1 8R /
 7 6R  3 3R  4 6 8  1 3R  2 5 8 /
7D /
 (1 1  2 3R  3 3R  4 3R  5 3R  6 3R) 3R /
 (7 7  8 3R  9 3R  10 3R  11 3R  12 3R) 3R /
 (13 13  14 3R  15 3R  16 3R  17 3R  18 3R) 4R /
0V NDXSRF
1D /
  15  4  14  15  8  4
2D /
 (*O-16  * *NA-23 * *CR-N  * *MN-55 * *FE-N  * *NI-N  * *MO-N  *
  *TA-181* *U-235 * *U-238 * *PU-239* *PU-240* *PU-241* *PU-242*
  *SSFP  * ) 2R /
 0.0 15R /
 15.862 22.786 52.01 54.466 55.845 58.705 95.066 179.39 233.025
 236.006 236.999 237.990 238.978 240.145 161.0 /
 0 6  5 5R  7 1 2 1 2 1 3 4 /
 (14  0 3R) 3R  7  0 3R /
 1 2 3 4 5 6 7 8 10 11 12 13 14 15 /
 (1 2 3 4 5 6 7 8 9 10 11 12 13 15) 2R /
 2 3 4 5 6 7 8  0 7R /
 1 2 3 4 5 6 7 8 0 9 10 11 12 13 14 /
 (1 2 3 4 5 6 7 8 9 10 11 12 13 0 14) 2R /
 0 1 2 3 4 5 6 7  0 7R /
3D /
 266983.6 223505.7 187884.9 157288.2 296002.6 208306.6 498851.2
 445948.4 /
 1.0 0.0  1.0 6R /
 55876.42 4R /
 1 0  3 4R 4 4 /
```

(CONT)

```
 2 4R /
 2 4R /
OV ZNATDN
1D /
 0.0  0  12  14  1
2D /
 1.804800E-02 8.218598E-03 2.945900E-03 4.325500E-04 1.134900E-02
 2.078700E-03 5.186498E-04 5.261999E-05 7.179096E-03 9.960700E-04
 2.896199E-04 2.796900E-05 7.217899E-06 5.223998E-04
 0.0 14R  1.804800E-02 /
 8.218598E-03 2.945900E-03 4.325500E-04 1.134900E-02 2.078700E-03
 5.186498E-04 5.261999E-05 2.124799E-05 8.596398E-03 1.841500E-04
 6.197200E-06 9.999999E-16 4.515100E-05 1.804800E-02 8.218598E-03
 2.945900E-03 4.325500E-04 1.134900E-02 2.078700E-03 5.186498E-04
 5.261999E-05 2.124799E-05 8.596398E-03 1.841500E-04 6.197200E-06
 9.999999E-16 4.515100E-05 1.804800E-02 8.218598E-03 2.945900E-03
 4.325500E-04 1.134900E-02 2.078700E-03 5.186498E-04 5.261999E-05
 2.124799E-05 8.596398E-03 1.841500E-04 6.197200E-06 9.999999E-16
 4.515100E-05 1.804800E-02 8.218598E-03 2.945900E-03 4.325500E-04
 1.134900E-02 2.078700E-03 5.186498E-04 5.261999E-05 2.124799E-05
 8.596398E-03 1.841500E-04 6.197200E-06 9.999999E-16 4.515100E-05
 4.359998E-03 1.149600E-02 1.688000E-03 4.428800E-02 8.111998E-03
 2.024000E-03 9.999999E-16 /
  0.0 7R                   4.359998E-03 1.149600E-02 1.688000E-03
 4.428800E-02 8.111998E-03 2.024000E-03 9.999999E-16
 0.0 7R  1.804800E-02 /
 8.218598E-03 2.945900E-03 4.325500E-04 1.134900E-02 2.078700E-03
 5.186498E-04 5.261999E-05 2.124799E-05 8.596398E-03 1.841500E-04
 6.197200E-06 9.999999E-16 4.515100E-05 1.804800E-02 8.218598E-03
 2.945900E-03 4.325500E-04 1.134900E-02 2.078700E-03 5.186498E-04
 5.261999E-05 2.124799E-05 8.596398E-03 1.841500E-04 6.197200E-06
 9.999999E-16 4.515100E-05 1.804800E-02 8.218598E-03 2.945900E-03
 4.325500E-04 1.134900E-02 2.078700E-03 5.186498E-04 5.261999E-05
 2.124799E-05 8.596398E-03 1.841500E-04 6.197200E-06 9.999999E-16
 4.515100E-05 1.804800E-02 8.218598E-03 2.945900E-03 4.325500E-04
 1.134900E-02 2.078700E-03 5.186498E-04 5.261999E-05 2.124799E-05
 8.596398E-03 1.841500E-04 6.197200E-06 9.999999E-16 4.515100E-05
OV SEARCH
1D /
  7  2  0 18R /
2D /
 1.01  0.0  0.00005  0.001  0.0 6R /
  9  0  0  0 3R  3  1  2  0  0  0  8  0 17R /
5D /
  1  2 /
*U-238 *  *PU-240*  *PU-239* /
 0.0001  0.0002  0.0003
1D /
  8  2  0 18R /
2D /
 1.01  0.0  0.00005  0.001  0.0 6R /
  5  0  7  6  3  1  0  0  2  0  0  0  0 18R /
3D /
 1.0  1.0  1.0  1.0  0.0  0.0 /
 0.0  0.0  0.5 /
 0.0
1D /
 -10  0 19R/
STOP
END
/*
//
```

Table 450-2. Input for Two Sample Problems in the Special Input Processors Format

```
//USERID   JOB (CHARG),'ADRES-NAME COL 25-44',
// MSGLEVEL=(1,1)
//*CLASS   CPU95=03M,REGION=0300K,IO=015,LINES=19,CARDS=00
//STEP EXEC BOLDVENT,
// NB1=1,NB2=1,B1=3520,B2=15360,NX=2,NS=50,N1=100,
// N2=4,N3=13,N4=1,N5=6,N6=10,N7=1,N8=1,N9=2,N10=2,N11=3,N12=5,N13=2,
// N14=1,N15=10,
// GOSIZE=300K
//GO.STEPLIB DD DSN=TBF.BOLD.VENTURE.NEW.WORKING
//GO.SYSIN DD *
=CONTROL1
 VENTURE SAMPLE PROBLEM RUN - USING THE SPECIAL INPUT PROCESSORS.
015000
  2  2  6  2  7  2  2  6  2  7  0
END
DCMACR
  3
CITATION MACROS TO MICROS.
008
  3  1  0
     1     1       1.677         0.0         0.0
         0.0     0.04378         0.0
     1     2      0.8696     0.02864     0.00755              0.8     -13
         0.0         0.0     0.04295
     1     3      0.3346      0.1132      0.1088               1.0     -12
         0.0         0.0         0.0
     2     1       1.831       0.013         0.0
         0.0      0.0043         0.0
     2     2       1.214       0.008         0.0
         0.0         0.0      0.0025
     2     3  1.0
         0.0         0.0         0.0
     3     1       1.367         0.0         0.0
         0.0     0.02016         0.0
     3     2       1.022      0.0029         0.0
         0.0         0.0     0.01392
     3     3      0.6602     0.00716         0.0
         0.0         0.0         0.0
     0
         0.6         0.4         0.0
END
DCRSPR
        1  1  1                                                        1  1
              3
ZONE 1
ZONE 2
ZONE 3
END
```

(CONT)

```
DVENTR
001
 0.0
                                                  1.6
 0.0
            1
  1  1                                  3  1
003
  8  3  3  1  2  1  1  1  0  3  1
 0.001
 0.0          0.0          0.4692
  2
004
  4 .1707963  8       1.4  4 .1707963  8       1.4
  6      30.0  4       5.0  4      10.0  6      25.0
005
  1  1  1  1
  2  1  2  1
  1  1  1  1
  3  3  3  3
012
  0
  1  3  1  1 1.0
  0
013
  3
  3
ZONE 1ZONE 2ZONE 3
020
  1  1
ZONE 1 1.0
  2  2
ZONE 2 1.0
  3  3
ZONE 3 1.0
  0
END
DCMACR
  3
CITATION MACROS TO MICROS.
008
  2  1  0
     1     1          1.5       0.0012        0.004                 5.      -14
         0.0       0.0033
     1     2          1.2       0.0047        0.063                 1.96875-13
         0.0          0.0
     2     1          1.7       0.0007       0.0004                    5.   -15
         0.0       0.0052
     2     2         1.13       0.0063        0.025                 6.25    -14
         0.0          0.0
     3     1          1.2      0.00052          0.0
         0.0       0.0067
```

(CONT)

```
     3      2          0.87        0.008          0.0
          0.0          0.0
     0
          1.0
END
DCRSPR
         1   1   1
                3
ZONE1
ZONE2
ZONE3
END
DVENTR
001
                                                10.0
 0.0
                                                0.09
     4      1      0          0      0 50
  1   1   1   1   1   1   1   1   0   0   1   1   2   4   1   1   1   1   0   2   1   5
003
 14   1   0   0   1   0   0   1   0   0   0
 0.0109045
004
  4        8.0   2        8.0   3        9.0
  9       18.0
  5       15.0
005
  1   1   1
006
   2
   5    6    1    9    1    5
   3
   7    9    1    9    1    5
   0
012
  0
  1   3   1   1 1.0
  0
013
  3
  3
ZONE1 ZONE2 ZONE3
020
  1   1
ZONE1   1.0
  2   2
ZONE2   1.0
  3   3
ZONE3   1.0
  0
END
/*
//
```

Table 450-3. Selected Printout for Sample Problems

```
BOLD VENTURE VERS-2 RUN AT K-25 ON 360/195, CONTROL MOD=CONTROL1, DATE=06-02-77, TIME=00.31.33, JOBNAME=T6F4

INITILIZATION, REFERENCE - REMAINING I/O=  24.94, CPU MIN=   3.00

RUN TITLE AND CONTROL MODULE DATA
*********************VENTURE RUN - SAMPLE PROBLEMS**********************
 18000     0     0     0     0     0     0     0     0 0 0 1 0 0 0
  1 6 7 1 7 1 6 7 9

MODULES TO BE ACCESSED IN ORDER
     1     6     7     1     7     1     6     7     9

                         INITIAL I/O FILE MANAGEMENT TABLES
                     FILE NAME SUPPLIED BY
                 ------------------------------
FILE NUMBER      SEEK   USER-EXIST   USER-STACK      VERSION      WRITTEN
    10          CONTRL                                  1            1

READ DATA AND ACCESS MODULE  1     - REMAINING I/O=  24.87, CPU MIN=   2.99

READ INPUT DATA ONLY (LOCK-AHEAD) - REMAINING I/O=  24.27, CPU MIN=   2.95

ACCESS MODULES  6  7  0  0  0      - REMAINING I/O=  24.14, CPU MIN=   2.94
     ITERATIONS, CONVERGENCE, SEARCH, PEAK POWER DENSITY, K -     18  -2.34779D-05    0.0            5.20034E-04    0.6119772
     ADJOINT - ITERATIONS, CONVERGENCE, K -     11   1.047360-05    0.6119764

ACCESS INPUT MODULE  1             - REMAINING I/O=  22.37, CPU MIN=   2.70

READ INPUT DATA ONLY (LOCK-AHEAD) - REMAINING I/O=  21.83, CPU MIN=   2.66

ACCESS MODULES  7  0  0  0  0      - REMAINING I/O=  21.43, CPU MIN=   2.66
     ITERATIONS, CONVERGENCE, SEARCH, PEAK POWER DENSITY, K -     30   3.72899D-06  -9.99986E-01   1.18286E-02    0.0900000
     ADJOINT - ITERATIONS, CONVERGENCE, K -     10   1.36358D-05    0.0900000
     PROMPT NEUTRON LIFETIME, K/(INTEGRAL(CHI,NUSIGF,PHI,PHI*)) -   2.22252E 01   1.86826E-09

ACCESS INPUT MODULE  1             - REMAINING I/O=  19.45, CPU MIN=   2.39

ACCESS MODULES  6  7  9  0  0      - REMAINING I/O=  19.32, CPU MIN=   2.29
     ITERATIONS, CONVERGENCE, SEARCH, PEAK POWER DENSITY, K -      1   1.08622D-08    0.0            3.22392E-03    1.0099993
     PRIMITIVE CONVERSION RATIO, ALSO FOR CRITICAL SYSTEM, FUEL CONSUMPTION(ATOMS/WATT-SEC) -   1.23325   1.26298   2.99028E 10
     ADJOINT - ITERATIONS, CONVERGENCE, K -     14  -3.69153D-05    1.0099993
     PROMPT NEUTRON LIFETIME, K/(INTEGRAL(CHI,NUSIGF,PHI,PHI*)) -   2.17066E-01   3.40568E-08
     FISSILE INVENTORY 9.947813E 02 KG, CONVERSION RATIO(RR)    1.23325, FISSILE CONSUMPTION RATE 1.17678OE-14 KG/W-SEC

                         FINAL I/O FILE MANAGEMENT TABLES
                     FILE NAME SUPPLIED BY
                 ------------------------------
FILE NUMBER      SEEK   USER-EXIST   USER-STACK      VERSION      WRITTEN
    10          CONTRL                                  1            1
    11          ISOTXS                                  1            1
    12          GEODST                                  1            1
    13          NDXSRF                                  1            1
    14          ZNATDN                                  1            1
    15          GRUPXS                                  1            1
    16          RTFLUX                                  1            1
    17          ATFLUX                                  1            1
    18          RZFLUX                                  1            1
    19          PWDINT                                  1            1
    20          PERTUB                                  1            1
    30          SEARCH                                  1            1
    31          ZNATDN                                  2            1
    32          GEODST                                  2            1
    33          NDXSRF                                  2            1
```

```
RUN TITLE -  PERIODIC BOUNDARY IN THETA-R GEOMETRY, CASE A4 WITH BLACK ABSORBER
             24X20X3 GROUP, 1440 POINTS  FWRD. + ADJ.

                        VENTURE NEUTRONICS CODE BLOCK - VERSION 2 --- APRIL 30, 1977.
                        ------------------------------------------------------------

REFERENCE REAL TIME FROM ZNATDN INTERFACE FILE =  0.0          DAYS

SOLUTION BY FINITE-DIFFERENCE DIFFUSION THEORY
EIGENVALUE PROBLEM
A REGULAR ADJOINT WILL FOLLOW FORWARD PROBLEM
GEOMETRY NO.  8   2-D THETA-R
NUMBER OF ENERGY GROUPS                                  3
NUMBER OF UPSCATTER GROUPS (MAX)                         0
NUMBER OF DOWNSCATTER GROUPS (MAX)                       1
NUMBER OF INTERVALS IN DIMENSION 1 (COLUMNS)            24
NUMBER OF INTERVALS IN DIMENSION 2 (ROWS)               20
NUMBER OF INTERVALS IN DIMENSION 3 (PLANES)              1
NUMBER OF ZONES                                          3
NUMBER OF REGIONS                                       16
NUMBER OF BLACK ABSORBER ZONES                           1
BOUNDARY INDICATORS-   LEFT  3  RIGHT  3
                        TOP  1 BOTTOM  2


                                    MEMORY REQUIREMENTS FOR DATA STORAGE

                                          TOTAL                  A          B          C          D
                                       MINIMUM   MAXIMUM
STORAGE AVAILABLE                        18000
MACRO CALCULATION                          187
EQUATION CONSTANTS CALCULATION
          CORE CONTAINED OR SPACE STORED  2909      2909
          PLANE STORED                    3870      3870
          ROW STORED                       944       944
          MULTI-LEVEL PLANE STORED        4344      4344
INITIAL FLUX
          CORE CONTAINED OR SPACE STORED  1733      1733
          OTHER MODES                     1733      1733
ITERATIVE PROCESS
          CORE CONTAINED                 14701                11654       990        92      1965
          SPACE STORED                    6836                 5805       990        41         0
        1 PLANES STORED                   8757                 7726       990        41         0
        1 PLANE STORED                    8757                 7726       990        41         0
       20 ROWS STORED                     6495                 5464       990        41         0
        1 ROW STORED                      1031                    0       990        41         0
        1 MULTI-LEVEL PLANES STORED      11151                 2880       990        41      7240
PERTURBATION CALCULATION                  2926

DATA WILL BE STORED FOR ALL GROUPS, ALL SPACE

MEMORY LOCATIONS RESERVED FOR DATA STORAGE---   18000
MAX MEMORY LOCATIONS REQUIRED FOR THIS PROB--   14701
MEMORY LOCATIONS NOT USED-------------------    3299

     SPECIAL SCRATCH DATASET REQUIREMENTS
     MAXIMUM PHYSICAL RECORD IS      7200 WORDS

RITE CONTAINER ARRAYS, CONTROL      36 DATA    3253
FILE 24 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      3    960   2880      1    373
```

```
A FLUX - EIGENVALUE PROBLEM FOLLOWS
     4 INNERS MIN,  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE     MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS   SOURCE        K-USED     K-CALC
   1    0     0     0    1.14667D 00    0.0       0.0      1.00000       0.0         0.0       9.82507E 13  1.0000000  0.6174905
   2    0     1     0    2.18367D 01   29.96185   0.0      1.00000       1.00000     0.0       5.91452E 13  1.0000000  0.6154622
NEW OVERRELAXATION COEFFICIENTS CALCULATED
  1.52392  1.39867  1.27840
   3    0     0     1    1.28188D 01    0.58299   0.0      1.00000       1.39800     0.0       3.52317E 13  0.7619642  0.6069385
   4    0     0     0    6.06513D-01    0.26841   0.0      1.00000       0.67278    -0.31287   2.85547E 13  0.6069385  0.6078110
   5    1     1     0   -5.90901D-02    0.0       0.0      1.00000       0.58715     0.0       2.85279E 13  0.6078110
   6    1     1     0   -6.10800D-02    0.0       0.0      1.00000       1.19875     0.38534   2.86253E 13  0.6098862
   7    1     0     0    2.56259D-02    0.42434   0.38548  1.00000       0.96593     0.23865   2.86863E 13  0.6111869
   8    1     0     0   -2.63525D-02    0.26451   1.04153  1.00000       0.91748     0.20812   2.87173E 13  0.6118475
   9    1     0     0    9.52763D-03    0.16461   0.35678  1.00000       0.90769     0.20196   2.87311E 13  0.6121408
  10    1     1     0    3.36171D-03    1.38295   0.40373  1.00000       0.90573     0.20072   2.87255E 13  0.6120563
  11    1     0     0   -3.40771D-03    0.66947   1.01539  1.00000       0.90533     0.20047   2.87237E 13  0.6120177
  12    1     0     0    3.06018D-03    0.54064   0.89649  1.00000       0.90525     0.20042   2.87234E 13  0.6120111
  13    1     0     0   -8.53942D-04    0.47321   0.27948  1.00000       0.90524     0.20041   2.87218E 13  0.6119944
  14    3     0     0    9.90606D-04    0.63773   1.15954  0.0           4.43912     0.05435   2.87207E 13  0.6119820
  15    0     0     1    1.26084D-03    0.0       0.0      1.00000      -2.06858     1.24633   2.87196E 13  0.6119703  0.6119756
  16    1     0     0   -2.37825D-04    0.0       0.0      1.00000       0.58715     0.0       2.87196E 13  0.6119756
  17    1     0     0    1.06612D-04    0.0       0.0      1.00000       0.90523     0.20041   2.87196E 13  0.6119768
  18    1     0     0   -2.34779D-05    0.36407   0.28474  1.00000       0.90523     0.20041   2.87196E 13  0.6119762

ESTIMATED ABSOLUTE POINT FLUX RELATIVE ERROR  1.23149D-04

FINAL CALCULATED KEFFECTIVE   0.6119772
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES-------------------------   0.6119764
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   0.6119915   0.6119628
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   0.6119877   0.6119585

NEUTRON BALANCE KEFFECTIVE   0.6119765

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  8.39890D-01
  1.52216  1.39842  1.27838

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.086   0.231

    LEAKAGE  3.17835E 09  TOTAL LOSSES  1.73671E 11  TOTAL PRODUCTIONS  1.06283E 11  REACTOR POWER(WATTS)  1.00000D 00

BOUNDARY NEUTRON LEAKAGE
GROUP     LEFT          RIGHT          TOP          BOTTOM         FRONT          BACK
 1  -2.32804D 08  2.32804D 08  0.0          6.02194D 08  0.0          0.0
 2  -1.21550D 08  1.21550D 08  0.0          1.12113D 09  0.0          0.0
 3  -1.37647D 08  1.37647D 08  0.0          1.45503D 09  0.0          0.0
SUM -4.92001E 08  4.92001E 08  0.0          3.17835E 09  0.0          0.0

GROUP NEUTRON BALANCE FOR EACH ZONE

ZONE GROUP ABSORPTIONS  B**2 LOSSES    1/V LOSS   OUT-SCATTER  IN-SCATTER  P1 IN-SCATTER   SOURCE      POWER(WATTS)  AVERAGE FLUX
   1    1   0.0        3.54166E 09  0.0          9.24590E 10  0.0         0.0             1.04203E 11  0.0           6.75735E 08
   1    2   6.24662E 10  1.89667E 09  0.0          9.36774E 10  9.24590E 10  0.0            6.94684E 10  1.74486E-01  6.97870E 08
   1    3   9.34480E 10  2.76217E 08  0.0          0.0          9.36774E 10  0.0            0.0           8.25513E-01  2.64136E 08
SUM         1.55914E 11  5.71454E 09  0.0          1.86136E 11  1.86136E 11  0.0            1.73671E 11  1.00000E 00

   2    1   1.06098E 09  5.50948E 07  0.0          1.29387E 08  0.0          0.0            0.0           0.0           5.42077E 08
   2    2   2.50768E 08  3.80541E 07  0.0          7.83651E 07  1.29387E 08  0.0            0.0           0.0           5.64704E 08
   2    3   3.89231E 08  0.0          0.0          0.0          7.83651E 07  0.0            0.0           0.0           0.0
```

```
SUM          1.70098E 09  9.31489E 07  0.0          2.07752E 08  2.07752E 08  0.0          0.0          0.0

   3   1     0.0          4.46061E 08  0.0          6.57834E 09  0.0          0.0          0.0          0.0          7.22551E 07
   3   2     1.48018E 09  5.21634E 08  0.0          7.10484E 09  6.57834E 09  0.0          0.0          0.0          1.13021E 08
   3   3     4.23208E 09  3.90226E 08  0.0          0.0          7.10484E 09  0.0          0.0          0.0          1.30883E 08
SUM          5.71225E 09  1.35792E 09  0.0          1.36832E 10  1.36832E 10  0.0          0.0          0.0

OVERALL NEUTRON BALANCE

     GROUP ABSORPTIONS  B**2 LOSSES    1/V LOSS    OUT-SCATTER  IN-SCATTER  P1 IN-SCATTER   SOURCE     POWER(WATTS)
       1   1.06098E 09  4.04282E 09  0.0          9.91667E 10  0.0          0.0          1.04203E 11  0.0
       2   6.41971E 10  2.45636E 09  0.0          1.00861E 11  9.91667E 10  0.0          6.94684E 10  1.74486E-01
       3   9.80693E 10  6.66443E 08  0.0          0.0          1.00861E 11  0.0          0.0          8.25513E-01
SUM        1.63327E 11  7.16561E 09  0.0          2.00027E 11  2.00027E 11  0.0          1.73671E 11  1.00000E 00

ZONE VOLUMES FOLLOW. TOTAL VOLUME  7.69688E 03
  3.12534E 03  5.55088E 01  4.51603E 03

POINT REGULAR FLUX INTERFACE FILE RTFLUX (VERSION  1) HAS BEEN WRITTEN ON UNIT NUMBER  16

GROUP FLUX VALUES AT PLANE  1 ROW  1 COLUMN 21 = POINT AT FIRST GROUP MAXIMUM
  1.10851E 09  1.14033E 09  4.28807E 08

MAXIMUM FIRST GROUP FLUXES BY ZONE
  1.10851E 09  5.91311E 08  2.14115E 08

THE MAXIMUM POWER DENSITY IS AT PLANE   1, ROW   1,  AND COLUMN  21  AND IS   5.20033725D-04  WATTS/CC.

THE MAXIMUM NEUTRON DENSITY IS AT PLANE   1, ROW   1, AND COLUMN  21  AND IS   2.67764711D 09  NEUTRONS/CC.

THE MAXIMUM POWER DENSITY (WATTS/CC) IN EACH ZONE IS
  5.20034E-04  0.0          0.0
ELAPSED CPU AND CLOCK MINUTES ARE  0.176   2.163
```

```
ADJOINT PROBLEM FOLLOWS
      4 INNERS MIN.  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE    MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS
   1    0     0     0    1.07398D 01    0.0      0.0      1.00000      0.0        0.0
   2    0     0     0    1.99489D-01    0.09976  0.0      1.00000      1.00000    0.0
   3    0     0     0   -8.28797D-03    0.03267  0.0      1.00000      0.03377    0.0
   4    0     0     0    2.49425D-03    0.23886  0.0      1.00000     -0.05456    0.00947
   5    0     0     0    5.79710D-04    0.33260  0.0      1.00000      0.52417   -0.00541
   6    0     0     0   -4.44277D-04    0.64808  0.0      1.00000     -6.41743    1.44847
   7    0     1     0   -4.80195D-04    1.08061  0.0      1.00000     -5.14787    1.22582
   8    0     1     0   -4.24693D-04    0.84344  0.0      1.00000      6.81788    3.00205
   9    0     1     0   -3.51050D-04    0.80972  0.0      1.00000      5.01598   -0.77969
  10    3     1     0   -1.56711D-03    0.79710  0.0      1.00000      6.32878   -1.78872
  11    0     0     0    1.04736D-05    0.0      0.0      1.00000      0.0        0.0

ESTIMATED ABSOLUTE POINT FLUX RELATIVE ERROR  5.49374D-05
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES-------------------------   0.6119765
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   0.6119836   0.6119707
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   0.6120025   0.6119717

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  8.39890D-01
  1.27838  1.39842  1.52216

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.040   0.168

ADJOINT FLUX ENERGY SPECTRUM BY GROUP, 1 TO MAX, (SUMMED OVER SPACE)
  3.77764D-05  3.92851D-05  5.28613D-05

ADJOINT FLUX SPACE FUNCTION BY ZONE (SUMMED OVER ENERGY)
  2.63328D-04  1.18921D-04  3.77339D-05

POINT ADJOINT FLUX INTERFACE FILE ATFLUX (VERSION  1) HAS BEEN WRITTEN ON UNIT NUMBER  17

DOPC USE OF CONTAINER ARRAYS, CONTROL      11, MAX DATA    2880

TOTAL CPU TIME IS  0.222 MINUTES AND TOTAL CLOCK TIME IS   2.533 MINUTES


CASE TITLE -  PERIODIC BOUNDARY IN THETA-R GEOMETRY, CASE A4 WITH BLACK ABSORBER
              24X20X3 GROUP, 1440 POINTS  FWRD. + ADJ.

MPARM    18000       0       0       0       0       0       0       0       0       0       0       0

****STANDARD FILE CARD INPUT****
CV CONTRL                                                                                    CARD     1
1D PROINS /                                                                                  CARD     2
* 3-D (X,Y,Z) BUCKLING SEARCH (OLD WHIRLAWAY CASE) - 9X9X5X2          *                       CARD     3
* RUNNING IN THE PLANE STORED MODE - * PLANES STORED                  *                       CARD     4
*      * *      *  0.0 74R  0 100R                                                            CARD     5
1D DVRINS  0.0 100R  18000  0 99R                                                            CARD     6
1D XCPINS  0.0 100R  0 23R  1  0 76R                                                         CARD     7
1D DTNINS  0.0  1.0  0.0  10.0  1.0 2R  0.09  0.0 3R  1.0-6  5.0-5                           CARD     8
  0.0 88R                                                                                    CARD     9
  0 3R  1  4  1  0 13R  50  0 8R  1 5R  0  1  0  1 6R  0 2R 5 1 1 0 3R                       CARD    10
  1  0  1  1  0 2R  0  1  2  0  2  4  0 38R                                                  CARD    11
1D *      *  0.0 100R  0 100R                                                                CARD    12
CV GRUPXS                                                                                    CARD    13
```

```
RUN TITLE -  3-D (X,Y,Z) BUCKLING SEARCH (OLD WHIRLAWAY CASE) - 9X9X5X2
             RUNNING IN THE PLANE STORED MODE - 4 PLANES STORED

                        VENTURE NEUTRONICS CODE BLOCK - VERSION 2 --- APRIL 30, 1977.
                        ------------------------------------------------------------

REFERENCE REAL TIME FROM ZNATON INTERFACE FILE =  0.0          DAYS

SOLUTION BY FINITE-DIFFERENCE DIFFUSION THEORY
DIRECT BUCKLING SEARCH PROBLEM
A REGULAR ADJOINT WILL FOLLOW FORWARD PROBLEM
PERTURBATION RESULTS ARE REQUESTED
GEOMETRY NO. 14    3-D X-Y-Z
NUMBER OF ENERGY GROUPS                                  2
NUMBER OF UPSCATTER GROUPS (MAX)                         0
NUMBER OF DOWNSCATTER GROUPS (MAX)                       1
NUMBER OF INTERVALS IN DIMENSION 1 (COLUMNS)             9
NUMBER OF INTERVALS IN DIMENSION 2 (ROWS)                9
NUMBER OF INTERVALS IN DIMENSION 3 (PLANES)              5
NUMBER OF ZONES                                          3
NUMBER OF REGIONS                                        3
NUMBER OF BLACK ABSORBER ZONES                           0
BOUNDARY INDICATORS-   LEFT  1  RIGHT  0
                        TOP  0 BOTTOM  1
                      FRONT  0   REAR  0
```

MEMORY REQUIREMENTS FOR DATA STORAGE

	TOTAL MINIMUM	TOTAL MAXIMUM	A	B	C	D
STORAGE AVAILABLE	18000					
MACRO CALCULATION	181					
EQUATION CONSTANTS CALCULATION						
CORE CONTAINED OR SPACE STORED	2679	2841				
PLANE STORED	1150	1312				
ROW STORED	482	644				
MULTI-LEVEL PLANE STORED	1220	1382				
INITIAL FLUX						
CORE CONTAINED OR SPACE STORED	1207	1531				
OTHER MODES	397	721				
ITERATIVE PROCESS						
CORE CONTAINED	11147		8444	450	56	2197
SPACE STORED	5928		5437	450	41	0
13 PLANES STORED	13873		13382	450	41	0
1 PLANE STORED	1969		1478	450	41	0
13 ROWS STORED	2079		1588	450	41	0
1 ROW STORED	491		0	450	41	0
13 MULTI-LEVEL PLANES STORED	15107		486	450	41	14130
PERTURBATION CALCULATION	3804					

DATA WILL BE STORED FOR ALL GROUPS, ALL SPACE

```
MEMORY LOCATIONS RESERVED FOR DATA STORAGE---   18000
MAX MEMORY LOCATIONS REQUIRED FOR THIS PROB--   11147
MEMORY LOCATIONS NOT USED-------------------    6853

     SPECIAL SCRATCH DATASET REQUIREMENTS
     MAXIMUM PHYSICAL RECORD IS      7200 WORDS
```

```
RITE CONTAINER ARRAYS, CONTROL       36 DATA     6807
FILE 24 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      2    810   1620      1   5187
FILE 27 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      2    810   1620   1621   3567
FILE 28 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      2    810   1620   3241   1947
DIRECT ACCESS FILE 40  REQUIRES      2 RECORDS      2196 WORDS IN LENGTH

DD PARAMETERS FOLLOW FOR  E1 = 3520  AND  B2 =   2592
N2=   3  N3=  10  N4=   1  N5=  12  N6=  10  N7=   2  N8=   2  N9=   2  N10=   2  N11=   3  N12=   1  N13=   2  N14=   1  N15=  10
N16=   3   (NOTE THAT IF THE FLUXES ARE TO BE EXPANDED FROM EXISTING RTFLUX, N10=   3)

REQUIRED DISK STORAGE SPACE FOR FLUX(UNITS 24,27,28) IS      10560 BYTES.
                             FOR CONSTANTS(UNIT 40) IS--      31104 BYTES.
                             FOR CONSTANTS(UNIT 23) IS--      35200 BYTES.
REQUIRED TOTAL DISK STORAGE SPACE IS-------------------    5505792 BYTES.

FOR THE ASSIGNED DATA STORAGE, THE REQUIRED REGION SIZE IS APPROXIMATELY  402K BYTES

TITLE FROM CROSS SECTION FILE / GRUPXS CROSS SECTIONS FOR VENTURE SAMPLE PROBLEM

*** WARNING *** NUCLIDE NAMES OR CLASSES ON NDXSRF AND GRUPXS DO NOT COMPARE

CROSS SECTION          UNIQUE                          ABSOLUTE                          CLASS
    ORDER NO.  NDXSRF          GRUPXS       NDXSRF          GRUPXS       NDXSRF          GRUPXS
            1  ZONE1   NOT EQ  ZONE1   OR  ZONE1   NOT EQ          OR       0  NOT EQ       0
            2  ZONE2   NOT EQ  ZONE2   OR  ZONE2   NOT EQ          OR       0  NOT EQ       0
            3  ZONE3   NOT EQ  ZONE3   OR  ZONE3   NOT EQ          OR       0  NOT EQ       0

         3 NUCLIDES HAVE ERRORS


PRINCIPAL MACROSCOPIC CROSS SECTIONS

GROUP    1
ZONE   D              SIGA          SIGNF         SIGWF         SIGAS         SIGNFS
    1  1.500001E 00  1.200000E-03  3.999997E-03  5.000000E-14  0.0           0.0
    2  1.700001E 00  6.999997E-04  3.999998E-04  4.999998E-15  0.0           0.0
    3  1.200000E 00  5.199998E-04  0.0           0.0           0.0           0.0

GROUP    2
ZONE   D              SIGA          SIGNF         SIGWF         SIGAS         SIGNFS
    1  1.200000E 00  4.699998E-03  6.299996E-02  1.968750E-13  0.0           0.0
    2  1.129999E 00  6.299999E-03  2.499999E-02  6.249997E-14  0.0           0.0
    3  8.700005E-01  7.999998E-03  0.0           0.0           0.0           0.0

FISSION SPECTRUM CONSTANT FOR ALL ZONES
  1.000000E 00  0.0

1/V CONSTANT FOR ALL ZONES
  1.000000E 00  1.000000E 00


SCATTERING MACROSCOPIC CROSS SECTIONS

GROUP    1  MBAND    1  MJJ    1
TP0
  0.0           0.0           0.0

GROUP    2  MBAND    2  MJJ    1
TP0
  0.0           3.299999E-03  0.0           5.199999E-03  0.0           6.699998E-03

SCATTERING REMOVAL
GROUP    1
  3.299999D-03  5.199999D-03  6.699998D-03
```

```
GROUP     2
  0.0             0.0             0.0

FINE MESH DESCRIPTION - POINT IS LOCATED AT THE CENTROID OF THE VOLUME ELEMENT
DISTANCE TO POINT - DIMENSION 1 (LEFT TO RIGHT)
    1   1.0000     2   3.0000     3   5.0000     4   7.0000     5  10.0000     6  14.0000     7  17.5000     8  20.5000
    9  23.5000
DISTANCE TO POINT - DIMENSION 2 (TOP TO BOTTOM)
    1   1.0000     2   3.0000     3   5.0000     4   7.0000     5   9.0000     6  11.0000     7  13.0000     8  15.0000
    9  17.0000
DISTANCE TO POINT - DIMENSION 3 (FRONT TO REAR)
    1   1.5000     2   4.5000     3   7.5000     4  10.5000     5  13.5000

SEARCH LIMITING FACTORS - SP1 =  -1.275115E 00 SP2 =  -5.591301E 01  SA =   8.28741BE-02 SNF =   0.0

DETERMINE INITIAL PARAMETERS FOR ITERATIVE PROCEDURE

REFERENCE POINT FOR INITIALIZATION WILL BE AT COLUMN =      2 ROW =      8 PLANE =      3 ZONE =      1
INITIAL OUTER ITERATION EIGENVALUE         0.049787  OPTION     0
INITIAL OVERRELAXATION COEFFICIENTS MAX.  1.596701  MIN.  1.584751  INNER ITERATIONS MAX.    4  MIN.    4  OPTION    0
MESH POINT SWEEP OPTION    1
OUTER ITERATION LIMIT TO BE USED    50  ESTIMATED    19

MAXIMUM STORAGE USED FOR CALCULATING INITIAL PARAMETERS WAS    2454

INITIAL FLUX IS FXK(J,K)*FY(I)*FZ(K9)

TOTAL CORE REQUIRED FOR DATA STORAGE IS  11094 WORDS
ELAPSED CPU AND CLOCK MINUTES ARE  0.052   0.952
```

```
A FLUX - EIGENVALUE PROBLEM FOLLOWS
      4 INNERS MIN,  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE     MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS        K        SEARCH FACTOR  S.F.-CALC
   1     0     0     0    5.67466D 00    0.0       0.0     1.00000       0.0          0.0        0.0430242  0.0            0.0
NEW OVERRELAXATION COEFFICIENTS CALCULATED
  1.40021  1.39680
   2     0     0     0    8.45159D 00    5.66444   0.0     1.00000       1.00000      0.0        0.0494369  0.0           -2.65383D 00
   3     0     0     0   -6.01462D-01    0.37190   0.0     1.00000       0.59209      0.0        0.0537092 -1.02009D-01 -2.39535D 00
   4     0     0     0   -4.62942D-01    0.53822   0.0     1.00000       0.74341      0.11542    0.0548734 -1.93817D-01 -2.37107D 00
   5     0     0     0   -4.43629D-01    0.73647   0.0     1.00000      15.99354     -4.05419    0.0559678 -2.76444D-01 -2.35303D 00
   6     0     0     0   -4.28708D-01    0.75201   0.0     1.00000       3.22178     -0.13121    0.0569559 -3.50808D-01 -2.37936D 00
   7     0     0     0   -4.15343D-01    0.76115   0.0     1.00000       6.60886     -2.47856    0.0578623 -4.17736D-01 -2.32771D 00
   8     0     0     0   -4.03053D-01    0.76889   0.0     1.00000      11.61119     -6.15168    0.0586981 -4.77971D-01 -2.31728D 00
   9     0     0     0   -3.82725D-01    0.75820   0.0     1.00000       1.06245      1.66775    0.0602377 -5.86395D-01 -2.29939D 00
  10     0     0     0   -3.48518D-01    0.73636   0.0     1.00000      -9.57098     10.22132    0.0628631 -7.59873D-01 -2.26944D 00
  11     0     0     0   -3.03553D-01    0.71921   0.0     1.00000       7.07794     -3.54228    0.0663090 -9.68045D-01 -2.23103D 00
  12     4     0     0   -4.48260D-01    0.72142   0.0     1.00000       1.08525      0.0        0.0686497 -1.02009D 00 -2.21666D 00
  13     0     1     0   -2.76270D-01    0.0       0.0     1.00000       0.0          0.0        0.0733752 -1.27512D 00 -2.10434D 00
  14     0     0     0   -3.44565D-01    1.07493   0.0     1.00000      -4.14183      3.91832    0.0673633 -1.02009D 00 -2.21321D 00
  15     0     0     0   -2.51334D-01    0.60375   0.0     1.00000       2.67335      6.53594    0.0701165 -1.17948D 00 -2.19255D 00
  16     0     0     0   -1.95692D-01    0.68077   0.0     1.00000       1.57165      0.27280    0.0747460 -1.40581D 00 -2.14454D 00
  17     0     0     0   -1.66745D-01    0.76871   0.0     1.00000      88.21709    -41.87192    0.0764145 -1.47610D 00 -2.12326D 00
  18     0     0     0   -1.44471D-01    0.79418   0.0     1.00000       5.24162     -0.94625    0.0780885 -1.54990D 00 -2.10749D 00
  19     0     0     0   -1.22421D-01    0.78616   0.0     1.00000       2.79310      0.72887    0.0799208 -1.62740D 00 -2.09048D 00
  20     0     0     0   -9.87286D-02    0.75711   0.0     1.00000      -3.58395      6.07318    0.0819299 -1.70877D 00 -2.07220D 00
  21     0     0     0   -7.36168D-02    0.70884   0.0     1.00000     -39.39581     37.96339    0.0841366 -1.79420D 00 -2.05265D 00
  22     0     0     0   -4.67523D-02    0.61170   0.0     1.00000     -19.07022     19.51677    0.0865677 -1.88391D 00 -2.03175D 00
  23     0     0     0   -1.89394D-02    0.39563   0.0     1.00000    -128.13467    123.61820    0.0892552 -1.97810D 00 -2.00940D 00
  24     0     0     0    1.36619D-02    0.42084   0.0     1.00000       0.60696      0.04537    0.0902513 -2.00940D 00 -1.99893D 00
  25     0     0     0    1.74330D-03    0.18852   0.0     1.00000      -0.65789      0.52492    0.0899836 -1.99893D 00 -1.99961D 00
  26     0     0     0    6.18074D-04    0.32152   0.0     1.00000       0.14418      0.05197    0.0899892 -1.99961D 00 -2.00006D 00
  27     0     0     0    2.32780D-04    0.34065   0.0     1.00000       0.56018     -0.01353    0.0900018 -2.00006D 00 -1.99999D 00
  28     0     0     0    3.92124D-05    0.21776   0.0     1.00000      -0.53358      0.32815    0.0900001 -1.99999D 00 -1.99998D 00
  29     0     0     0    1.09695D-05    0.27404   0.0     1.00000       0.17925      0.04006    0.0899998 -1.99998D 00 -1.99999D 00
  30     0     0     0    3.72899D-06    0.32957   0.0     1.00000       0.94382     -0.11445    0.0900000 -1.99999D 00 -1.99999D 00

ESTIMATED ABSOLUTE POINT FLUX RELATIVE ERROR  9.65656D-06

FINAL CALCULATED KEFFECTIVE   0.0900000
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES--------------------------   0.0900000
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   0.0900003   0.0899997
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   0.0900003   0.0899999

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  7.21416D-01
  1.39996  1.39656

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.082   0.181

    LEAKAGE  1.83970E 13  TOTAL LOSSES  1.47888E 13  TOTAL PRODUCTIONS  1.33100E 12  REACTOR POWER(WATTS)  1.00000D 01

BUCKLINGS WERE MULTIPLIED BY -9.9996621D-01, FRACTION LOSS TO SEARCH PARAMETER -0.2660146

BOUNDARY NEUTRON LEAKAGE
GROUP    LEFT          RIGHT          TOP          BOTTOM         FRONT          BACK
 1   0.0          2.99386D 11  2.59557D 12  0.0          7.25090D 12  7.25090D 12
 2   0.0          4.54990D 10  1.44948D 11  0.0          4.04924D 11  4.04924D 11
SUM  0.0          3.44885E 11  2.74051E 12  0.0          7.65583E 12  7.65583E 12
```

GROUP NEUTRON BALANCE FOR EACH ZONE

ZONE	GROUP	ABSORPTIONS	B**2 LOSSES	1/V LOSS	OUT-SCATTER	IN-SCATTER	P1 IN-SCATTER	SOURCE	POWER(WATTS)	AVERAGE FLUX
1	1	1.82956E 11	-2.49377E 12	0.0	5.03129E 11	0.0	0.0	1.29073E 13	7.62316E 00	7.05848E 10
1	2	4.11660E 10	-1.14610E 11	0.0	0.0	5.03129E 11	0.0	0.0	1.72437E 00	4.05497E 09
SUM		2.24122E 11	-2.60838E 12	0.0	5.03129E 11	5.03129E 11	0.0	1.29073E 13	9.34754E 00	
2	1	4.00927E 10	-1.06174E 12	0.0	2.97833E 11	0.0	0.0	1.88159E 12	2.86378E-01	2.65165E 10
2	2	3.69012E 10	-7.21734E 10	0.0	0.0	2.97833E 11	0.0	0.0	3.66083E-01	2.71173E 09
SUM		7.69939E 10	-1.13391E 12	0.0	2.97833E 11	2.97833E 11	0.0	1.88159E 12	6.52461E-01	
3	1	6.77394E 09	-1.70459E 11	0.0	8.72798E 10	0.0	0.0	0.0	0.0	5.36084E 09
3	2	1.79551E 10	-2.12921E 10	0.0	0.0	8.72798E 10	0.0	0.0	0.0	9.23618E 08
SUM		2.47291E 10	-1.91751E 11	0.0	8.72798E 10	8.72798E 10	0.0	0.0	0.0	

OVERALL NEUTRON BALANCE

GROUP	ABSORPTIONS	B**2 LOSSES	1/V LOSS	OUT-SCATTER	IN-SCATTER	P1 IN-SCATTER	SOURCE	POWER(WATTS)
1	2.29822E 11	-3.72597E 12	0.0	8.88242E 11	0.0	0.0	1.47888E 13	7.90954E 00
2	9.60223E 10	-2.08075E 11	0.0	0.0	8.88242E 11	0.0	0.0	2.09046E 00
SUM	3.25845E 11	-3.93404E 12	0.0	8.88242E 11	8.88242E 11	0.0	1.47888E 13	1.00000E 01

ZONE VOLUMES FOLLOW. TOTAL VOLUME 6.75000E 03
2.16000E 03 2.16000E 03 2.43000E 03

ZONE AVERAGE FLUX INTERFACE FILE RZFLUX (VERSION 1) HAS BEEN WRITTEN ON UNIT NUMBER 18

BUCKLINGS CALCULATED ALONG PLANE 2 FOLLOW

ZONE BUCKLINGS FOR GROUP 1
4.24407E-02 4.24407E-02 4.24407E-02

ZONE BUCKLINGS FOR GROUP 2
4.24407E-02 4.24407E-02 4.24407E-02

ZONE AVERAGE BUCKLINGS FOR EACH GROUP
4.24407E-02 4.24407E-02

ZONE AVERAGE DIFFUSION COEFFICIENTS FOR EACH GROUP
1.53388E 00 1.13175E 00

GROSS BUCKLING 4.24407E-02

BUCKLINGS CALCULATED ALONG PLANE 4 FOLLOW

ZONE BUCKLINGS FOR GROUP 1
4.24407E-02 4.24407E-02 4.24407E-02

ZONE BUCKLINGS FOR GROUP 2
4.24407E-02 4.24407E-02 4.24407E-02

ZONE AVERAGE BUCKLINGS FOR EACH GROUP
4.24407E-02 4.24407E-02

ZONE AVERAGE DIFFUSION COEFFICIENTS FOR EACH GROUP
1.53388E 00 1.13175E 00

GROSS BUCKLING 4.24407E-02

POINT POWER DISTRIBUTION (WATTS/CC)

PLANE NUMBER 1

	1	2	3	4	5	6	7	8	9
1	3.198D-04	3.046D-04	2.747D-04	2.309D-04	2.402D-05	1.542D-05	0.0	0.0	0.0
2	9.497D-04	9.046D-04	8.158D-04	6.857D-04	7.132D-05	4.580D-05	0.0	0.0	0.0
3	1.551D-03	1.477D-03	1.332D-03	1.120D-03	1.165D-04	7.478D-05	0.0	0.0	0.0
4	2.105D-03	2.005D-03	1.808D-03	1.520D-03	1.581D-04	1.015D-04	0.0	0.0	0.0
5	2.595D-03	2.471D-03	2.229D-03	1.873D-03	1.949D-04	1.251D-04	0.0	0.0	0.0
6	3.006D-03	2.863D-03	2.582D-03	2.170D-03	2.257D-04	1.449D-04	0.0	0.0	0.0
7	3.325D-03	3.168D-03	2.857D-03	2.401D-03	2.498D-04	1.604D-04	0.0	0.0	0.0
8	3.544D-03	3.376D-03	3.045D-03	2.559D-03	2.662D-04	1.709D-04	0.0	0.0	0.0
9	3.655D-03	3.482D-03	3.140D-03	2.639D-03	2.745D-04	1.763D-04	0.0	0.0	0.0

PLANE NUMBER 2

	1	2	3	4	5	6	7	8	9
1	8.372D-04	7.975D-04	7.193D-04	6.045D-04	6.288D-05	4.037D-05	0.0	0.0	0.0
2	2.486D-03	2.368D-03	2.136D-03	1.795D-03	1.867D-04	1.199D-04	0.0	0.0	0.0
3	4.060D-03	3.867D-03	3.488D-03	2.931D-03	3.049D-04	1.958D-04	0.0	0.0	0.0
4	5.510D-03	5.249D-03	4.733D-03	3.979D-03	4.138D-04	2.657D-04	0.0	0.0	0.0
5	6.793D-03	6.470D-03	5.835D-03	4.905D-03	5.102D-04	3.276D-04	0.0	0.0	0.0
6	7.869D-03	7.496D-03	6.760D-03	5.682D-03	5.910D-04	3.795D-04	0.0	0.0	0.0
7	8.706D-03	8.293D-03	7.479D-03	6.286D-03	6.539D-04	4.198D-04	0.0	0.0	0.0
8	9.279D-03	8.839D-03	7.971D-03	6.700D-03	6.969D-04	4.474D-04	0.0	0.0	0.0
9	9.570D-03	9.116D-03	8.221D-03	6.910D-03	7.187D-04	4.615D-04	0.0	0.0	0.0

PLANE NUMBER 3

	1	2	3	4	5	6	7	8	9
1	1.035D-03	9.858D-04	8.891D-04	7.473D-04	7.772D-05	4.990D-05	0.0	0.0	0.0
2	3.073D-03	2.927D-03	2.640D-03	2.219D-03	2.308D-04	1.482D-04	0.0	0.0	0.0
3	5.018D-03	4.780D-03	4.311D-03	3.623D-03	3.769D-04	2.420D-04	0.0	0.0	0.0
4	6.811D-03	6.488D-03	5.851D-03	4.918D-03	5.115D-04	3.284D-04	0.0	0.0	0.0
5	8.396D-03	7.998D-03	7.213D-03	6.063D-03	6.306D-04	4.049D-04	0.0	0.0	0.0
6	9.726D-03	9.265D-03	8.356D-03	7.023D-03	7.305D-04	4.690D-04	0.0	0.0	0.0
7	1.076D-02	1.025D-02	9.245D-03	7.771D-03	8.082D-04	5.189D-04	0.0	0.0	0.0
8	1.147D-02	1.093D-02	9.853D-03	8.282D-03	8.614D-04	5.531D-04	0.0	0.0	0.0
9	1.183D-02	1.127D-02	1.016D-02	8.541D-03	8.884D-04	5.704D-04	0.0	0.0	0.0

PLANE NUMBER 4

	1	2	3	4	5	6	7	8	9
1	8.372D-04	7.975D-04	7.193D-04	6.045D-04	6.288D-05	4.037D-05	0.0	0.0	0.0
2	2.486D-03	2.368D-03	2.136D-03	1.795D-03	1.867D-04	1.199D-04	0.0	0.0	0.0
3	4.060D-03	3.867D-03	3.488D-03	2.931D-03	3.049D-04	1.958D-04	0.0	0.0	0.0
4	5.510D-03	5.249D-03	4.733D-03	3.979D-03	4.138D-04	2.657D-04	0.0	0.0	0.0
5	6.793D-03	6.470D-03	5.835D-03	4.905D-03	5.102D-04	3.276D-04	0.0	0.0	0.0
6	7.869D-03	7.496D-03	6.760D-03	5.682D-03	5.910D-04	3.795D-04	0.0	0.0	0.0
7	8.706D-03	8.293D-03	7.479D-03	6.286D-03	6.539D-04	4.198D-04	0.0	0.0	0.0
8	9.279D-03	8.839D-03	7.971D-03	6.700D-03	6.969D-04	4.474D-04	0.0	0.0	0.0
9	9.570D-03	9.116D-03	8.221D-03	6.910D-03	7.187D-04	4.615D-04	0.0	0.0	0.0

PLANE NUMBER 5

	1	2	3	4	5	6	7	8	9
1	3.198D-04	3.046D-04	2.747D-04	2.309D-04	2.402D-05	1.542D-05	0.0	0.0	0.0
2	9.497D-04	9.046D-04	8.158D-04	6.857D-04	7.132D-05	4.580D-05	0.0	0.0	0.0
3	1.551D-03	1.477D-03	1.332D-03	1.120D-03	1.165D-04	7.478D-05	0.0	0.0	0.0
4	2.105D-03	2.005D-03	1.808D-03	1.520D-03	1.581D-04	1.015D-04	0.0	0.0	0.0
5	2.595D-03	2.471D-03	2.229D-03	1.873D-03	1.949D-04	1.251D-04	0.0	0.0	0.0
6	3.006D-03	2.863D-03	2.582D-03	2.170D-03	2.257D-04	1.449D-04	0.0	0.0	0.0
7	3.325D-03	3.168D-03	2.857D-03	2.401D-03	2.498D-04	1.604D-04	0.0	0.0	0.0
8	3.544D-03	3.376D-03	3.045D-03	2.559D-03	2.662D-04	1.709D-04	0.0	0.0	0.0
9	3.655D-03	3.482D-03	3.140D-03	2.639D-03	2.745D-04	1.763D-04	0.0	0.0	0.0

```
ADJOINT PROBLEM FOLLOWS
      4 INNERS MIN,  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF,   ICVR=0,1-YES,NO INNERS CONVR,   OCVR=0,1-YES,NO OUTERS CONVR,
ITER  PROC  ICVR  OCVR   FLUX CHANGE     MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS
  1     0     0     0    1.84590D 01    0.0       0.0      1.00000       0.0         0.0
  2     0     0     0    2.84369D 00    1.57590   0.0      1.00000       1.00000     0.0
  3     0     0     0    2.42313D-01    0.20637   0.0      1.00000       0.26003     0.0
  4     0     0     0    3.50240D-02    0.16205   0.0      1.00000       0.25395    -0.01320
  5     0     0     0    1.00632D-02    0.28821   0.0      1.00000      -0.16950     0.07907
  6     0     0     0    2.58423D-03    0.26968   0.0      1.00000       0.33822     0.00918
  7     0     0     0    6.85700D-04    0.27313   0.0      1.00000       0.30541     0.01888
  8     0     0     0    1.85374D-04    0.27471   0.0      0.0           0.57363    -0.05311
  9     0     0     0    5.01235D-05    0.27516   0.0      0.0           0.49579    -0.03189
 10     0     0     0    1.36358D-05    0.27541   0.0      0.0           0.63535    -0.07021

ESTIMATED ABSOLUTE POINT FLUX RELATIVE ERROR  5.18295D-06
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES-------------------------   0.0900000
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   0.0900012   0.0899988
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   0.0900092   0.0899961

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  2.75414D-01
  1.39656  1.39996

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.024   0.064

ADJOINT FLUX ENERGY SPECTRUM BY GROUP, 1 TO MAX, (SUMMED OVER SPACE)
  1.37455D-05  1.34403D-04

ADJOINT FLUX SPACE FUNCTION BY ZONE (SUMMED OVER ENERGY)
  3.03576D-04  1.29435D-04  2.66235D-05


REGULAR, ADJOINT FLUX INTERGRALS---(DELTA K)/(K*DELTA S WHERE S REPERSENTS MACRO. CROSS SECTIONS. BIG DADDY =  1.868256D-09

 ZONE  GRP  SIGA,SIGR,DB**2      B**2            NU*SIGF       DIFF. COEF.
   1    1    -1.104552E 01  -1.656830E 01   1.227281E 02  -5.922714E-01
        2    -6.721860E 00  -8.066224E 00   7.000970E 00  -3.475140E-01
   2    1    -2.113946E 00  -3.593710E 00   2.348830E 01  -1.449168E-01
        2    -1.962744E 00  -2.217898E 00   2.345262E 00  -1.184277E-01
   3    1    -1.873039E-01  -2.247646E-01   2.081155E 00  -2.000686E-02
        2    -1.937901E-01  -1.685975E-01   3.451945E-01  -1.991272E-02

VOLUME INTEGRALS  FLUX*ADJOINT FLUX -2.22251E 01  CHI*ADJOINT FLUX, NU-SIGF*FLUX  1.000000D 00

GRP. TO GRP.   DELTA-K/(K*DELTA-SIGS) FOR ALL ZONES 1,2,3,.... - (THE IN-GROUP TERMS MAKE NO CONTRIBUTION.)
  1        1  1.104552E 01  2.113946E 00  1.873039E-01
  2        1  6.300871E-01  2.110735E-01  3.106750E-02
  1        2  1.178712E 02  1.977725E 01  1.175513E 00
  2        2  6.721860E 00  1.962744E 00  1.937901E-01

PROMPT-NEUTRON LIFETIME IS  2.222520 01  SEC.


*****************************************************************************************
NORMALIZATION OF IMPORTANCE MAPS IS TO UNIT FISSION SOURCE IMPORTANCE FOR THE ACTUAL PROBLEM.      *
MULTIPLY BY THE FRACTION OF THE CORE TREATED IF THE VALUES ARE TO BE MADE RELATIVE TO THE          *
TOTAL, BUT TAKE CARE TO UNDERSTAND THAT THIS IS APPROPRIATE IN A SPECIFIC SITUATION.               *
*****************************************************************************************
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MACRO. ABSORP. CROSS SECTION IMPORTANCE MAP (SIGA/K)(DELTA K/DELTA SIGA).

PLANE NUMBER 1

	1	2	3	4	5	6	7	8	9
1	7.353D-08	6.758D-08	5.678D-08	4.308D-08	2.654D-08	1.065D-08	4.571D-09	1.217D-09	1.141D-10
2	6.484D-07	5.960D-07	5.007D-07	3.799D-07	2.341D-07	9.396D-08	4.031D-08	1.073D-08	1.006D-09
3	1.729D-06	1.589D-06	1.335D-06	1.013D-06	6.241D-07	2.505D-07	1.075D-07	2.861D-08	2.682D-09
4	3.184D-06	2.927D-06	2.459D-06	1.866D-06	1.149D-06	4.614D-07	1.980D-07	5.271D-08	4.941D-09
5	4.840D-06	4.448D-06	3.737D-06	2.836D-06	1.747D-06	7.013D-07	3.009D-07	8.010D-08	7.509D-09
6	6.495D-06	5.970D-06	5.016D-06	3.806D-06	2.345D-06	9.412D-07	4.038D-07	1.075D-07	1.008D-08
7	7.951D-06	7.308D-06	6.140D-06	4.658D-06	2.870D-06	1.152D-06	4.943D-07	1.316D-07	1.234D-08
8	9.031D-06	8.301D-06	6.974D-06	5.292D-06	3.260D-06	1.309D-06	5.615D-07	1.495D-07	1.401D-08
9	9.606D-06	8.829D-06	7.418D-06	5.628D-06	3.467D-06	1.392D-06	5.972D-07	1.590D-07	1.490D-08

PLANE NUMBER 2

	1	2	3	4	5	6	7	8	9
1	5.040D-07	4.632D-07	3.892D-07	2.953D-07	1.819D-07	7.303D-08	3.133D-08	8.341D-09	7.819D-10
2	4.444D-06	4.085D-06	3.432D-06	2.604D-06	1.604D-06	6.440D-07	2.763D-07	7.356D-08	6.895D-09
3	1.185D-05	1.089D-05	9.151D-06	6.943D-06	4.277D-06	1.717D-06	7.367D-07	1.961D-07	1.839D-08
4	2.183D-05	2.006D-05	1.686D-05	1.279D-05	7.879D-06	3.163D-06	1.357D-06	3.613D-07	3.387D-08
5	3.317D-05	3.049D-05	2.562D-05	1.944D-05	1.197D-05	4.807D-06	2.062D-06	5.490D-07	5.147D-08
6	4.452D-05	4.092D-05	3.438D-05	2.608D-05	1.607D-05	6.451D-06	2.768D-06	7.368D-07	6.907D-08
7	5.449D-05	5.009D-05	4.208D-05	3.193D-05	1.967D-05	7.896D-06	3.388D-06	9.020D-07	8.455D-08
8	6.190D-05	5.689D-05	4.780D-05	3.627D-05	2.234D-05	8.970D-06	3.848D-06	1.025D-06	9.604D-08
9	6.584D-05	6.052D-05	5.085D-05	3.858D-05	2.377D-05	9.541D-06	4.093D-06	1.090D-06	1.022D-07

PLANE NUMBER 3

	1	2	3	4	5	6	7	8	9
1	7.700D-07	7.077D-07	5.946D-07	4.511D-07	2.779D-07	1.116D-07	4.787D-08	1.274D-08	1.195D-09
2	6.790D-06	6.241D-06	5.244D-06	3.979D-06	2.451D-06	9.839D-07	4.221D-07	1.124D-07	1.054D-08
3	1.810D-05	1.664D-05	1.398D-05	1.061D-05	6.535D-06	2.623D-06	1.126D-06	2.996D-07	2.809D-08
4	3.335D-05	3.065D-05	2.575D-05	1.954D-05	1.204D-05	4.832D-06	2.073D-06	5.520D-07	5.174D-08
5	5.068D-05	4.658D-05	3.914D-05	2.970D-05	1.829D-05	7.344D-06	3.151D-06	8.389D-07	7.864D-08
6	6.802D-05	6.252D-05	5.253D-05	3.985D-05	2.455D-05	9.856D-06	4.229D-06	1.126D-06	1.055D-07
7	8.326D-05	7.653D-05	6.430D-05	4.878D-05	3.005D-05	1.206D-05	5.176D-06	1.378D-06	1.292D-07
8	9.457D-05	8.693D-05	7.304D-05	5.541D-05	3.414D-05	1.370D-05	5.880D-06	1.565D-06	1.467D-07
9	1.006D-04	9.246D-05	7.768D-05	5.894D-05	3.631D-05	1.458D-05	6.254D-06	1.665D-06	1.561D-07

PLANE NUMBER 4

	1	2	3	4	5	6	7	8	9
1	5.040D-07	4.632D-07	3.892D-07	2.953D-07	1.819D-07	7.303D-08	3.133D-08	8.341D-09	7.819D-10
2	4.444D-06	4.085D-06	3.432D-06	2.604D-06	1.604D-06	6.440D-07	2.763D-07	7.356D-08	6.895D-09
3	1.185D-05	1.089D-05	9.151D-06	6.943D-06	4.277D-06	1.717D-06	7.367D-07	1.961D-07	1.839D-08
4	2.183D-05	2.006D-05	1.686D-05	1.279D-05	7.879D-06	3.163D-06	1.357D-06	3.613D-07	3.387D-08
5	3.317D-05	3.049D-05	2.562D-05	1.944D-05	1.197D-05	4.807D-06	2.062D-06	5.490D-07	5.147D-08
6	4.452D-05	4.092D-05	3.438D-05	2.608D-05	1.607D-05	6.451D-06	2.768D-06	7.368D-07	6.907D-08
7	5.449D-05	5.009D-05	4.208D-05	3.193D-05	1.967D-05	7.896D-06	3.388D-06	9.020D-07	8.455D-08
8	6.190D-05	5.689D-05	4.780D-05	3.627D-05	2.234D-05	8.970D-06	3.848D-06	1.025D-06	9.604D-08
9	6.584D-05	6.052D-05	5.085D-05	3.858D-05	2.377D-05	9.541D-06	4.093D-06	1.090D-06	1.022D-07

PLANE NUMBER 5

	1	2	3	4	5	6	7	8	9
1	7.353D-08	6.758D-08	5.678D-08	4.308D-08	2.654D-08	1.065D-08	4.571D-09	1.217D-09	1.141D-10
2	6.484D-07	5.960D-07	5.007D-07	3.799D-07	2.341D-07	9.396D-08	4.031D-08	1.073D-08	1.006D-09
3	1.729D-06	1.589D-06	1.335D-06	1.013D-06	6.241D-07	2.505D-07	1.075D-07	2.861D-08	2.682D-09
4	3.184D-06	2.927D-06	2.459D-06	1.866D-06	1.149D-06	4.614D-07	1.980D-07	5.271D-08	4.941D-09
5	4.840D-06	4.448D-06	3.737D-06	2.836D-06	1.747D-06	7.013D-07	3.009D-07	8.010D-08	7.509D-09
6	6.495D-06	5.970D-06	5.016D-06	3.806D-06	2.345D-06	9.412D-07	4.038D-07	1.075D-07	1.008D-08
7	7.951D-06	7.308D-06	6.140D-06	4.658D-06	2.870D-06	1.152D-06	4.943D-07	1.316D-07	1.234D-08
8	9.031D-06	8.301D-06	6.974D-06	5.292D-06	3.260D-06	1.309D-06	5.615D-07	1.495D-07	1.401D-08
9	9.606D-06	8.829D-06	7.418D-06	5.628D-06	3.467D-06	1.392D-06	5.972D-07	1.590D-07	1.490D-08

THE FOLLOWING ARE CHANGES DUE TO 100 PERCENT CHANGE IN MACROSCOPIC CROSS SECTIONS.
(DIVIDE BY 100 TO GET THE EFFECT OF A 1 PERCENT CHANGE).

FOR INSCATTER

GRP.	TO GRP.	FOR ALL ZONES		
1	1	0.0	0.0	0.0
2	1	0.0	0.0	0.0
1	2	3.889747E-01	1.028417E-01	7.875938E-03
2	2	0.0	0.0	0.0

SUM OF ALL INSCATTER IS 4.996923D-01

ZONE	GRP	REMOVAL
1	1	-3.645021E-02
	2	0.0
2	1	-1.099252E-02
	2	0.0
3	1	-1.254936E-03
	2	0.0

SUM IS -4.869766D-02

ZONE	GRP	ABSORPTIONS	SCATTERING	FISSION SOURCE	TRANSPORT	OVERALL
1	1	-1.325461D-02	3.525244D-01	4.909117D-01	4.442039D-01	1.274385D 00
	2	-3.159272D-02	0.0	4.410607D-01	2.085083D-01	6.179763D-01
2	1	-1.479756D-03	9.184915D-02	9.395313D-03	1.231793D-01	2.229440D-01
	2	-1.236528D-02	0.0	5.663152D-02	6.691158D-02	1.131778D-01
3	1	-9.739773D-05	6.620999D-03	0.0	1.200411D-02	1.852771D-02
	2	-1.550321D-03	0.0	0.0	8.662038D-03	7.111717D-03
BY ZONE						
1		-4.484732D-02	3.525244D-01	9.319724D-01	6.527122D-01	1.892362D 00
2		-1.384504D-02	9.184915D-02	6.802683D-02	1.900909D-01	3.361218D-01
3		-1.647718D-03	6.620999D-03	0.0	2.066615D-02	2.563943D-02
BY GROUP						
	1	-1.483176D-02	4.509945D-01	5.003070D-01	5.793873D-01	1.515857D 00
	2	-4.550832D-02	0.0	4.996922D-01	2.840819D-01	7.382658D-01
TOTALS		-6.034008D-02	4.509945D-01	9.999992D-01	8.634692D-01	2.254123D 00

THE FOLLOWING ARE UNCERTAINTY ASSOCIATED WITH A 100 PERCENT UNCERTAINTY IN THE DATA (UNCORRELATED). BUT NET SCATTERING IN THE ABOVE TABLE TREATED AS AN ENTITY.

	ABSORPTIONS	SCATTERING	FISSION SOURCE	TRANSPORT	OVERALL
BY ZONE					
1	3.426053D-02	3.525244D-01	6.599460D-01	4.907063D-01	1.537437D 00
2	1.245351D-02	9.184913D-02	5.937951D-02	1.401795D-01	3.038617D-01
3	1.553377D-03	6.620999D-03	0.0	1.480303D-02	2.297740D-02
BY GROUP					

```
RUN TITLE -  2-D  17X10 - 5 GROUP SEARCH PROBLEM
             PRIMARY SEARCH = NUCLIDE(DIRECT) - SECONDARY SEARCH = DIMENSION

                        VENTURE NEUTRONICS CODE BLOCK - VERSION 2 --- APRIL 30, 1977.
                        -------------------------------------------------------------

REFERENCE REAL TIME FROM ZNATON INTERFACE FILE =  0.0          DAYS

SOLUTION BY FINITE-DIFFERENCE DIFFUSION THEORY
SEARCH PROBLEM
     DIRECT CONCENTRATION SEARCH
A REGULAR ADJOINT WILL FOLLOW FORWARD PROBLEM
PERTURBATION RESULTS ARE REQUESTED
GEOMETRY NO.  7   2-D R-Z
NUMBER OF ENERGY GROUPS                                  5
NUMBER OF UPSCATTER GROUPS (MAX)                         0
NUMBER OF DOWNSCATTER GROUPS (MAX)                       4
NUMBER OF INTERVALS IN DIMENSION 1 (COLUMNS)            17
NUMBER OF INTERVALS IN DIMENSION 2 (ROWS)               10
NUMBER OF INTERVALS IN DIMENSION 3 (PLANES)              1
NUMBER OF ZONES                                          8
NUMBER OF REGIONS                                       18
NUMBER OF BLACK ABSORBER ZONES                           0
BOUNDARY INDICATORS-   LEFT  1  RIGHT  2
                        TOP  2 BOTTOM  1
```

MEMORY REQUIREMENTS FOR DATA STORAGE

	TOTAL MINIMUM	TOTAL MAXIMUM	A	B	C	D
STORAGE AVAILABLE	18000					
MACRO CALCULATION	968					
EQUATION CONSTANTS CALCULATION						
CORE CONTAINED OR SPACE STORED	1397	1397				
PLANE STORED	1737	1737				
ROW STORED	705	705				
MULTI-LEVEL PLANE STORED	1889	1889				
INITIAL FLUX						
CORE CONTAINED OR SPACE STORED	774	774				
OTHER MODES	774	774				
ITERATIVE PROCESS						
CORE CONTAINED	8229		6257	782	482	708
SPACE STORED	3052		2068	782	202	0
1 PLANES STORED	3732		2748	782	202	0
1 PLANE STORED	3732		2748	782	202	0
10 ROWS STORED	2966		1982	782	202	0
1 ROW STORED	984		0	782	202	0
1 MULTI-LEVEL PLANES STORED	4564		1020	782	202	2560
PERTURBATION CALCULATION	2330					

```
DATA WILL BE STORED FOR ALL GROUPS, ALL SPACE

MEMORY LOCATIONS RESERVED FOR DATA STORAGE---   18000
MAX MEMORY LOCATIONS REQUIRED FOR THIS PROB--    8229
MEMORY LOCATIONS NOT USED-------------------     9771

     SPECIAL SCRATCH DATASET REQUIREMENTS
     MAXIMUM PHYSICAL RECORD IS     7200 WORDS
```

```
RITE CONTAINER ARRAYS, CONTROL       36 DATA     9725
FILE 24 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      5    340   1700      1   8025
FILE 27 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      5    340   1700   1701   6325
FILE 28 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      5    340   1700   3401   4625
FILE 40 DEFAULTS TO CORE - NO.RECS, REC.LNTH, TOT.LNTH, START LOC, CORE LEFT.      5    707   3535   5101   1089

DO PARAMETERS FOLLOW FOR  B1 = 3520  AND  B2 =   5440
N2=   3  N3=  10  N4=   1  N5=   6  N6=  10  N7=   1  N8=   1  N9=   1  N10=   1  N11=   1  N12=   1  N13=   1  N14=   1  N15=  1
N16=   3   (NOTE THAT IF THE FLUXES ARE TO BE EXPANDED FROM EXISTING RTFLUX, N10=   3)

REQUIRED DISK STORAGE SPACE FOR FLUX(UNITS 24,27,28) IS      10560 BYTES.
                              FOR CONSTANTS(UNIT 40) IS--     32640 BYTES.
                              FOR CONSTANTS(UNIT 23) IS--     35200 BYTES.
REQUIRED TOTAL DISK STORAGE SPACE IS-------------------   5518720 BYTES.

FOR THE ASSIGNED DATA STORAGE, THE REQUIRED REGION SIZE IS APPROXIMATELY  402K BYTES

TITLE FROM CROSS SECTION FILE / 5 GROUP LMFBR CROSS SECTION SET.


PRINCIPAL MACROSCOPIC CROSS SECTIONS

GROUP    1
ZONE   D              SIGA            SIGNF           SIGWF           SIGAS           SIGNFS
    1  2.516465E 00   5.792666E-03   1.421664E-02   1.536809E-13   9.401215E-04   2.849508E-03
    2  2.491580E 00   4.330136E-03   9.215195E-03   1.034325E-13   0.0            0.0
    3  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    4  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    5  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    6  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    7  2.121200E 00   8.190463E-04   6.389623E-06   0.0            0.0            0.0
    8  2.121200E 00   8.190463E-04   6.389623E-06   0.0            0.0            0.0

GROUP    2
ZONE   D              SIGA            SIGNF           SIGWF           SIGAS           SIGNFS
    1  1.453617E 00   3.342617E-03   4.837800E-03   5.416419E-14   6.200797E-04   1.484710E-03
    2  1.438300E 00   1.975165E-03   9.110016E-04   1.033252E-14   0.0            0.0
    3  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    4  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    5  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    6  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    7  1.276845E 00   5.057480E-04   0.0            0.0            0.0            0.0
    8  1.276845E 00   5.057480E-04   0.0            0.0            0.0            0.0

GROUP    3
ZONE   D              SIGA            SIGNF           SIGWF           SIGAS           SIGNFS
    1  9.447532E-01   6.746028E-03   5.472325E-03   6.199490E-14   8.871062E-04   1.604511E-03
    2  9.359486E-01   5.115528E-03   1.075083E-03   1.238740E-14   0.0            0.0
    3  9.359536E-01   5.115535E-03   1.075084E-03   1.238741E-14   0.0            0.0
    4  9.359536E-01   5.115535E-03   1.075084E-03   1.238741E-14   0.0            0.0
    5  9.359536E-01   5.115535E-03   1.075084E-03   1.238741E-14   0.0            0.0
    6  9.359536E-01   5.115535E-03   1.075084E-03   1.238741E-14   0.0            0.0
    7  6.192686E-01   1.612214E-03   0.0            0.0            0.0            0.0
    8  6.192686E-01   1.612214E-03   0.0            0.0            0.0            0.0

GROUP    4
ZONE   D              SIGA            SIGNF           SIGWF           SIGAS           SIGNFS
    1  6.452593E-01   1.574807E-02   1.068695E-02   1.212021E-13   2.050783E-03   3.078995E-03
    2  6.413477E-01   1.179417E-02   2.138645E-03   2.472050E-14   0.0            0.0
    3  6.413473E-01   1.179422E-02   2.138647E-03   2.472052E-14   0.0            0.0
    4  6.413473E-01   1.179422E-02   2.138647E-03   2.472052E-14   0.0            0.0
    5  6.413473E-01   1.179422E-02   2.138647E-03   2.472052E-14   0.0            0.0
    6  6.413473E-01   1.179422E-02   2.138647E-03   2.472052E-14   0.0            0.0
    7  3.954161E-01   7.729638E-03   0.0            0.0            0.0            0.0
    8  3.954161E-01   7.729638E-03   0.0            0.0            0.0            0.0
```

```
GROUP    5
ZONE   D              SIGA           SIGNF          SIGWF          SIGAS          SIGNFS
    1  6.781518E-01  3.251838E-02  2.651023E-02  3.233347E-13  5.601514E-03  8.106362E-03
    2  6.903558E-01  1.931511E-02  5.696688E-03  6.586382E-14  0.0           0.0
    3  6.903527E-01  1.931519E-02  5.696688E-03  6.586387E-14  0.0           0.0
    4  6.903527E-01  1.931519E-02  5.696688E-03  6.586387E-14  0.0           0.0
    5  6.903527E-01  1.931519E-02  5.696688E-03  6.586387E-14  0.0           0.0
    6  6.903527E-01  1.931519E-02  5.696688E-03  6.586387E-14  0.0           0.0
    7  3.869154E-01  1.466906E-02  0.0           0.0           0.0           0.0
    8  3.869154E-01  1.466906E-02  0.0           0.0           0.0           0.0

FISSION SPECTRUM CONSTANT FOR ALL ZONES
  7.550370E-01  2.380250E-01  6.937999E-03  0.0           0.0

1/V CONSTANT FOR ALL ZONES
  3.876078E-04  1.121930E-03  3.081634E-03  9.142663E-03  2.393971E-02


SCATTERING MACROSCOPIC CROSS SECTIONS

GROUP    1  MBAND    1  MJJ    1
TPO
  0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0

GROUP    2  MBAND    2  MJJ    1
TPO
  0.0           3.099186E-02  0.0           3.272266E-02  0.0           3.272273E-02  0.0           3.272273E-02
  0.0           3.272273E-02  0.0           3.272273E-02  0.0           2.414452E-02  0.0           2.414452E-02

GROUP    3  MBAND    3  MJJ    1
TPO
  0.0           6.354101E-03  5.214883E-04  0.0           6.463207E-03  5.669191E-04  0.0           6.463237E-03
  5.669224E-04  0.0           6.463237E-03  5.669224E-04  0.0           6.463237E-03  5.669224E-04  0.0
  6.463237E-03  5.669224E-04  0.0           4.524011E-03  6.934805E-04  0.0           4.524011E-03  6.934805E-04

GROUP    4  MBAND    4  MJJ    1
TPO
  0.0           5.591076E-03  7.068575E-06  1.036582E-05  0.0           5.589414E-03  7.527391E-06  1.062008E-05
  0.0           5.589440E-03  7.527407E-06  1.062010E-05  0.0           5.589440E-03  7.527407E-06  1.062010E-05
  0.0           5.589440E-03  7.527407E-06  1.062010E-05  0.0           5.589440E-03  7.527407E-06  1.062010E-05
  0.0           7.264681E-03  1.163266E-05  3.452154E-05  0.0           7.264681E-03  1.163266E-05  3.452154E-05

GROUP    5  MBAND    5  MJJ    1
TPO
  0.0           3.247920E-03  2.834759E-06  1.405918E-08  9.156958E-08  0.0           3.246953E-03  3.342082E-06
  1.405917E-08  9.156952E-08  0.0           3.246958E-03  3.342087E-06  1.405918E-08  9.156958E-08  0.0
  3.246958E-03  3.342087E-06  1.405918E-08  9.156958E-08  0.0           3.246958E-03  3.342087E-06  1.405918E-08
  9.156958E-08  0.0           3.246958E-03  3.342087E-06  1.405918E-08  9.156958E-08  0.0           4.516136E-03
  0.0           5.486510E-08  3.573390E-07  0.0           4.516136E-03  0.0           5.486510E-08  3.573390E-07

SCATTERING REMOVAL
GROUP    1
  3.152381D-02  3.330029D-02  3.330036D-02  3.330036D-02  3.330036D-02  3.330036D-02  2.487288D-02  2.487288D-02
GROUP    2
  6.361184D-03  6.470749D-03  6.470779D-03  6.470779D-03  6.470779D-03  6.470779D-03  4.535699D-03  4.535699D-03
GROUP    3
  5.593911D-03  5.592756D-03  5.592783D-03  5.592783D-03  5.592783D-03  5.592783D-03  7.264681D-03  7.264681D-03
GROUP    4
  3.247920D-03  3.246953D-03  3.246958D-03  3.246958D-03  3.246958D-03  3.246958D-03  4.516136D-03  4.516136D-03
GROUP    5
  0.0           0.0           0.0           0.0           0.0           0.0           0.0           0.0

FINE MESH DESCRIPTION - POINT IS LOCATED AT THE CENTROID OF THE VOLUME ELEMENT
DISTANCE TO POINT - DIMENSION I (LEFT TO RIGHT)
```

```
    1   6.2410     2  10.8097     3  20.7514     4  31.3091     5  39.1139     6  45.3280     7  50.5416     8  55.2654
    9  61.3612    10  68.4633    11  74.8950    12  81.7364    13  88.8928    14  95.5146    15 101.3582    16 106.5518
   17 111.5037
DISTANCE TO POINT - DIMENSION 2 (TOP TO BOTTOM)
    1   2.0400     2   6.1200     3  10.2000     4  15.2567     5  21.2900     6  27.3233     7  33.5550     8  39.9850
    9  46.4150    10  52.8450

SEARCH LIMITING FACTORS - SP1 =  -5.805285E 00 SP2 =  -1.039481E 01  SA =   1.009960E-02 SNF =   1.712409E-02

DETERMINE INITIAL PARAMETERS FOR ITERATIVE PROCEDURE

REFERENCE POINT FOR INITIALIZATION WILL BE AT COLUMN =     2 ROW =     9 PLANE =     1 ZONE =     1
INITIAL OUTER ITERATION EIGENVALUE        0.521879  OPTION     0
INITIAL OVERRELAXATION COEFFICIENTS MAX.  1.361220  MIN.  1.200000  INNER ITERATIONS MAX.    4  MIN.    4  OPTION    0
MESH POINT SWEEP OPTION    1
OUTER ITERATION LIMIT TO BE USED    35  ESTIMATED    15

MAXIMUM STORAGE USED FOR CALCULATING INITIAL PARAMETERS WAS    1261

INITIAL FLUX IS FXK(J,K)*FY(I)*FZ(KB)

TOTAL CORE REQUIRED FOR DATA STORAGE IS   8193 WORDS
ELAPSED CPU AND CLOCK MINUTES ARE  0.062   0.917
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A FLUX - EIGENVALUE PROBLEM FOLLOWS
     4 INNERS MIN,  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
   SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE    MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS      K      SEARCH FACTOR  S.F.-CALC
  1    0     0     0    1.53640D 00    0.0      0.0      1.00000      0.0         0.0        0.7471086  0.0           0.0
NEW OVERRELAXATION COEFFICIENTS CALCULATED
  1.24588  1.35644  1.24912  1.15511  1.13327
  2    0     0     0   -4.46711D-01    0.14731  0.0      1.00000      1.00000     0.0        0.7577998  0.0           2.85357D 00
  3    0     0     0   -4.06942D-01    0.70750  0.0      1.00000      2.41884     0.0        0.7982813  2.85357D-01   2.68730D 00
  4    0     0     0   -3.65643D-01    0.71569  0.0      1.00000      2.52512    -0.00537    0.8316870  5.25552D-01   2.55413D 00
  5    0     0     0   -3.17456D-01    0.70948  0.0      1.00000      1.25731     0.86650    0.8591307  7.28410D-01   2.45021D 00
  6    0     0     0   -2.71624D-01    0.71982  0.0      1.00000      0.59694     1.34944    0.8817867  9.00590D-01   2.36872D 00
  7    0     0     0   -2.31462D-01    0.73641  0.0      1.00000    -18.92863    14.70988    0.9006261  1.04740D 00   2.30395D 00
  8    0     0     0   -1.97354D-01    0.75396  0.0      1.00000     21.01284   -12.33746    0.9164021  1.17306D 00   2.25174D 00
  9    0     0     0   -1.77213D-01    0.80934  0.0      1.00000     -3.62400     4.59751    0.9422742  1.38879D 00   2.17460D 00
 10    0     0     0   -1.56394D-01    0.80432  0.0      1.00000      3.79136     0.26502    0.9785125  1.70312D 00   2.07237D 00
 11    0     0     0   -1.01238D-01    0.59671  0.0      1.00000     -1.16269     4.38010    1.0114103  1.99852D 00   1.98180D 00
 12    4     0     0   -2.55388D-02    0.14299  0.0      1.00000      0.02087     0.0        1.0101636  1.98180D 00   1.97886D 00
 13    0     0     0   -7.24038D-03    0.0      0.0      1.00000      0.0         0.0        1.0100194  1.97692D 00   1.97668D 00
 14    0     0     0   -3.20786D-03    0.38132  0.0      1.00000      0.65149    -0.01180    1.0101246  1.97668D 00   1.97520D 00
 15    0     0     0   -1.35372D-03    0.49451  0.0      1.00000     -4.07548     1.57450    1.0100250  1.97520D 00   1.97490D 00

**********SEARCH EIGENVALUE RANGE VIOLATED - CALCULATED  1.97490D 00  USING  1.00000D 00

NEW ZNATON INTERFACE VERSION   2  HAS BEEN WRITTEN ON I/O UNIT NUMBER  31
DENSITIES UPDATED FOR DIRECT SEARCH WITH CHANGE EIGENVALUE  1.00000E 00
PROCEEDING WITH SECONDARY SEARCH

TITLE FROM CROSS SECTION FILE / 5 GROUP LMFBR CROSS SECTION SET.


PRINCIPAL MACROSCOPIC CROSS SECTIONS

GROUP    1
ZONE   D              SIGA           SIGNF          SIGWF          SIGAS          SIGNFS
    1  2.461064E 00   6.732788E-03   1.706615E-02   1.832810E-13   0.0            0.0
    2  2.491580E 00   4.330136E-03   9.215195E-03   1.034325E-13   0.0            0.0
    3  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    4  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    5  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    6  2.491576E 00   4.330140E-03   9.215225E-03   1.034326E-13   0.0            0.0
    7  2.121200E 00   8.190463E-04   6.389623E-06   0.0            0.0            0.0
    8  2.121200E 00   8.190463E-04   6.389623E-06   0.0            0.0            0.0

GROUP    2
ZONE   D              SIGA           SIGNF          SIGWF          SIGAS          SIGNFS
    1  1.421424E 00   3.962696E-03   6.322514E-03   7.079309E-14   0.0            0.0
    2  1.438300E 00   1.975165E-03   9.110016E-04   1.033252E-14   0.0            0.0
    3  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    4  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    5  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    6  1.438299E 00   1.975170E-03   9.110027E-04   1.033252E-14   0.0            0.0
    7  1.276845E 00   5.057480E-04   0.0            0.0            0.0            0.0
    8  1.276845E 00   5.057480E-04   0.0            0.0            0.0            0.0

GROUP    3
ZONE   D              SIGA           SIGNF          SIGWF          SIGAS          SIGNFS
    1  9.229326E-01   7.633135E-03   7.076833E-03   8.019117E-14   0.0            0.0
    2  9.359486E-01   5.115528E-03   1.075083E-03   1.238740E-14   0.0            0.0
```

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A FLUX - EIGENVALUE PROBLEM FOLLOWS
      4 INNERS MIN.  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE     MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS   SOURCE        K-USED     K-CALC
   1    0     0     0   -2.46017D-01    0.0       0.0      1.00000       0.0          0.0      5.75668E 15  1.0099993  0.8951658
NEW OVERRELAXATION COEFFICIENTS CALCULATED
  1.24532  1.35376  1.24692  1.15431  1.13277
   2    0     0     0   -2.09484D-01    0.74676   0.0      1.00000       1.00000      0.0      5.17947E 15  1.0099993  0.8971673
   3    0     0     0   -1.05115D-01    0.44922   0.0      1.00000       0.81561      0.0      4.64157E 15  0.9502457  0.9008052
   4    0     0     0   -3.69691D-02    0.33322   0.0      1.00000       0.97461     -0.25825  4.41739E 15  0.9008052  0.9041489
   5    0     0     0   -2.05438D-02    0.35219   0.0      1.00000       0.43515      0.03513  4.43275E 15  0.9041489  0.9042664
   6    0     0     0   -5.56791D-03    0.32682   0.0      1.00000       0.03960      0.16318  4.43344E 15  0.9042664  0.9043765
   7    0     0     0   -1.75756D-03    0.40304   0.0      1.00000      -0.23625      0.26414  4.43399E 15  0.9043765  0.9044171

NOTE RELAXED FLUX CHANGE ON FIRST PASS OF INDIRECT SEARCH

FINAL CALCULATED KEFFECTIVE   0.9044171
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES--------------------------   0.9044533
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   0.9060067   0.9028275
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   0.9093089   0.8955730

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  0.0
  1.24531  1.35366  1.24691  1.15431  1.13277

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.024   0.113

COURSE MESH CHANGE EIGENVALUE IS  3.96292D-01
ELAPSED CPU AND CLOCK MINUTES ARE  0.197   2.382

A FLUX - EIGENVALUE PROBLEM FOLLOWS
      4 INNERS MIN.  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE     MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS   SOURCE        K-USED     K-CALC
   1    0     0     0   -4.66637D-01    0.0       0.0      1.00000       0.0          0.0      1.01553E 16  1.0099993  0.9791812
NEW OVERRELAXATION COEFFICIENTS CALCULATED
  1.24435  1.34408  1.24055  1.15252  1.13167
   2    0     0     0   -4.77607D-01    0.78470   0.0      1.00000       1.00000      0.0      9.90520E 15  1.0099993  0.9947174
   3    0     0     0   -3.21417D-01    0.51227   0.0      1.00000       1.05030      0.0      9.76997E 15  1.0099993  1.0004116
   4    0     0     0   -1.65776D-01    0.43288   0.0      1.00000       1.19493     -0.25711  9.68472E 15  1.0099993  1.0029786
   5    0     0     0   -6.26366D-02    0.45717   0.0      1.00000       0.58299      0.10739  9.62183E 15  1.0099993  1.0042616
   6    0     0     0   -4.50883D-02    0.52308   0.0      1.00000      -7.22099      3.34088  9.57027E 15  1.0099993  1.0049737
   7    0     0     0   -2.81791D-02    0.61089   0.0      1.00000       9.13755     -3.22962  9.52508E 15  1.0099993  1.0054032
   8    3     0     0   -1.35038D-01    0.69575   0.0      1.00000       8.66276     -2.87214  9.48381E 15  1.0099993  1.0056776
   9    0     0     0   -6.68943D-03    0.0       0.0      1.00000       0.0          0.0      9.22824E 15  1.0084193  1.0066880
  10    0     0     0    4.53654D-03    0.67590   0.0      1.00000       0.31107      0.28717  9.21333E 15  1.0066880  1.0066648
  11    0     0     0    2.85904D-03    0.70013   0.0      1.00000       2.42185     -0.05445  9.21307E 15  1.0066648  1.0065876
  12    0     0     0    2.05100D-03    0.71021   0.0      1.00000       3.86549     -0.95724  9.21235E 15  1.0065876  1.0065348
  13    0     0     0    1.43734D-03    0.70363   0.0      1.00000       1.33169      0.75715  9.21186E 15  1.0065348  1.0064976
  14    0     0     0    1.00332D-03    0.70155   0.0      1.00000       3.30997     -0.67973  9.21151E 15  1.0064976  1.0064716
  15    3     0     0    2.50480D-03    0.70098   0.0      0.0           3.13297     -0.55608  9.21127E 15  1.0064716  1.0064534
  16    0     0     0   -3.36457D-06    0.0       0.0      1.00000       0.0          0.0      9.21070E 15  1.0064107  1.0064107

ESTIMATED ABSOLUTE POINT FLUX RELATIVE ERROR  7.88758D-06

FINAL CALCULATED KEFFECTIVE   1.0064107
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES--------------------------   1.0064107
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   1.0064141   1.0064073
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   1.0064248   1.0063965

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  7.00984D-01
  1.24434  1.34400  1.24055  1.15252  1.13167

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.042   0.217

COURSE MESH CHANGE EIGENVALUE IS  4.10235D-01
ELAPSED CPU AND CLOCK MINUTES ARE  0.274   3.293
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A FLUX - EIGENVALUE PROBLEM FOLLOWS
     4 INNERS MIN,  4 INNERS MAX - CHEBYCHEV  BETA ON INNERS
    SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF.   ICVR=0,1-YES,NO INNERS CONVR.   OCVR=0,1-YES,NO OUTERS CONVR.
ITER  PROC  ICVR  OCVR   FLUX CHANGE    MU-BAR  OTHER-MU  SEM-IND   ACCELERATION PARAMETERS   SOURCE        K-USED    K-CALC
  1    0     0     0    1.08622D-06    0.0      0.0      1.00000      0.0        0.0      9.45941E 15  1.0099993  1.0099993

FINAL CALCULATED KEFFECTIVE   1.0099993
MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES--------------------------   1.0099992
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE------------   1.0100004   1.0099982
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS-------   1.0100614   1.0099685

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS     4  0.0
  1.24422  1.34360  1.24029  1.15242  1.13159

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE  0.005   0.063

FINAL COURSE MESH INTERVAL BOUNDARIES
XMESH  0.0            1.765121D 01  6.007519D 01  8.128718D 01  1.101779D 02  1.309249D 02  1.461649D 02
YMESH  0.0            1.224000D 01  3.034000D 01  6.138575D 01
ZMESH  0.0            1.000000D 00

DISTANCES TO FINE MESH INTERFACES
1/XX    1    0.0       2   12.4813    3   17.6512    4   37.5595    5   50.0986    6   60.0752    7   67.8863
1/XX    8   74.8871    9   81.2872   10   91.9318   11  101.4658   12  110.1779   13  117.5013   14  124.3943
1/XX   15  130.9249   16  136.1945   17  141.2677   18  146.1649
2/YY    1    0.0       2    4.0800    3    8.1600    4   12.2400    5   18.2733    6   24.3067    7   30.3400
2/YY    8   38.1014    9   45.8629   10   53.6243   11   61.3857
3/ZZ    1    0.0       2    1.0000

DISTANCES TO FLUX POINTS
1/X     1    8.8256    2   15.2864    3   29.3452    4   44.2752    5   55.3123    6   64.0999    7   71.4725
1/X     8   78.1527    9   86.7729   10   96.8163   11  105.9115   12  113.8985   13  120.9969   14  127.7014
1/X    15  133.5657   16  138.7543   17  143.7372
2/Y     1    2.0400    2    6.1200    3   10.2000    4   15.2567    5   21.2900    6   27.3233    7   34.2207
2/Y     8   41.9822    9   49.7436   10   57.5050
3/Z     1    0.5000

    LEAKAGE  7.47042E 12  TOTAL LOSSES  1.04243E 14  TOTAL PRODUCTIONS  1.05285E 14  REACTOR POWER(WATTS)  2.34500D 03

PRIMITIVE FISSILE CONVERSION RATIO IS  1.23325D 00. ESTIMATE FOR CRITICAL SYSTEM IS  1.26298D 00
FISSILE DESTRUCTION PER UNIT ENERGY (ATOMS/WATT-SEC) IS  2.99028D 10

BOUNDARY NEUTRON LEAKAGE
GROUP    LEFT          RIGHT          TOP          BOTTOM         FRONT          BACK
 1   0.0          2.90580D 10  4.94736D 11  0.0          0.0          0.0
 2   0.0          3.64110D 11  4.11276D 12  0.0          0.0          0.0
 3   0.0          1.51483D 11  1.53639D 12  0.0          0.0          0.0
 4   0.0          6.20004D 10  5.67394D 11  0.0          0.0          0.0
 5   0.0          1.67724D 10  1.35721D 11  0.0          0.0          0.0
SUM  0.0          6.23424E 11  6.84699E 12  0.0          0.0          0.0

GROUP NEUTRON BALANCE FOR EACH ZONE

ZONE GROUP ABSORPTIONS  B**2 LOSSES    1/V LOSS   OUT-SCATTER  IN-SCATTER  P1 IN-SCATTER   SOURCE     POWER(WATTS)  AVERAGE FLUX
  1   1   1.07637E 13  0.0          0.0          5.13343E 13  0.0          0.0          7.13496E 13  2.93012E 02  2.48069E 09
  1   2   2.30175E 13  0.0          0.0          3.72454E 13  5.04648E 13  0.0          2.24929E 13  4.11206E 02  9.01306E 09
  1   3   2.07127E 13  0.0          0.0          1.52592E 13  3.80564E 13  0.0          6.55628E 11  2.17601E 02  4.21055E 09
  1   4   1.27917E 13  0.0          0.0          2.34508E 12  1.53096E 13  0.0          0.0          1.12228E 02  1.11517E 09
  1   5   2.43421E 12  0.0          0.0          0.0          2.35311E 12  0.0          0.0          2.65244E 01  9.90854E 07
```

SUM		6.97198E 13	0.0	0.0	1.06184E 14	1.06184E 14	0.0	9.44981E 13	1.06057E 03	
2	1	5.58655E 11	0.0	0.0	4.29626E 12	0.0	0.0	2.36686E 12	1.33444E 01	2.39135E 08
2	2	1.71328E 12	0.0	0.0	5.61281E 12	4.22173E 12	0.0	7.46152E 11	8.96256E 00	1.60778E 09
2	3	2.80928E 12	0.0	0.0	3.07136E 12	5.67941E 12	0.0	2.17490E 10	6.80275E 00	1.01790E 09
2	4	2.32774E 12	0.0	0.0	6.40832E 11	3.07742E 12	0.0	0.0	4.87894E 00	3.65821E 08
2	5	5.91655E 11	0.0	0.0	0.0	6.42691E 11	0.0	0.0	2.01752E 00	5.67770E 07
SUM		8.00062E 12	0.0	0.0	1.36213E 13	1.36213E 13	0.0	3.13476E 12	3.60061E 01	
3	1	9.63481E 11	0.0	0.0	7.40952E 12	0.0	0.0	3.76174E 12	2.30144E 01	5.92201E 08
3	2	2.67771E 12	0.0	0.0	8.77235E 12	7.28100E 12	0.0	1.18589E 12	1.40077E 01	3.60817E 09
3	3	4.16135E 12	0.0	0.0	4.54958E 12	8.88827E 12	0.0	3.45665E 10	1.00768E 01	2.16507E 09
3	4	3.40081E 12	0.0	0.0	9.36246E 11	4.55943E 12	0.0	0.0	7.12805E 00	7.67434E 08
3	5	8.65680E 11	0.0	0.0	0.0	9.39004E 11	0.0	0.0	2.95193E 00	1.19285E 08
SUM		1.20690E 13	0.0	0.0	2.16677E 13	2.16677E 13	0.0	4.98219E 12	5.71788E 01	
4	1	1.23852E 11	0.0	0.0	9.52479E 11	0.0	0.0	6.53534E 11	2.95842E 00	9.09341E 07
4	2	4.75642E 11	0.0	0.0	1.55823E 12	9.35949E 11	0.0	2.06026E 11	2.48818E 00	7.65596E 08
4	3	8.62779E 11	0.0	0.0	9.43270E 11	1.57263E 12	0.0	6.00529E 09	2.08924E 00	5.36207E 08
4	4	7.86859E 11	0.0	0.0	2.16623E 11	9.44823E 11	0.0	0.0	1.64925E 00	2.12106E 08
4	5	2.28056E 11	0.0	0.0	0.0	2.17192E 11	0.0	0.0	7.77659E-01	3.75376E 07
SUM		2.47719E 12	0.0	0.0	3.67059E 12	3.67059E 12	0.0	8.65566E 11	9.96275E 00	
5	1	6.77219E 10	0.0	0.0	5.20806E 11	0.0	0.0	4.33502E 11	1.61765E 00	3.20566E 07
5	2	3.11073E 11	0.0	0.0	1.01999E 12	5.11772E 11	0.0	1.36661E 11	1.62729E 00	3.22811E 08
5	3	6.21793E 11	0.0	0.0	6.79803E 11	1.02677E 12	0.0	3.98343E 09	1.50569E 00	2.49141E 08
5	4	5.96050E 11	0.0	0.0	1.64093E 11	6.80748E 11	0.0	0.0	1.24931E 00	1.03587E 08
5	5	1.81503E 11	0.0	0.0	0.0	1.64503E 11	0.0	0.0	6.18916E-01	1.92608E 07
SUM		1.77814E 12	0.0	0.0	2.38379E 12	2.38379E 12	0.0	5.74146E 11	6.61885E 00	
6	1	2.05186E 10	0.0	0.0	1.57795E 11	0.0	0.0	1.41492E 11	4.90121E-01	1.66594E 07
6	2	9.93934E 10	0.0	0.0	3.25619E 11	1.55058E 11	0.0	4.46054E 10	5.19948E-01	1.76916E 08
6	3	2.04553E 11	0.0	0.0	2.23636E 11	3.27926E 11	0.0	1.30017E 09	4.95331E-01	1.40582E 08
6	4	2.05038E 11	0.0	0.0	5.64470E 10	2.23932E 11	0.0	0.0	4.29756E-01	6.11193E 07
6	5	6.64343E 10	0.0	0.0	0.0	5.65818E 10	0.0	0.0	2.26538E-01	1.20923E 07
SUM		5.95937E 11	0.0	0.0	7.63498E 11	7.63498E 11	0.0	1.87398E 11	2.16169E 00	
7	1	2.98625E 10	0.0	0.0	9.06869E 11	0.0	0.0	1.74157E 08	0.0	4.43814E 07
7	2	1.81796E 11	0.0	0.0	1.63040E 12	8.80313E 11	0.0	5.49029E 07	0.0	4.37555E 08
7	3	3.71995E 11	0.0	0.0	1.67622E 12	1.65148E 12	0.0	1.60032E 06	0.0	2.80865E 08
7	4	8.81738E 11	0.0	0.0	5.15166E 11	1.68166E 12	0.0	0.0	0.0	1.38856E 08
7	5	3.81766E 11	0.0	0.0	0.0	5.15199E 11	0.0	0.0	0.0	3.16794E 07
SUM		1.84716E 12	0.0	0.0	4.72865E 12	4.72865E 12	0.0	2.30660E 08	0.0	
8	1	2.46245E 09	0.0	0.0	7.47798E 10	0.0	0.0	1.43609E 07	0.0	4.61124E 06
8	2	2.19033E 10	0.0	0.0	1.96435E 11	7.25901E 10	0.0	4.52726E 06	0.0	6.64255E 07
8	3	5.24519E 10	0.0	0.0	2.36350E 11	1.98014E 11	0.0	1.31961E 05	0.0	4.98997E 07
8	4	1.39386E 11	0.0	0.0	8.14380E 10	2.36957E 11	0.0	0.0	0.0	2.76579E 07
8	5	6.79327E 10	0.0	0.0	0.0	8.14414E 10	0.0	0.0	0.0	7.10290E 06
SUM		2.84136E 11	0.0	0.0	5.89003E 11	5.89003E 11	0.0	1.90201E 07	0.0	

OVERALL NEUTRON BALANCE

GROUP	ABSORPTIONS	B**2 LOSSES	1/V LOSS	OUT-SCATTER	IN-SCATTER	P1 IN-SCATTER	SOURCE	POWER(WATTS)
1	1.25303E 13	0.0	0.0	6.56528E 13	0.0	0.0	7.87068E 13	3.34436E 02
2	2.84983E 13	0.0	0.0	5.63602E 13	6.45232E 13	0.0	2.48123E 13	4.38811E 02
3	2.97969E 13	0.0	0.0	2.66393E 13	5.74009E 13	0.0	7.23234E 11	2.38571E 02
4	2.11293E 13	0.0	0.0	4.95592E 12	2.67145E 13	0.0	0.0	1.27564E 02
5	4.81723E 12	0.0	0.0	0.0	4.96972E 12	0.0	0.0	3.31170E 01
SUM	9.67720E 13	0.0	0.0	1.53608E 14	1.53608E 14	0.0	1.04242E 14	1.17250E 03

ZONE VOLUMES FOLLOW. TOTAL VOLUME 4.12005E 06

6.44460E 05 5.39510E 05 3.75727E 05 3.14540E 05 4.87876E 05 2.84437E 05 8.21518E 05 6.51990E 05

POINT NEUTRON DENSITY (NEUTRONS/CC)

	1	2	3	4	5	6	7	8	9	10	11
1	6.413D 06	6.262D 06	5.800D 06	4.834D 06	3.975D 06	3.248D 06	2.643D 06	2.125D 06	1.517D 06	9.744D 05	6.232D 05
2	1.415D 07	1.382D 07	1.280D 07	1.067D 07	8.772D 06	7.168D 06	5.833D 06	4.690D 06	3.349D 06	2.152D 06	1.377D 06
3	2.113D 07	2.063D 07	1.911D 07	1.593D 07	1.309D 07	1.069D 07	8.695D 06	6.985D 06	4.983D 06	3.197D 06	2.042D 06
4	2.653D 07	2.590D 07	2.399D 07	1.999D 07	1.642D 07	1.340D 07	1.088D 07	8.732D 06	6.219D 06	3.978D 06	2.533D 06
5	3.390D 07	3.310D 07	3.065D 07	2.553D 07	2.095D 07	1.796D 07	1.382D 07	1.106D 07	7.871D 06	5.003D 06	3.164D 06
6	4.164D 07	4.065D 07	3.764D 07	3.133D 07	2.569D 07	2.087D 07	1.686D 07	1.347D 07	9.696D 06	6.142D 06	3.856D 06
7	4.810D 07	4.695D 07	4.348D 07	3.616D 07	2.960D 07	2.398D 07	1.929D 07	1.541D 07	1.175D 07	7.456D 06	4.648D 06
8	5.776D 07	5.638D 07	5.220D 07	4.340D 07	3.549D 07	2.869D 07	2.301D 07	1.833D 07	1.395D 07	8.799D 06	5.444D 06
9	6.556D 07	6.399D 07	5.925D 07	4.925D 07	4.024D 07	3.250D 07	2.602D 07	2.067D 07	1.565D 07	9.815D 06	6.040D 06
10	6.978D 07	6.812D 07	6.306D 07	5.241D 07	4.281D 07	3.456D 07	2.765D 07	2.194D 07	1.657D 07	1.036D 07	6.359D 06

	12	13	14	15	16	17
1	4.098D 05	2.748D 05	1.820D 05	1.180D 05	6.992D 04	2.851D 04
2	9.059D 05	6.089D 05	4.062D 05	2.647D 05	1.570D 05	6.362D 04
3	1.343D 06	9.049D 05	6.120D 05	4.037D 05	2.405D 05	9.740D 04
4	1.663D 06	1.125D 06	7.814D 05	5.634D 05	3.383D 05	1.374D 05
5	2.067D 06	1.396D 06	9.778D 05	7.282D 05	4.434D 05	1.810D 05
6	2.504D 06	1.684D 06	1.180D 06	8.845D 05	5.411D 05	2.213D 05
7	2.998D 06	2.007D 06	1.402D 06	1.052D 06	6.436D 05	2.634D 05
8	3.488D 06	2.323D 06	1.617D 06	1.211D 06	7.405D 05	3.030D 05
9	3.853D 06	2.556D 06	1.775D 06	1.327D 06	8.108D 05	3.316D 05
10	4.047D 06	2.680D 06	1.858D 06	1.388D 06	8.478D 05	3.467D 05

THE RELATIVE NEUTRON DENSITY TRAVERSE LEFT-TO-RIGHT IS
1.00000D 00 9.76170D-01 9.03719D-01 7.51065D-01 6.13526D-01 4.95267D-01 3.96226D-01 3.14403D-01 2.37407D-01
1.48466D-01 9.11229D-02 5.80010D-02 3.84094D-02 2.66267D-02 1.98937D-02 1.21490D-02 4.96798D-03

THE RELATIVE NEUTRON DENSITY TRAVERSE TOP-TO-BOTTOM IS
9.19046D-02 2.02829D-01 3.02861D-01 3.80211D-01 4.85793D-01 5.96689D-01 6.89213D-01 8.27668D-01 9.39425D-01
1.00000D 00

POWER DENSITY INTERFACE FILE PWDINT (VERSION 1) HAS BEEN WRITTEN ON UNIT NUMBER 19

POINT FLUXES WERE WRITTEN ON R2FLUX UNIT 18 FOR ZONES(NON-ZERO) 1 0
ELAPSED CPU AND CLOCK MINUTES ARE 0.480 5.574

ADJOINT PROBLEM FOLLOWS
4 INNERS MIN, 4 INNERS MAX - CHEBYCHEV BETA ON INNERS
SIGMA-1 ORDERING
PROCEDURE=0,1,2,3,4-NORMAL,CHEBYSHEV,SEMEX,DEMEX,SEMEXF, ICVR=0,1-YES,NO INNERS CONVR, OCVR=0,1-YES,NO OUTERS CONVR.

ITER	PROC	ICVR	OCVR	FLUX CHANGE	MU-BAR	OTHER-MU	SEM-IND	ACCELERATION PARAMETERS		
1	0	0	0	7.61062D 00	0.0	0.0	1.00000	0.0	0.0	
2	0	0	0	5.76472D 00	3.63981	0.0	1.00000	1.00000	0.0	
3	0	0	0	1.02778D 00	0.69218	0.0	1.00000	2.24865	0.0	
4	0	0	0	2.63858D-01	0.38871	0.0	1.00000	1.01638	-0.52301	
5	0	0	0	9.13895D-02	0.39200	0.0	1.00000	0.63243	0.00476	
6	0	0	0	3.61362D-02	0.41348	0.0	1.00000	-2.04502	1.03992	
7	0	0	0	1.60981D-02	0.45353	0.0	1.00000	7.50225	-2.57043	
8	0	0	0	8.07634D-03	0.63415	0.0	1.00000	-2.53159	1.29499	
9	0	0	0	4.50545D-03	0.67492	0.0	1.00000	2.47672	-0.22572	
10	3	0	0	9.05676D-03	0.68541	0.0	1.00000	2.74040	-0.42145	
11	0	0	0	-1.75973D-04	0.0	0.0	1.00000	0.0	0.0	
12	0	0	0	-9.71227D-05	0.74277	0.0	1.00000	0.04169	0.04752	
13	0	0	0	-5.90328D-05	0.68962	0.0	1.00000	2.20927	0.01133	
14	0	0	0	-3.69163D-05	0.73916	0.0	1.00000	1.10210	1.00361	

MULTIPLICATION RELIABILITY ESTIMATORS
BY THE SUM OF THE SQUARES OF THE RESIDUES---------- 1.0100001
UPPER AND LOWER BOUNDS ESTIMATES BY MAX REL FLUX CHANGE---------- 1.0100366 1.0099620
UPPER AND LOWER BOUNDS ESTIMATES OVER ALL SIGNIFICANT POINTS------- 1.0101039 1.0099666

NUMBER OF INNER ITERATIONS, OUTER ITERATION ERROR EIGENVALUE, AND OVERRELAXATION COEFFICIENTS 4 0.0
1.13159 1.25915 1.24029 1.34360 1.24422

CPU AND CLOCK MINUTES REQUIRED FOR THIS EIGENVALUE PROBLEM ARE 0.029 0.083

ADJOINT FLUX ENERGY SPECTRUM BY GROUP, 1 TO MAX. (SUMMED OVER SPACE)
6.60436D-08 5.26797D-08 4.06474D-08 3.74816D-08 4.58632D-08

ADJOINT FLUX SPACE FUNCTION BY ZONE (SUMMED OVER ENERGY)
1.11085D-06 1.51137D-07 3.48209D-07 6.82841D-08 2.83696D-08 1.55039D-08 3.48538D-08 5.15614D-09

REGULAR, ADJOINT FLUX INTERGRALS---(DELTA K)/(K*DELTA S WHERE S REPERSENTS MACRO. CROSS SECTIONS. BIG DADDY = 3.4056750-08

ZONE	GRP	SIGA,SIGR,DB**2	B**2	NU*SIGF	DIFF. COEF.
1	1	-1.733592E 01	-4.266484E 01	1.643025E 01	-1.574868E-02
	2	-5.177005E 01	-7.358720E 01	5.921536E 01	-4.300096E-02
	3	-2.055159E 01	-1.896774E 01	2.741919E 01	-1.521267E-02
	4	-5.361812E 00	-3.385130E 00	7.194757E 00	-3.112436E-03
	5	-5.786460E-01	-3.796329E-01	6.286317E-01	8.172856E-06
2	1	-2.915669E-01	-7.264621E-01	2.712569E-01	-2.274885E-03
	2	-1.401424E 00	-2.015669E 00	1.717647E 00	-6.606374E-03
	3	-5.539829E-01	-5.185004E-01	1.054754E 00	-2.494419E-03
	4	-1.461644E-01	-9.374225E-02	3.704312E-01	-5.176908E-04
	5	-2.572955E-02	-1.776254E-02	5.574602E-02	-3.363781E-06
3	1	-1.064334E 00	-2.651871E 00	9.942831E-01	-6.073229E-03
	2	-4.820760E 00	-6.933695E 00	5.813613E 00	-1.755508E-02
	3	-1.933080E 00	-1.813952E 00	3.417875E 00	-6.429151E-03
	4	-5.091053E-01	-3.265134E-01	1.184844E 00	-1.140644E-03
	5	-8.742809E-02	-6.035626E-02	1.783171E-01	8.293083E-05
4	1	-3.145770E-02	-7.837921E-02	2.903038E-02	-2.152585E-04
	2	-1.844627E-01	-2.653126E-01	2.330874E-01	-9.658416E-04
	3	-7.114786E-02	-6.659108E-02	1.595870E-01	-3.788003E-04
	4	-1.901380E-02	-1.219445E-02	6.188696E-02	-9.322974E-05
	5	-3.959861E-03	-2.733699E-03	1.068392E-02	-1.353698E-05
5	1	-6.876949E-03	-1.713445E-02	6.282918E-03	-3.872743E-05
	2	-4.743854E-02	-6.823081E-02	6.238237E-02	-2.378838E-04
	3	-1.732897E-02	-1.621911E-02	4.768630E-02	-8.803567E-05
	4	-4.958004E-03	-3.179802E-03	1.959505E-02	-2.227447E-05
	5	-1.181444E-03	-8.156127E-04	3.585390E-03	-4.321888E-06
6	1	-1.178603E-03	-2.936577E-03	1.074526E-03	-7.451557E-06
	2	-8.466080E-03	-1.217676E-02	1.123334E-02	-4.827997E-05
	3	-3.065787E-03	-2.869435E-03	8.849930E-03	-1.764596E-05
	4	-9.150908E-04	-5.868911E-04	3.791617E-03	-4.684232E-06
	5	-2.334698E-04	-1.611765E-04	7.355916E-04	-9.736086E-07
7	1	-5.116911E-02	-1.085399E-01	4.724521E-02	-7.224926E-04
	2	-3.534289E-01	-4.512740E-01	4.447575E-01	-4.659235E-03
	3	-1.213174E-01	-7.512808E-02	2.865556E-01	-2.322922E-03
	4	-3.167681E-02	-1.252552E-02	1.390291E-01	-5.940930E-04
	5	-6.606486E-03	-2.556151E-03	3.086758E-02	-9.476466E-05
8	1	-3.175887E-04	-6.736694E-04	2.896739E-04	-4.462982E-06
	2	-3.078479E-03	-3.930740E-03	4.070532E-03	-3.506265E-05
	3	-9.295901E-04	-5.756659E-04	3.131441E-03	-1.566144E-05
	4	-2.777411E-04	-1.098233E-04	1.718139E-03	-4.679201E-06
	5	-7.034487E-05	-2.721751E-05	4.334138E-04	-9.487598E-07

VOLUME INTEGRALS FLUX*ADJOINT FLUX -1.07407E 02 CHI*ADJOINT FLUX, NU-SIGF*FLUX 1.000000 00

GRP. TO GRP. DELTA-K/(K*DELTA-SIGS) FOR ALL ZONES 1,2,3,.... - (THE IN-GROUP TERMS MAKE NO CONTRIBUTION.)

1	1	1.733592E 01	2.915669E-01	1.064334E 00	3.145770E-02	6.876949E-03	1.178603E-03	5.116911E-02	3.175887E-04
2	1	6.248271E 01	1.847520E 00	6.226573E 00	2.526859E-01	6.828427E-02	1.232193E-01	4.819056E-01	4.463557E-03
3	1	2.893364E 01	1.134909E 00	3.661591E 00	1.730412E-01	5.219994E-02	9.707797E-03	3.103123E-01	3.432878E-03
4	1	7.592584E 00	3.986908E-01	1.269696E 00	6.711620E-02	2.145073E-02	4.159320E-03	1.505734E-01	1.883631E-03
5	1	6.634637E-01	6.002142E-02	1.911704E-01	1.158927E-02	3.925174E-03	8.069715E-04	3.343940E-02	4.752248E-04
1	2	1.436705E 01	2.218960E-01	8.261285E-01	2.301396E-02	4.778989E-03	8.099740E-04	3.757754E-02	2.192322E-04
2	2	5.177005E 01	1.401424E 00	4.820760E 00	1.844627E-01	4.743854E-02	8.466080E-03	3.534289E-01	3.078479E-03
3	2	2.396725E 01	8.594061E-01	2.831506E 00	1.261911E-01	3.625689E-02	6.669067E-03	2.280517E-01	2.370986E-03

1/V (NEUTRON IMPORTANCE) MAP (1/V/K)(DELTA K/DELTA 1/V).

	1	2	3	4	5	6	7	8	9	10	11
1	1.781D-09	1.698D-09	1.456D-09	1.010D-09	6.789D-10	4.479D-10	2.906D-10	1.817D-10	8.626D-11	3.278D-11	1.253D-11
2	8.538D-09	8.138D-09	6.980D-09	4.839D-09	3.253D-09	2.145D-09	1.388D-09	8.644D-10	4.060D-10	1.527D-10	5.803D-11
3	2.303D-08	2.195D-08	1.883D-08	1.305D-08	8.770D-09	5.774D-09	3.728D-09	2.308D-09	1.068D-09	3.965D-10	1.494D-10
4	4.955D-08	4.723D-08	4.051D-08	2.807D-08	1.884D-08	1.238D-08	7.966D-09	4.899D-09	2.226D-09	8.121D-10	3.027D-10
5	1.029D-07	9.807D-08	8.410D-08	5.823D-08	3.902D-08	2.554D-08	1.628D-08	9.829D-09	4.220D-09	1.461D-09	5.264D-10
6	2.047D-07	1.951D-07	1.672D-07	1.157D-07	7.740D-08	5.046D-08	3.191D-08	1.889D-08	7.445D-09	2.407D-09	8.301D-10
7	4.065D-07	3.874D-07	3.321D-07	2.296D-07	1.534D-07	9.967D-08	6.270D-08	3.672D-08	1.287D-08	3.840D-09	1.263D-09
8	6.466D-07	6.161D-07	5.281D-07	3.648D-07	2.432D-07	1.575D-07	9.852D-08	5.715D-08	1.959D-08	5.616D-09	1.786D-09
9	8.545D-07	8.143D-07	6.979D-07	4.819D-07	3.209D-07	2.074D-07	1.293D-07	7.462D-08	2.535D-08	7.144D-09	2.234D-09
10	9.750D-07	9.290D-07	7.962D-07	5.496D-07	3.658D-07	2.362D-07	1.470D-07	8.468D-08	2.867D-08	8.026D-09	2.491D-09

	12	13	14	15	16	17
1	5.147D-12	2.205D-12	9.081D-13	3.519D-13	1.197D-13	2.386D-14
2	2.378D-11	1.019D-11	4.201D-12	1.565D-12	5.092D-13	9.508D-14
3	6.103D-11	2.624D-11	1.098D-11	3.889D-12	1.214D-12	2.181D-13
4	1.230D-10	5.310D-11	2.318D-11	8.638D-12	2.560D-12	4.441D-13
5	2.096D-10	8.965D-11	3.943D-11	1.540D-11	4.699D-12	7.949D-13
6	3.223D-10	1.358D-10	5.944D-11	2.341D-11	7.035D-12	1.212D-12
7	4.769D-10	1.975D-10	8.558D-11	3.368D-11	1.011D-11	1.741D-12
8	6.590D-10	2.685D-10	1.151D-10	4.514D-11	1.352D-11	2.323D-12
9	8.126D-10	3.277D-10	1.395D-10	5.453D-11	1.630D-11	2.796D-12
10	9.011D-10	3.616D-10	1.534D-10	5.984D-11	1.786D-11	3.062D-12

THE FOLLOWING ARE CHANGES DUE TO 100 PERCENT CHANGE IN MACROSCOPIC CROSS SECTIONS.
(DIVIDE BY 100 TO GET THE EFFECT OF A 1 PERCENT CHANGE).

FOR INSCATTER

GRP.	TO GRP.	FOR ALL ZONES							
1	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
2	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	2	4.535113E-01	7.261019E-03	2.703318E-02	7.530795E-04	1.563815E-04	2.650455E-05	9.072917E-04	5.293257E-06
2	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
3	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
1	3	6.578401E-03	8.241706E-05	3.247622E-04	7.439161E-06	1.297124E-06	2.114031E-07	1.386075E-05	5.962352E-08
2	3	2.844839E-01	5.871281E-03	2.141525E-02	6.746298E-04	1.466446E-04	2.516752E-05	8.468891E-04	5.432684E-06
3	3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
4	3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
5	3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

```
TOTALS
            -6.393325D-01  -1.690778D-01   9.999997D-01   9.510199D-02   2.866913D-01


THE FOLLOWING ARE UNCERTAINTY ASSOCIATED WITH A 100 PERCENT UNCERTAINTY IN THE DATA (UNCORRELATED), BUT NET
SCATTERING IN THE ABOVE TABLE TREATED AS AN ENTITY.


              ABSORPTIONS      SCATTERING   FISSION SOURCE    TRANSPORT       OVERALL


BY ZONE
   1          2.998547D-01   1.074305D-01   5.165113D-01   3.570623D-02   9.595027D-01
   2          4.529337D-03   4.043814D-03   3.272802D-03   5.656295D-03   1.750125D-02
   3          1.578305D-02   1.292364D-02   1.153069D-02   1.502711D-02   5.526450D-02
   4          5.831165D-04   6.051456D-04   4.090419D-04   7.659639D-04   2.363168D-03
   5          1.465084D-04   1.778618D-04   1.066939D-04   1.826050D-04   6.136691D-04
   6          2.623831D-05   3.256576D-05   1.940656D-05   3.690868D-05   1.151193D-04
   7          3.759057D-04   9.257791D-04   3.018790D-07   3.157001D-03   4.458988D-03
   8          3.226688D-06   9.405221D-06   1.850907D-09   2.340703D-05   3.604079D-05


   BY GROUP
        1     1.168170D-01   9.680520D-02   2.805622D-01   2.101172D-02   5.151961D-01
        2     2.053889D-01   4.827012D-02   3.744307D-01   3.225598D-02   6.603457D-01
        3     1.572122D-01   2.731450D-03   1.940793D-01   7.761940D-03   3.617848D-01
        4     9.563890D-02   4.151070D-03   9.907826D-02   1.068366D-03   1.999366D-01
        5     2.212841D-02   0.0            2.304303D-02   3.447132D-05   4.520591D-02

TOTALS
            3.003047D-01   1.082864D-01   5.166505D-01   3.928525D-02   6.085885D-01

     PERTURBATION INTERFACE FILE PERTUB HAS BEEN WRITTEN ON NEW UNIT NUMBER  34

DOPC USE OF CONTAINER ARRAYS. CONTROL       21. MAX DATA     8635

TOTAL CPU TIME IS  0.576 MINUTES AND TOTAL CLOCK TIME IS   6.571 MINUTES


START EXECUTING REACTION RATE MODULE

CASE TITLE -  2-D  17X10 - 5 GROUP SEARCH PROBLEM
              PRIMARY SEARCH = NUCLIDE(DIRECT) - SECONDARY SEARCH = DIMENSION

RITE CONTAINER ARRAYS. CONTROL        6 DATA        1

MAXIMUM ARRAY SIZE USED FOR INITIAL PROCESSING IS      684

STORAGE REQUIRED FOR BASIC DATA IS      570

        STORAGE SUPPLIED IS     18000
MAXIMUM STORAGE REQUIRED IS      2027
MINIMUM STORAGE REQUIRED IS      1270

 MODZSZ =  0 MODZ   =  0 MODZC  =  0

INTERFACE FILE RZFLUX
 TIME  =  0.0           POWER =  1.172500E 03
 VOL   =  4.120052E 06  EFFK  =  1.009999E 00
 EIVS  =  0.0           DKDS  =  0.0
 TNL   =  1.042425E 14  TNA   =  9.677212E 13
 TNSL  =  7.470420E 12  TNBL  =  0.0
 TNBAL =  0.0           TNCRA =  0.0
```

REACTION RATE AND POWER PRODUCTION BY ZONE
REACTION RATES HAVE UNITS OF EVENTS/SEC

ZONE 1 ZONE CLASS 1

POS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	3.063401E 02	1.748128E 11	0.0	0.0	1.748128E 11	0.0	0.0
2	2	NA-23	NA-23	6	2.003930E 02	1.468139E 11	2.025560E 07	4.051120E 07	1.467937E 11	0.0	0.0
3	3	CR-N	CR-N	5	1.639540E 02	4.700712E 11	0.0	0.0	4.700712E 11	0.0	0.0
4	4	MN-55	MN-55	5	2.521034E 01	2.977258E 11	7.420685E 07	1.484137E 08	2.976515E 11	0.0	0.0
5	5	FE-N	FE-N	5	6.782012E 02	1.420202E 12	0.0	0.0	1.420202E 12	0.0	0.0
6	6	NI-N	NI-N	5	1.305822E 02	4.861385E 11	0.0	0.0	4.861385E 11	0.0	0.0
7	7	MO-N	MO-N	5	5.276143E 01	1.178826E 12	1.231851E 09	2.463703E 09	1.177594E 12	0.0	0.0
8	8	TA-181	TA-181	7	1.010103E 01	3.579353E 11	3.174569E 08	6.349138E 08	3.576178E 11	0.0	0.0
10	10	U-238	U-238	2	1.838305E 03	2.731009E 13	3.903846E 12	1.087492E 13	2.340625E 13	1.234592E 02	0.0
11	11	PU-239	PU-239	1	3.286941E 02	3.120116E 13	2.589349E 13	7.592482E 13	5.307685E 12	8.437651E 02	0.0
12	12	PU-240	PU-240	2	1.246909E 02	4.274848E 12	2.034969E 12	6.218701E 12	2.239878E 12	6.680196E 01	0.0
13	13	PU-241	PU-241	1	7.152403E 00	9.059393E 11	7.798456E 11	2.349472E 12	1.260937E 11	2.577467E 01	0.0
14	14	PU-242	PU-242	3	1.854817E 00	4.924589E 10	2.354220E 10	7.184554E 10	2.570370E 10	7.712895E-01	0.0
15	15	SSFP	SSFP	4	9.000073E 01	1.446068E 12	0.0	0.0	1.446068E 12	0.0	0.0

ZONE 2 ZONE CLASS 1

POS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	2.564529E 02	1.410738E 10	0.0	0.0	1.410738E 10	0.0	0.0
2	2	NA-23	NA-23	6	1.677592E 02	3.154746E 10	1.634629E 06	3.269257E 06	3.154582E 10	0.0	0.0
3	3	CR-N	CR-N	5	1.372542E 02	1.165535E 11	0.0	0.0	1.165535E 11	0.0	0.0
4	4	MN-55	MN-55	5	2.110484E 01	9.115140E 10	5.988496E 06	1.197700E 07	9.114544E 10	0.0	0.0
5	5	FE-N	FE-N	5	5.677561E 02	2.975261E 11	0.0	0.0	2.975261E 11	0.0	0.0
6	6	NI-N	NI-N	5	1.093170E 02	6.609450E 10	0.0	0.0	6.609450E 10	0.0	0.0
7	7	MO-N	MO-N	5	4.416920E 01	2.968283E 11	9.941050E 07	1.988211E 08	2.967287E 11	0.0	0.0
8	8	TA-181	TA-181	7	8.456093E 00	8.214276E 10	2.561878E 07	5.123758E 07	8.211713E 10	0.0	0.0
9	9	U-235	U-235	1	4.435482E 00	1.185970E 11	8.946116E 10	2.190578E 11	2.913586E 10	2.816327E 00	0.0
10	10	U-238	U-238	2	1.817440E 03	6.019611E 12	3.728684E 11	1.038438E 12	5.646745E 12	1.179197E 01	0.0
11	11	PU-239	PU-239	1	3.909656E 01	8.294493E 11	6.536975E 11	1.899489E 12	1.757522E 11	2.130138E 01	0.0
12	12	PU-240	PU-240	2	1.321218E 00	9.338290E 09	2.940383E 09	8.864186E 09	6.397907E 09	9.652388E-02	0.0
13	13	PU-241	PU-241	1	2.140813E-10	6.460495E 00	5.434174E 00	1.626456E 01	1.026321E 00	1.796049E-10	0.0
15	15	SSFP	SSFP	4	6.511993E 00	2.768930E 10	0.0	0.0	2.768930E 10	0.0	0.0

ZONE 3 ZONE CLASS 1

POS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	1.785995E 02	2.433022E 10	0.0	0.0	2.433022E 10	0.0	0.0
2	2	NA-23	NA-23	6	1.168312E 02	4.706759E 10	2.819150E 06	5.638300E 06	4.706478E 10	0.0	0.0
3	3	CR-N	CR-N	5	9.558687E 01	1.721010E 11	0.0	0.0	1.721010E 11	0.0	0.0
4	4	MN-55	MN-55	5	1.469789E 01	1.340247E 11	1.032801E 07	2.065602E 07	1.340144E 11	0.0	0.0
5	5	FE-N	FE-N	5	3.953982E 02	4.434024E 11	0.0	0.0	4.434024E 11	0.0	0.0
6	6	NI-N	NI-N	5	7.613077E 01	1.038643E 11	0.0	0.0	1.038643E 11	0.0	0.0
7	7	MO-N	MO-N	5	3.076045E 01	4.382862E 11	1.714475E 08	3.428951E 08	4.381145E 11	0.0	0.0
8	8	TA-181	TA-181	7	5.889006E 00	1.220045E 11	4.418326E 07	8.836653E 07	1.219604E 11	0.0	0.0
9	9	U-235	U-235	1	3.088970E 00	1.782612E 11	1.348848E 11	3.305013E 11	4.337639E 10	4.246308E 00	0.0
10	10	U-238	U-238	2	1.265706E 03	9.093514E 12	6.427779E 11	1.790225E 12	8.450739E 12	2.032785E 01	0.0
11	11	PU-239	PU-239	1	2.722772E 01	1.256629E 12	9.957817E 11	2.896461E 12	2.608482E 11	3.244853E 01	0.0
12	12	PU-240	PU-240	2	9.201263E-01	1.428054E 10	4.755751E 09	1.436876E 10	9.524806E 09	1.561171E-01	0.0
13	13	PU-241	PU-241	1	1.490909E-10	9.724388E 00	8.197697E 00	2.455251E 01	1.526691E 00	2.709419E-10	0.0
15	15	SSFP	SSFP	4	4.535096E 00	4.127208E 10	0.0	0.0	4.127208E 10	0.0	0.0

ZONE 4 ZONE CLASS 1

POS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	1.495147E 02	3.127572E 09	0.0	0.0	3.127572E 09	0.0	0.0
2	2	NA-23	NA-23	6	9.780537E 01	1.013864E 10	3.623927E 05	7.247854E 05	1.013828E 10	0.0	0.0
3	3	CR-N	CR-N	5	8.002066E 01	3.869637E 10	0.0	0.0	3.869637E 10	0.0	0.0

6	6	NI-N	NI-N	5	5.155432E 02	1.374272E 10	0.0	0.0	1.374272E 10	0.0	0.0
7	7	MO-N	MO-N	5	2.083040E 02	1.053737E 11	9.040344E 06	1.808067E 07	1.053647E 11	0.0	0.0
8	8	TA-181	TA-181	7	1.942050E-10	1.295576E-01	1.134552E-05	2.269103E-05	1.295463E-01	0.0	0.0

REACTION RATE AND POWER PRODUCTION BY ZONE CLASS
REACTION RATES HAVE UNITS OF EVENTS/SEC

ZONE CLASS 1

PCS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	1.258021E 03	2.186060E 11	0.0	0.0	2.186060E 11	0.0	0.0
2	2	NA-23	NA-23	6	1.066005E 03	2.557479E 11	2.559518E 07	5.119043E 07	2.557223E 11	0.0	0.0
3	3	CR-N	CR-N	5	2.136170E 03	1.135099E 12	0.0	0.0	1.135099E 12	0.0	0.0
4	4	MN-55	MN-55	5	3.284717E 02	8.682019E 11	9.994576E 07	1.998916E 08	8.681020E 11	0.0	0.0
5	5	FE-N	FE-N	5	8.836340E 03	2.995386E 12	0.0	0.0	2.995386E 12	0.0	0.0
6	6	NI-N	NI-N	5	1.701387E 03	8.111117E 11	0.0	0.0	8.111117E 11	0.0	0.0
7	7	MO-N	MO-N	5	6.874412E 02	2.885502E 12	1.659123E 09	3.318248E 09	2.883842E 12	0.0	0.0
8	8	TA-181	TA-181	7	4.148103E 01	6.152023E 11	3.969846E 08	7.939697E 08	6.148053E 11	0.0	0.0
9	9	U-235	U-235	1	1.645981E 01	3.700022E 11	2.788672E 11	6.828031E 11	9.113495E 10	8.779020E 00	0.0
10	10	U-238	U-238	2	8.582711E 03	4.604025E 13	5.061293E 12	1.409842E 13	4.097899E 13	1.600635E 02	0.0
11	11	PU-239	PU-239	1	4.737786E 02	3.378498E 13	2.792643E 13	8.183174E 13	5.858598E 12	9.100110E 02	0.0
12	12	PU-240	PU-240	2	1.295939E 02	4.303987E 12	2.044063E 12	6.246122E 12	2.259921E 12	6.710051E 01	0.0
13	13	PU-241	PU-241	1	7.152403E 00	9.059393E 11	7.798456E 11	2.349472E 12	1.260937E 11	2.577467E 01	0.0
14	14	PU-242	PU-242	3	1.854817E 00	4.924589E 10	2.354220E 10	7.184554E 10	2.570370E 10	7.712895E-01	0.0
15	15	SSFP	SSFP	4	1.141663E 02	1.532713E 12	0.0	0.0	1.532713E 12	0.0	0.0

TOTAL REACTION RATE AND POWER PRODUCTION BY UNIQUE ISOTOPE FOR WHOLE REACTOR
REACTION RATES HAVE UNITS OF EVENTS/SEC

PCS. RRT.	POS. SIG.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	CLASS	INVENTORY (KGS)	ABSORPTION	FISSION	PRODUCTION	CAPTURE(N,G)	FISS. POWER (WATTS)	CAPT. POWER (WATTS)
1	1	O-16	O-16	0	2.516042E 03	4.372120E 11	0.0	0.0	4.372120E 11	0.0	0.0
2	2	NA-23	NA-23	6	2.132009E 03	5.114958E 11	5.119037E 07	1.023809E 08	5.114446E 11	0.0	0.0
3	3	CR-N	CR-N	5	4.272340E 03	2.270198E 12	0.0	0.0	2.270198E 12	0.0	0.0
4	4	MN-55	MN-55	5	6.569434E 02	1.736403E 12	1.998915E 08	3.997832E 08	1.736204E 12	0.0	0.0
5	5	FE-N	FE-N	5	1.767268E 04	5.990773E 12	0.0	0.0	5.990773E 12	0.0	0.0
6	6	NI-N	NI-N	5	3.402774E 03	1.622223E 12	0.0	0.0	1.622223E 12	0.0	0.0
7	7	MO-N	MO-N	5	1.374882E 03	5.771004E 12	3.318247E 09	6.636495E 09	5.767684E 12	0.0	0.0
8	8	TA-181	TA-181	7	8.296207E 01	1.230404E 12	7.939692E 08	1.587939E 09	1.229611E 12	0.0	0.0
9	9	U-235	U-235	1	3.291962E 01	7.400045E 11	5.577344E 11	1.365606E 12	1.822699E 11	1.755803E 01	0.0
10	10	U-238	U-238	2	1.716542E 04	9.208051E 13	1.012259E 13	2.819685E 13	8.195798E 13	3.201270E 02	0.0
11	11	PU-239	PU-239	1	9.475571E 02	6.756997E 13	5.585286E 13	1.636635E 14	1.171720E 13	1.820022E 03	0.0
12	12	PU-240	PU-240	2	2.591875E 02	8.607974E 12	4.088125E 12	1.249224E 13	4.519843E 12	1.342010E 02	0.0
13	13	PU-241	PU-241	1	1.430481E 01	1.811879E 12	1.559691E 12	4.698944E 12	2.521874E 11	5.154935E 01	0.0
14	14	PU-242	PU-242	3	3.709635E 00	9.849176E 10	4.708440E 10	1.436911E 11	5.140741E 10	1.542579E 00	0.0
15	15	SSFP	SSFP	4	2.283326E 02	3.065426E 12	0.0	0.0	3.065426E 12	0.0	0.0
		TOTALS				1.935440E 14	7.223244E 13	2.105695E 14	1.213116E 14	2.345000E 03	0.0

2-D 17X10 - 5 GROUP SEARCH PROBLEM
PRIMARY SEARCH = NUCLIDE(DIRECT) - SECONDARY SEARCH = DIMENSION
SUMMARY TABLE OF NEUTRON LOSSES FLUX WEIGHTED
NORMALIZED WITH 2.084852E 14 K-EFFECTIVE IS 1.009999

ZONE CLASS ID.	FISSILE 1	FERTILE 2	O. ACTINIDE 3	FISSION PROD 4	STRUCTURAL 5	COOLANT 6	CONTROL ROD 7	OTHER 8
1	0.3363396	0.4829526	0.0004724	0.0147033	0.0834141	0.0024534	0.0059016	0.0020971
SUM	0.3363396	0.4829526	0.0004724	0.0147033	0.0834141	0.0024534	0.0059016	0.0020971

SUMMARY TABLE OF OTHER INFORMATION

ZONE CLASS ID.	ABSORPTION LOSSES	FISSILE INVENTORY (KGS)	CONVERSION RATIO	FISSION POWER (WATTS)	TOTAL POWER (WATTS)
1	0.9283339	9.947813E 02	1.23325	2.345000E 03	2.345000E 03
SUM	0.9283339	9.947813E 02	1.23325	2.345000E 03	2.345000E 03
OTHER LOSSES	0.0716661				
TOTAL LOSSES	1.0000000				

A BETTER ESTIMATE OF THE FUEL CONVERSION RATIO FOR A CRITICAL SYSTEM IS 1.26298
(BUT NOT MADE CRITICAL BY CHANGING CONTROL ABSORPTIONS OR LEAKAGE)

FISSILE CONSUMPTION/UNIT ENERGY GENERATION IS 1.176780E-14 KGS/WATT-SEC
FISSILE CONSUMPTION RATE IS 2.759550E-11 KGS/SEC

PRIMITIVE DOUBLING TIME (YEARS) OF THE ABOVE FISSILE INVENTORY (ONE PLANT) IS**********

NOTE - CONVERSION RATIO = (CAPTURE IN FERTILE)/(ABSORPTION IN FISSILE)

ENERGY PRODUCING UNIQUE ISOTOPES -- EQUIVALENT FUEL
BASED ON FISSION POWER

POS.	IDENTIFIER UNIQUE	IDENTIFIER ABSOLUTE	AMOUNT (KGS)	DESTRUCTION RATE (KGS/SEC)	WEIGHT (ENERGY)	WEIGHTED ABSORPTION (ATOM/SEC)	UNWEIGHTED CAPTURE (ATOM/SEC)
1	O-16	O-16	2.516042E 03	1.151521E-14	0.0	0.0	4.372120E 11
2	NA-23	NA-23	2.132009E 03	1.935227E-14	0.0	0.0	5.114446E 11
3	CR-N	CR-N	4.272340E 03	1.960525E-13	0.0	0.0	2.270198E 12
4	MN-55	MN-55	6.569434E 02	1.570354E-13	0.0	0.0	1.736204E 12
5	FE-N	FE-N	1.767268E 04	5.555061E-13	0.0	0.0	5.990773E 12
6	NI-N	NI-N	3.402774E 03	1.581274E-13	0.0	0.0	1.622223E 12
7	MO-N	MO-N	1.374882E 03	9.109571E-13	0.0	0.0	5.767684E 12
8	TA-181	TA-181	8.296207E 01	3.664949E-13	0.0	0.0	1.229611E 12
9	U-235	U-235	3.291962E 01	2.863246E-13	8.959059E-01	6.629744E 11	1.822699E 11
10	U-238	U-238	1.716542E 04	3.608382E-11	1.296149E-01	1.193500E 13	8.195798E 13
11	PU-239	PU-239	9.475571E 02	2.659022E-11	1.000000E 00	6.756997E 13	1.171720E 13
12	PU-240	PU-240	2.591875E 02	3.401565E-12	5.763941E-01	4.961586E 12	4.519943E 12
13	PU-241	PU-241	1.430481E 01	7.189667E-13	1.047513E 00	1.897966E 12	2.521874E 11
14	PU-242	PU-242	3.719635E 00	3.927311E-14	5.738484E-01	5.651934E 10	5.140741E 10
15	SSFP	SSFP	2.283326E 02	8.194803E-13	0.0	0.0	3.065426E 12
	TOTAL				4.223276D 00	8.708402D 13	

WEIGHTED EQUIVALENT FUEL CONSUMPTION/UNIT ENERGY GENERATION IS 1.460983E-14 KGS/WATT-SEC (BASED ON PU-239)
CORRESPONDING CONSUMPTION RATE IS 3.426005D-11 KGS/SEC

END OF REACTION RATE MODULE - MAX ARRAY SIZE USED IS 2027 WORDS

MATHEMATICAL FORMULATIONS

Presented in this part of the documentation of the VENTURE code block are the mathematical equations programmed along with background material and certain displays to convey the nature of some of the formulations. Relatively simple approximations have generally been used; these tend to become more sophisticated with development and as experience in application grows. As with any of the more active programs, modifications continue to be made to extend the capability. The originators plan to upgrade the coverage of the programmed equations as appropriate; others who introduce changes are urged to do the same to keep the users fully informed about the version of the code in local use, and to notify us of the changes they have found to be desirable.

END OF SECTION

Section 701: The Discrete-Energy Group Diffusion Equation

Presented here is the basic equation which accounts for the various reactions of neutrons with material in a macroscopic sense, scattering and the diffusion approximation to neutron transport. Quite generally, an accounting of the neutrons in a system at one location and at one energy may be done in the form

$$\frac{1}{v}\frac{\partial N}{\partial t} = \text{Sources} - \text{Losses} - \text{Net Transport Loss} \ , \qquad (701\text{-}1)$$

where v is the neutron velocity, and $\frac{\partial N}{\partial t}$ is the time rate of change of the neutron density. We are not concerned here with the dynamic problem, but rather with a steady-state condition or static approximation to the neutron density. For a steady-state condition, it is necessary that the rate at which neutrons are added is equal to the rate at which they are removed, locally, and therefore over the whole system treated. At any location there may be generation of neutrons through the fission process and other sources not related to neutron reactions, inscattering to any energy from other energies, removal by absorption or outscattering, and transport in and transport out.

The neutron density in an operating reactor is at steady state on the average due to natural reactivity compensation and control. In a large fraction of the neutronics problems solved, it is the intent to approximate this condition. Any problem describing a geometry, nuclide concentrations and cross sections, may represent a situation far from a steady state. The neutron population would actually rise or fall, and a steady-state solution only approximates the neutron distribution.

To effect this steady-state condition, the multiplication factor is introduced. The rate at which source neutrons are generated from fission is divided by the multiplication factor causing the loss rate to equal this adjusted source rate, a pseudo steady-state condition. The multiplication factor is defined as

$$k_e = \frac{\text{neutron generation rate}}{\text{neutron loss rate}} \quad . \tag{701-2}$$

A critical condition is one at steady state for which k_e is unity. The pseudo steady-state equation with the diffusion approximation to transport for the neutron flux at geometric location r and energy E using usual macroscopic nuclear properties is expressed as

$$- \nabla D_{r,E} \nabla \phi_{r,E} + (\Sigma_{a,r,E} + \Sigma_{s,r,E} + D_{r,E} B^2_{\perp E}) \phi_{r,E}$$

$$= \int_{E'} \left(\Sigma_{r,E' \to E} + \frac{1}{k_e} \chi_{r,E} (\nu\Sigma)_{f,r,E'} \right) \phi_{r,E'} dE' \quad . \tag{701-3}$$

The continuous energy spectrum is divided into discrete energy groups, and usually a simplification is made in the transport term,

$$- D_{r,g} \nabla^2 \phi_{r,g} + \left(\Sigma_{a,r,g} + \sum_n \Sigma_{s,r,g \to n} + D_{r,g} B^2_{\perp g} \right) \phi_{r,g}$$

$$= \sum_n \left(\Sigma_{s,r,n \to g} + \frac{1}{k_e} \chi_{r,g} (\nu\Sigma)_{f,r,n} \right) \phi_{r,n} \quad . \tag{701-4}$$

Where

∇^2 = the Laplacian geometric operator, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in slab geometry, cm^{-2},

$\phi_{r,g}$ = the neutron flux at location r and in energy group g, $n/sec\text{-}cm^2$,

$\Sigma_{a,r,g}$ = the macroscopic cross section for absorption, normally weighted over a representative flux energy spectrum, cm^{-1},

$\Sigma_{s,r,g\to n}$ = the macroscopic cross section for scattering of neutrons from energy group g to energy group n[a] (a set of these makes up a scattering kernel), cm^{-1},

$D_{r,g}$ = the diffusion coefficient, normally one-third of the reciprocal of the transport cross section,[b] cm,

$B^2_{\perp g}$ = the buckling term to account for the effect of the Laplacian operator (leakage) in one or more orthogonal coordinates not treated explicitly, cm^{-2},

$\nu\Sigma_{f,r,g}$ = the macroscopic production cross section (ν is the number of neutrons produced by a fission and Σ_f is the cross section for fission), cm^{-1},

$\chi_{r,g}$ = the distribution function for source neutrons (normally $\sum_g \chi_{r,g} = 1.0$, but provision is made for it not),

k_e = the effective multiplication factor, the ratio of the rate of production of neutrons to the rate of loss of neutrons from all causes, an unknown to be determined.

Equation (701-4) is called the usual neutron flux eigenvalue problem in this report. There is no provision in the above expression for fixed, external sources. The level of the neutron flux is not defined by the equation above. It can be whatever the investigator wants; however, there is no account made of temperature effects associated with changes

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[a]The in-group term g→g is excluded from the calculation.

[b]Coordinate-direction dependence is permitted without effect on the value of D used for the buckling loss.

in the power density on the nuclear properties, so the equation is appropriate to the extent that the macroscopic properties are representative.

The multiplication factor is an extremely useful measure of the degree a calculated system deviates from critical. The more positive the value of $(k_e - 1)$, the faster the flux level would increase; the more negative, the faster it would decrease. The effectiveness of control rods is directly measured by the decrease in k_e associated with rod insertion.

The difficulty associated with determining critical conditions and associated high cost of computation to support analysis effort have directly caused extensive application of this usual flux eigenvalue formulation in analysis of reactors. It is important to recognize, however, that the conditions estimated for a system which is not critical only approximate the real situation of reactor operation.

A Simple P_1 Treatment

A first order correction to diffusion theory is possible by application of the consistent P_1 equations. These are examined here for the usual eigenvalue problem in the form

$$\nabla\cdot J + \Sigma_t \phi = \frac{1}{k}\chi \int \nu\Sigma_f \phi dE' + \int \Sigma_s^o \phi dE' \;;$$
$$\nabla\phi + 3\Sigma_t J = \int \Sigma_s^1 J dE' \;, \qquad (701\text{-}5)$$

where the equations are for a point in space and energy, the integrals run over the energy range of interest, J is the current, ϕ is the scalar flux, Σ_s^o is the inscattering cross section, and Σ_s^1 is its first moment.

The diffusion theory approximation of the neutron current gives

$$J = -D\nabla\phi; \tag{701-6}$$

$$-\nabla D\nabla\phi + \Sigma_t\phi = \frac{1}{k}\chi\int\nu\Sigma_f\phi dE' + \int\Sigma_s^{o}\phi dE' , \tag{701-7}$$

In one-dimension, J has only one direction component but the integral over direction is required in general. For the one-dimensional case,

$$D = \frac{1}{3\left\{\Sigma_t - \frac{1}{3J}\int\Sigma_s^{1} J dE'\right\}} , \tag{701-8}$$

Where changes in macroscopic properties have been ignored. A common approximation is

$$D \simeq \frac{1}{3\left\{\Sigma_a + (1 - \bar{\mu}_o)\Sigma_s^{o}\right\}} .$$

In a simple P_1 form, the equations may be cast as

$$-\frac{1}{3\Sigma_t}\nabla^2\phi + \Sigma_t\phi = \frac{1}{k}\chi\int\nu\Sigma_f\phi dE' + \int\Sigma_s^{o}\phi dE' - \frac{1}{3\Sigma_t}\int\Sigma_s^{1}\nabla\cdot J dE' , \tag{701-9}$$

and the $\nabla\cdot J$ term is given by

$$\nabla\cdot J = \frac{1}{k}\chi\int\nu\Sigma_f\phi dE' + \int\Sigma_s^{o}\phi dE' - \Sigma_t\phi . \tag{701-10}$$

In multigroup form the P_1 equations chosen for implementation, with in-group corrections, are

$$-D(n,r)\,\nabla^2\phi(n,r) + \Sigma_r(n,r)\,\phi(n,r) = S(n,r)$$

$$-D(n,r)\sum_{m\neq n}\Sigma_s^{1}(m\rightarrow n)\,\nabla\cdot J(m) \tag{701-11}$$

where

$$S(n,r) = \frac{1}{k}\chi(n,r)\sum_m \nu\Sigma_f(m,r)\phi(m,r) + \sum_{\substack{m \\ m\neq n}} \Sigma_s^{o}(m\to n,r)\phi(m,r) \ ,$$

$$\nabla\cdot J(n,r) = S(n,r) - \Sigma_r(n,r)\phi(n,r) \ ,$$

$$D(n,r) = \frac{1}{3\left[\Sigma_t(n,r) - \frac{1}{3}\Sigma_s^{1}(m\to n,r)\right]} \ , \quad \text{and}$$

$$\Sigma_r(n,r) = \Sigma_t(n,r) - \Sigma_s^{o}(m\to n,r) \ ,$$

where the argument r refers to space and n and m to energy.

We note that if the finite-difference equations are summed, the P_1 scattering term does not cancel out, so an overall neutron balance does not result. This may restrict practical application. The apparent advantage of the scheme is that the diffusion coefficient to be used is obtained directly at each energy without requiring some weighting on what happens at other energies.

If one examines the spherical harmonics equations for P_1 truncation, there is one more first-order equation than coordinates treated; for example, four equations treat three space coordinates. As implemented, a simple equation for the net current is used along with a second order equation for the flux. There is a piece of information lost, even if only one coordinate is treated. That is, the in-group correction is the same regardless of the direction of the net current at another energy. In fact, anisotropic scattering at one energy has a direct effect on the angular flux at the energy scattered into. This effect can only be accounted for by applying a better formulation. The utility of the programmed equations remains to be demonstrated.

A remark is in order about the representation of boundary conditions. The simple P_1 approximation is programmed to use only the usual diffusion theory boundary conditions. Reflected, periodic and rotational symmetry conditions require no special attention: the approximations are consistent with the formulation for internal points. The extrapolated or nonreturn boundary condition may require special attention. The leakage of neutrons in this approximation is not simply related to the scalar flux derivative. As is usual in the application of diffusion theory, the representation of conditions near a control rod should be tested against a higher-order transport approximation; a best value for the extrapolation distance must be established by test, and this test should be with the P_1 formulation implemented, not regular diffusion theory. As is usual with the application of diffusion theory, external boundaries should be located sufficiently remote from the core proper that the actual leakage which will be calculated will not have much effect on the flux distribution in the core. The estimate of surface leakage is probably not especially improved by the programmed equations; rather, careful attention to what will result from the formulation may be necessary.

We look forward to learning about the results of experience with application given sufficient detailed information to permit thorough assessment. Meanwhile, a superior treatment is sought to bridge the gap between diffusion theory and a more explicit representation of transport theory which can be applied at a reasonable cost of computation.

END OF SECTION

Section 702: Finite Difference Representation of the Laplacian Operator

The Laplacian operator is to be represented in a finite-difference form. First, the finite-difference mesh will be examined. The equations will be developed for the three-dimensional slab; for fewer dimensions, the extent in the untreated orthogonal directions is considered to be infinite and contributions from these simply drop out of the equations.

Consider a traverse in space direction r. A region is traversed between r_1 and r_2 boundaries or material interfaces. Input data specifies the number of mesh points to be located between r_1 and r_2 and the spacing $\Delta = r_2 - r_1$ across the region.

Figure 702-1 presents a three-dimensional sketch showing the flux location at mesh point (i,j,m) and the surrounding six flux locations, nearest neighbors. The finite-difference volume about mesh point (i,j,m) is $(x_i - x_{i-1})(y_j - y_{j-1})(z_m - z_{m-1})$ where these are locations of the surfaces of the finite-difference element.

Neutron leakage from (i,j,m) to (i,j,m-1), $L(z_{m-1})$, through the front face of area $(x_i - x_{i-1})(y_j - y_{j-1})$ is approximated as follows. Let A_1 equal the unknown flux at the interface. Leakage out is given by approximating the flux slope at the surface by the average within the element (between the central point and the surface),

$$L(z_{m-1}) = D_{i,j,m}[\phi_{i,j,m} - A_1]\left[\frac{(y_j - y_{j-1})(x_i - x_{i-1})}{\left(\frac{z_m - z_{m-1}}{2}\right)}\right],$$

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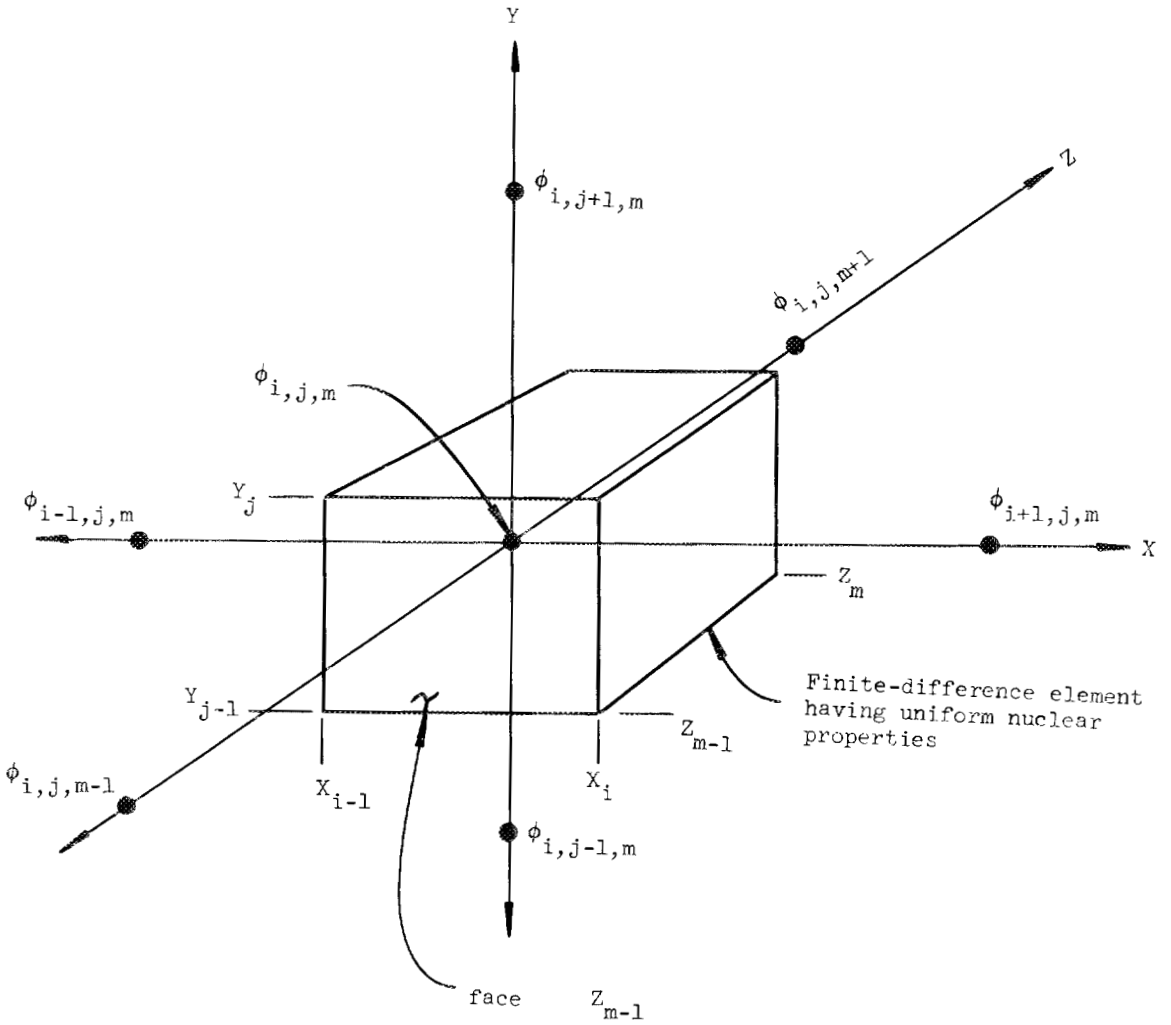

Fig. 702-1. The Seven-Point Finite Difference Mesh.

where $D_{i,j,m}$ is the diffusion constant at (i,j,m). Similarly for inward leakage from the adjacent finite element,

$$-L(z_{m-1}) = D_{i,j,m-1}\,[\phi_{i,j,m-1} - A_1]\left[\frac{(y_j - y_{j-1})(x_i - x_{i-1})}{\left(\frac{z_{m-1} - z_{m-2}}{2}\right)}\right] .$$

Eliminating A_1 from the equations gives

$$L(z_{m-1}) = \left[\frac{2(y_j - y_{j-1})(x_i - x_{i-1})}{\frac{z_m - z_{m-1}}{D_{i,j,m}} + \frac{z_{m-1} - z_{m-2}}{D_{i,j,m-1}}}\right][\phi_{i,j,m} - \phi_{i,j,m-1}] \quad . \qquad (702\text{-}1)$$

Since the term which multiplies the flux difference is simply some constant, Eq. 702-1 reduces to the form

$$L(z_{m-1}) = C_{i,j,m,m-1}\,[\phi_{i,j,m} - \phi_{i,j,m-1}] \quad . \qquad (702\text{-}2)$$

It may be noted that within a region having uniform nuclear properties and uniform mesh spacing,

$$C_{i,j,m,m-1} = \frac{(y_j - y_{j-1})(x_i - x_{i-1})\,D_{i,j,m}}{(z_m - z_{m-1})} \text{, internal, slab geometry.}$$

Provision is incorporated for the diffusion constant D to depend on coordinate direction; value of D simply depends on the particular coordinate treated and the assigned transport cross section.

The leakage from the whole element is given by

$$L(z_m) + L(z_{m-1}) + L(x_i) + L(x_{i-1}) + L(y_j) + L(y_{j-1})$$

$$= \phi_{i,j,m} [C_{i,j,m,m+1} + C_{i,j,m,m-1} + C_{i,j,m,i+1} + C_{i,j,m,i-1}$$

$$+ C_{i,j,m,j+1} + C_{i,j,m,j-1}] - C_{i,j,m,m+1} \phi_{i,j,m+1} - C_{i,j,m,m-1} \phi_{i,j,m-1}$$

$$- C_{i,j,m,i+1} \phi_{i+1,j,m} - C_{i,j,m,i-1} \phi_{i-1,j,m}$$

$$- C_{i,j,m,j+1} \phi_{i,j+1,m} - C_{i,j,m,j-1} \phi_{i,j-1,j} \quad . \qquad (702\text{-}3)$$

For a zero gradient boundary condition, the associated $C_{i,j,m,m-1}$ constant is set to zero.

For an extrapolated boundary condition, external or internal black boundary, the flux slope within the finite-difference element is extended. The boundary condition to be satisfied at the element surface is

$$-\frac{D}{\phi_s} \frac{\partial\phi}{\partial x} \bigg|_s = C_s \quad , \qquad (702\text{-}4)$$

where C_s is a specified constant.[a]

Let ϕ_i be the internal flux, ϕ_s be the boundary flux, and Δ be the distance to the boundary from the internal point.

A linear approximation of the flux within the element gives

$$-\frac{\partial\phi}{\partial x} = \frac{\phi_i - \phi_s}{\Delta}$$

---

[a]A default value of 0.4692 is used for C_s. Suitable group-dependent values which will reproduce the leakage condition must come from appropriate neutron transport calculations for a specific situation. An approximation which may be useful is $C_s \simeq 0.4692/(1 - \bar{\mu} + \frac{\Sigma_a}{\Sigma_s})$. There is also a correction for a curved surface; multiply C_s by something like (R+.5)/(R+1.) for a black sphere to reduce it as R decreases.

or

$$-\frac{D_i}{\phi_s}\frac{\partial\phi}{\partial x}\bigg|_s = \frac{D_i}{\Delta\phi_s}(\phi_i - \phi_s) = C_s \ .$$

Representing the normal area by A_n, the boundary leakage from one face of an element volume is given by

$$L_{s,n} = -D_i A_n \frac{\partial\phi}{\partial x}\bigg|_b = \frac{A_n\phi_i}{\left(\frac{1}{C_s} + \frac{\Delta}{D_i}\right)} , \qquad (702\text{-}5)$$

which gives the required constant for Eq. (702-3). Of course, the external leakage is considered lost from the system, but leakage into an internal black absorber is accounted for as an absorption in the region.

An alternative formulation for the extrapolated boundary condition is possible. Consider Eq. (702-4). Direct integration yields

$$\phi \propto e^{-C_s x/D} , \qquad (702\text{-}6)$$

and the leakage constant is given by

$$L_{s,n} = -D_i A \frac{\partial\phi}{\partial x}\bigg|_b = A_n C_s \phi_i e^{-C_s\Delta/D_i} \qquad (702\text{-}7)$$

This assumes an exponential shape of the flux between the internal point and the surface, rather than linear. We have tested this formulation but elected to use Eq. (702-5) because of wide practice in interpreting higher order transport theory results.

The repeating boundary condition causes flux values at opposite ends of a row to be coupled so that the row is a closed loop. For 90° rotational symmetry, coupling is from the right-hand edge column to the bottom edge row. Similarly, 120° rotational symmetry is treated for the

triangular mesh problem. In all such problems, the appropriate physical boundaries abut and the adjacent point flux values couple as across any internal interface. For 180° rotational symmetry, the right-hand edge column couples with itself inverted.

For curvilinear geometries, the surface areas of the finite-difference element faces must be used which lead to somewhat more involved equations than above. The finite-difference element is illustrated in Fig. 702-2.

For the special treatment of hexagonal and triagonal finite-difference elements, leakages across the individual volume element faces are formulated in the same manner as for slab geometry. The three-dimensional problem in hexagonal geometry involves eight nearest neighbors, six on the plane of the hexagons. In triangular geometry there are five nearest neighbors, three on the plane of the triangle. The hexagonal formulation is a high-order approximation to the situation (which may allow a relatively coarse mesh). The triangular formulation is of low-order and somewhat less reliable, especially since the next ring of points beyond the nearest neighbors are relatively close but not considered.

The mesh-point layout for the various geometries treated is indicated in the compact display in Table 702-1.

The special boundary conditions considered are shown in Fig. 702-3. These are for two-dimensional problems or on planes of three-dimensional problems. Note that the coordinate axes in triangular geometry are at either 120° or 60°. Fig. 702-4 shows the orientations for triangular geometry in detail, and Fig. 702-5 the layout for hexagonal geometry.

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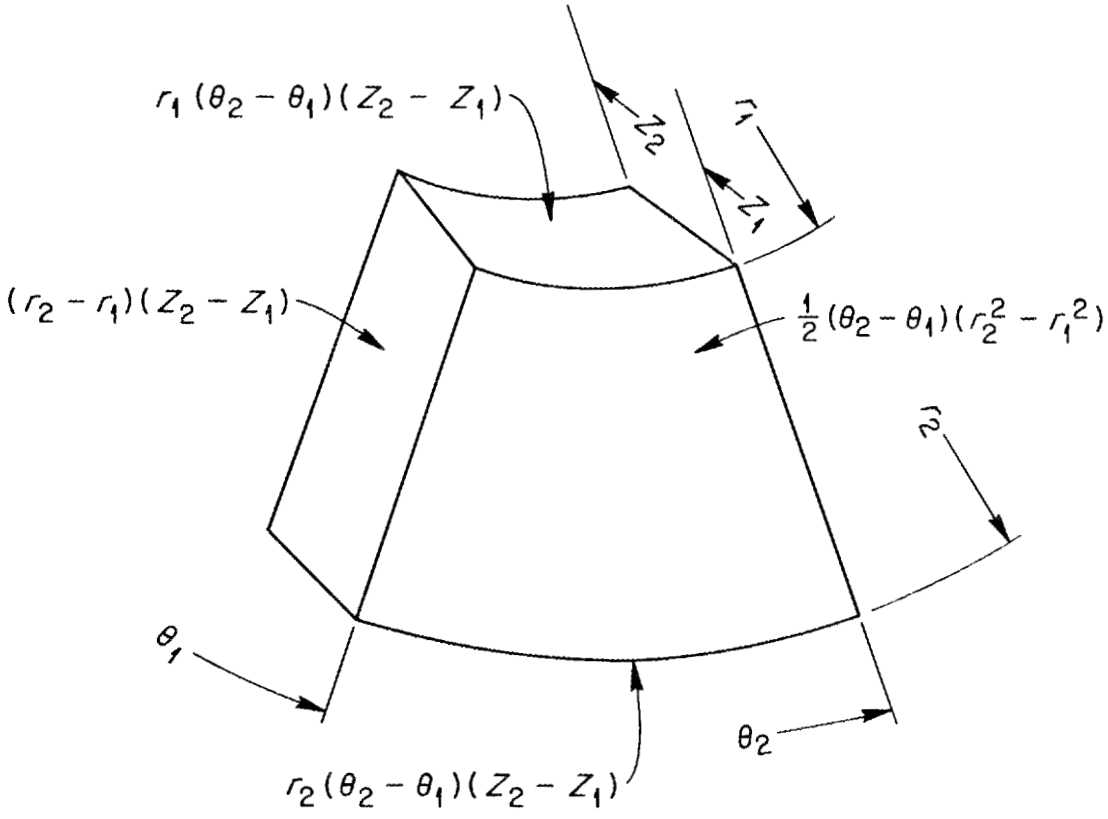


NOTE: θ IS IN RADIANS; WHEN THE CIRCLE IS CLOSED, θ SPANS 2π RADIANS

Figure 702-2. Cylindrical Finite-Difference Element

Table 702-1. Layout of Mesh Points[a]

System	Slab	Cylinder	Cylinder	Sphere	Hexagonal[b]	Triagonal[c]
Reference	$X\ Y\ Z$	$\Theta\ R\ Z$	$R\ Z$	R	$X\ Y\ Z$	$X\ Y\ Z$
Geometry	X-Y-Z	Θ-R-Z	R-Z	R	H-Z	T-Z
Specified region dimensions	Δ_x	Δ_r	Δ_r	Δ_r	Δ_x	Δ_x
	Δ_y	Δ_Θ	Δ_z		$\Delta_y = \Delta_x$	$\Delta_y = \Delta_x$
	Δ_z	Δ_z			Δ_z	Δ_z
Specified internal mesh points	J_x, I_y, M_z	J_r, I_z, M_Θ	J_r, I_z	J_r	J_x, I_y, M_z	J_x, I_x, M_z
Volume of region	$\Delta_x\Delta_y\Delta_z$	$\frac{\Delta_z\Delta_\Theta}{2}(r_2^2-r_1^2)$	$\pi\Delta_z(r_2^2-r_1^2)$	$\frac{4\pi}{3}(r_2^3-r_1^3)$	$\Delta_x\Delta_y\Delta_z\frac{\sqrt{3}}{2}$	$\Delta_x\Delta_y\Delta_z\frac{\sqrt{3}}{2}$

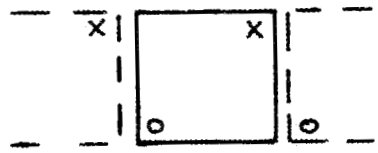
[a]Volume about each mesh point = volume of region ÷ number of internal points; mesh point locations are at finite-difference centroids.

[b]On a plane the Y coordinate is rotated 60° from the X coordinate.

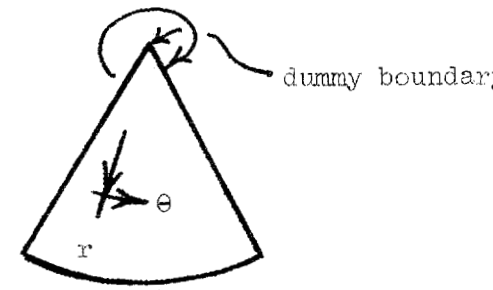
[c]On a plane, the Y coordinate is rotated 120° from the X coordinate in one option, 60° in another option, or 30°, or 90° as special cases (shown in Figure 702-4).

Special boundary conditions are keyed to the right-hand or third side indexed clockwise beginning with the left side. The coordinate axis intersect at the upper left hand corner in all cases.

REPEATING OR PERIODIC BOUNDARY

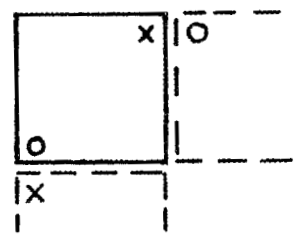


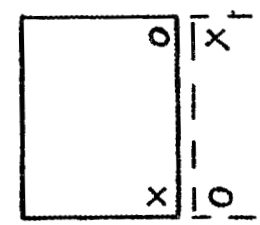
SLAB



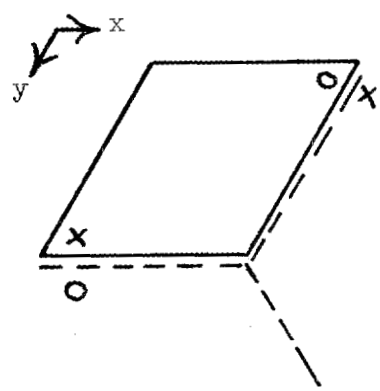
CYLINDER

90° AND 180° ROTATIONAL SYMMETRY

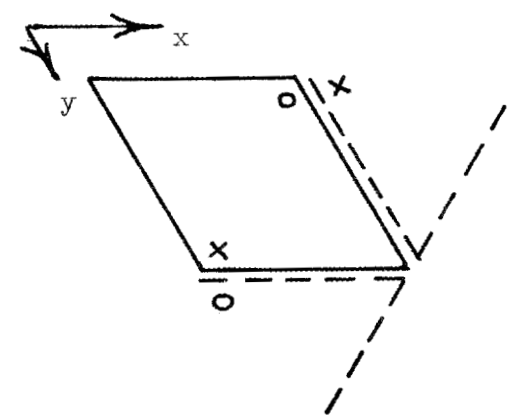




120° AND 60° ROTATIONAL SYMMETRY



Triangular, 120° Coordinates



Triangular, 60° Coordinates

Fig. 702-3. Special Boundary Conditions.

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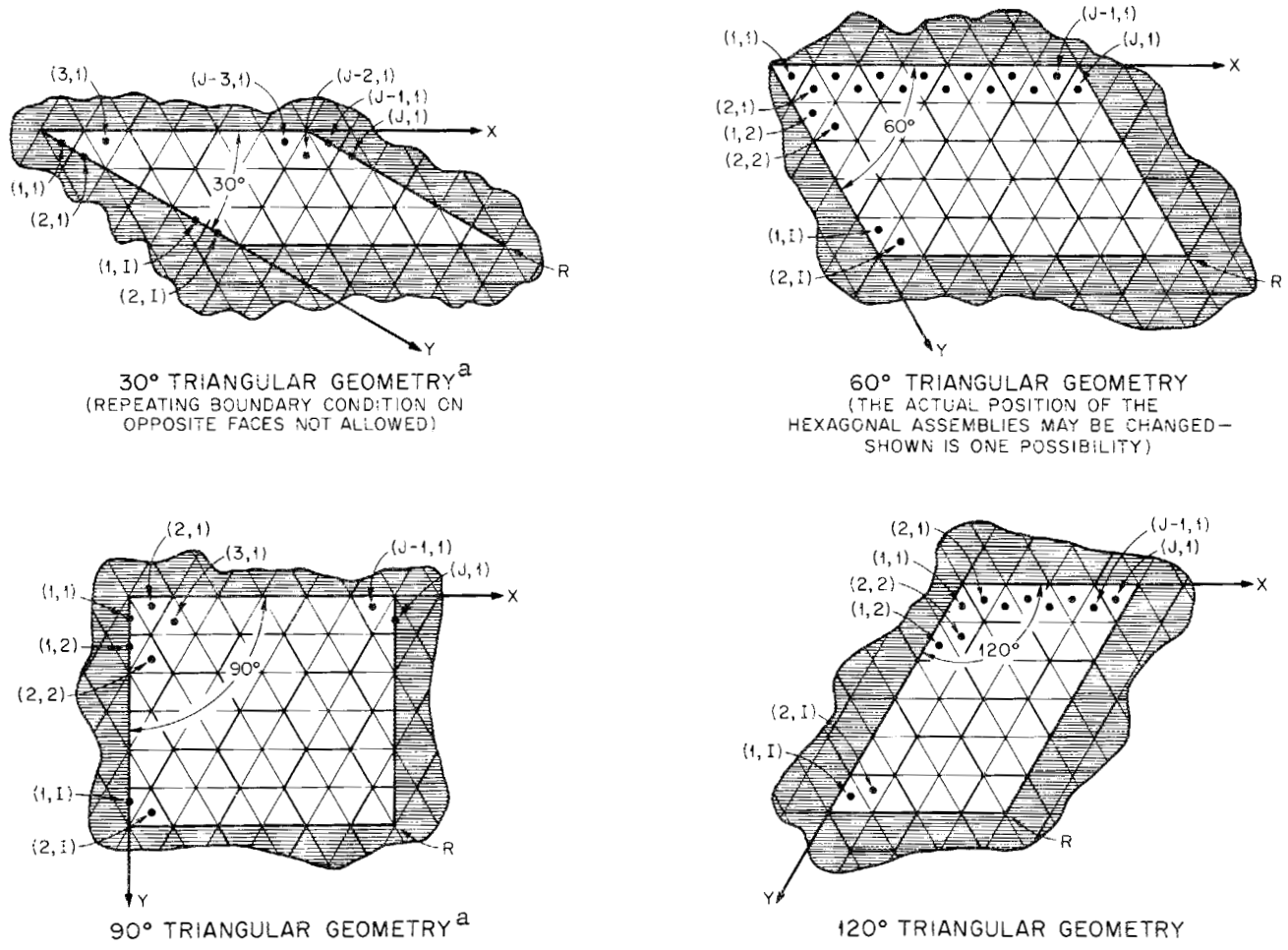

[a]Neither 30° nor 90° has been implemented; a superior formulation to mesh-centered difference is being implemented in another code.

Fig. 702-4. Orientation for Triangular Geometry

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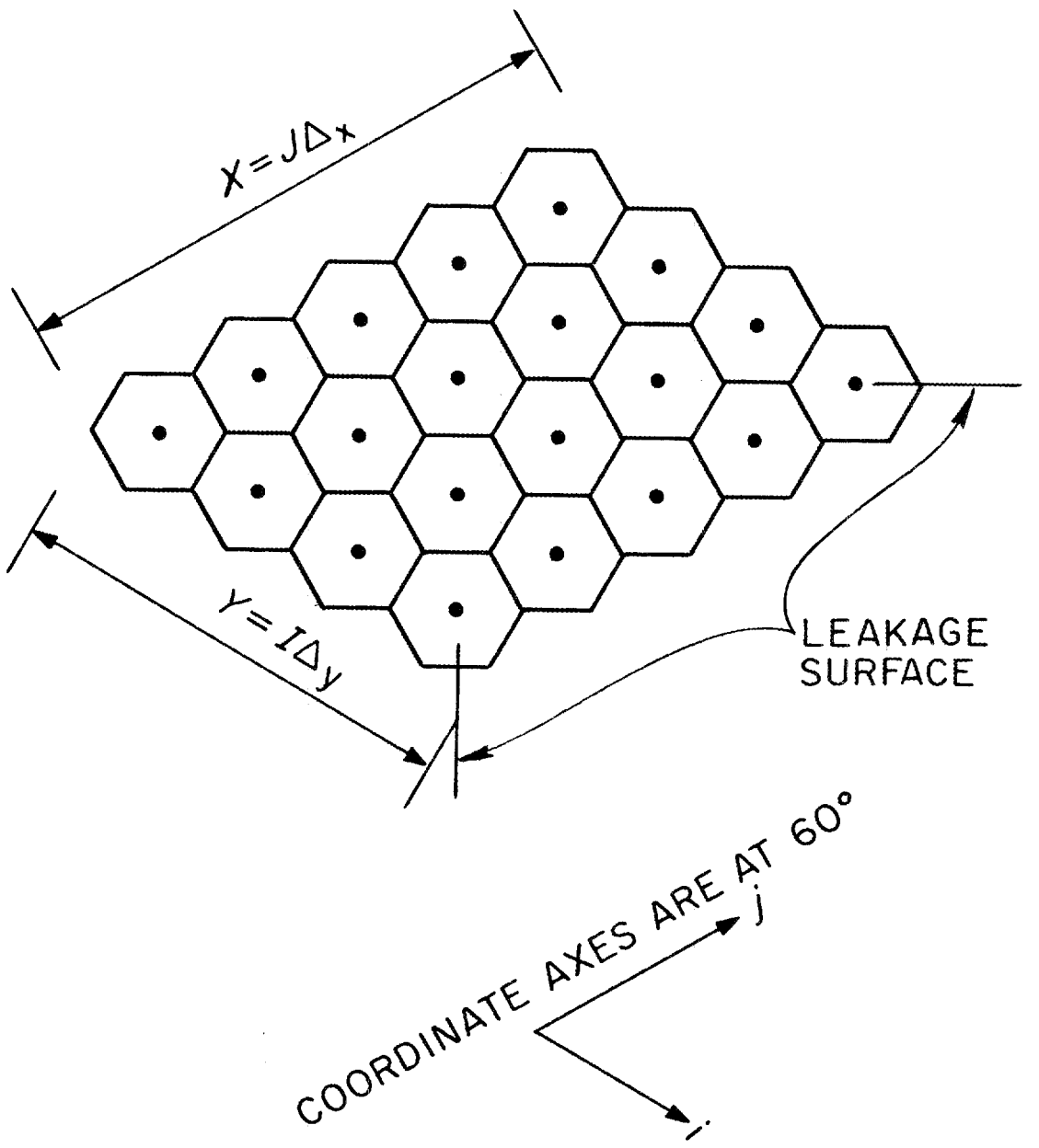

Figure 702-5. The Layout of Hexagonal Geometry.

Accuracy

It is well-known that the finite-difference approximation to the Laplacian operator is accurate to the order of the mesh spacing squared. We recognize that the accuracy of the mesh points centered approximation is slightly lower than that obtained with mesh points located on material interfaces. Of course they are identical within a homogeneous medium with uniform spacing. With mesh-centered points, reaction rates are properly located (rather than smearing abutting materials within the finite-difference volume element), a gain with this approximation; this makes such approximations as that of simple P_1 more realistic.

Still the analyst wants to know how accurate are integral quantities (k) as well as estimates of local properties (power density). We believe that experience is the best guide here. It is possible to increase the number of mesh points and solve the new fine-mesh problem, which normally improves the estimate of both integral and local quantities, but not necessarily. Care must be taken in allocation of mesh points and in selecting an energy group structure to get the best results. Generally it is desirable to increase the number of points in each direction (not just in one), and within each zone of uniform composition. About the same mean free neutron path length between adjacent points is desirable in all directions; therefore increasing of the number of mesh points should be done with this objective — decreasing large steps in the spacing.

Regarding local properties, it is a fallacy to believe that use of a very small finite-difference volume at one location will cause the estimate of local properties to have a high accuracy. We recommend against use of large changes in mesh spacing. Further, the interpretation of local quantities should be of mesh-average properties rather than local at the actual mesh point site.

Finite-Difference Approximation Error

The solution obtained by application of a finite-difference formulation is not precise; an error is associated with the approximation. This error may be larger than a casual user may anticipate. It is more serious regarding certain specific results than others, and has a dependence on the actual problem not readily predicted.

Some information is available from simple problems for which explicit solutions are available. Consider the one-group bare homogeneous cube in three dimensions, half-length L. The precise and finite-difference solutions for the flux are separable in space, the precise solution being $\phi(x,y,z) \propto \cos(\pi x/2L) \cos(\pi y/2L) \cos(\pi z/2L)$ with reflection at the start of each coordinate and zero flux at the extreme. Normalizing the flux such that its volume integral is unity,

$$\phi(x,y,z) = \left(\frac{\pi}{2L}\right)^3 \cos\left(\frac{\pi x}{2L}\right) \cos\left(\frac{\pi y}{2L}\right) \cos\left(\frac{\pi z}{2L}\right).$$

The leakage rate at one surface is, typically,

$$-D \int_y \int_z \frac{\partial\phi(x,y,z)}{\partial x}\bigg|_{x=L} dy\, dz = D\left(\frac{\pi}{2L}\right)^2 ,$$

and

$$k_e = \frac{\nu\Sigma_f}{\Sigma_a + 3D\left(\frac{\pi}{2L}\right)^2} ,$$

containing the familiar buckling term, $B_e = 3\,(\pi/2L)^2$.

The result for a finite-difference formulation depends on the location of the mesh points. Generally,

$$k_n = \frac{\nu\Sigma_f}{\Sigma_a + DB_n^2} ,$$

and

$$B_n^2 = \frac{-\int \left.\frac{\partial\phi}{\partial n}\right|_s ds}{\int\int\int \phi \, dx \, dy \, dz}$$

where the numerator is a surface integral of the normal derivative. For the situation here, assume the same representation along each coordinate,

$$B_n^2 = \frac{-3 \left.\frac{\partial\phi}{\partial x}\right|_{x=L}}{\int \phi \, dx} .$$

Consider mesh-centered points. Given N internal points along each coordinate space L/N, the end points located L/2N from boundaries, the solution is

$$\phi(n,j,i) = A \cos\left[\frac{\pi}{4N}(2n-1)\right] \cos\left[\frac{\pi}{4N}(2j-1)\right] \cos\left[\frac{\pi}{4N}(2i-1)\right] .$$

The surface leakage at x = L is estimated by assuming zero flux at x = L,

$$-\frac{\partial\phi}{\partial x}\bigg|_s \simeq -\frac{\Delta\phi}{\Delta x}\bigg|_s \simeq \left(\frac{2N}{L}\right)\phi(N,j,i)$$

$$= A\left(\frac{2N}{L}\right)\cos\left[\frac{\pi}{4N}(2N-1)\right]\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right]$$

$$= A\left(\frac{2N}{L}\right)\left\{\cos\left(\frac{\pi}{2}\right)\cos\left(\frac{\pi}{4N}\right)+\sin\left(\frac{\pi}{2}\right)\sin\left(\frac{\pi}{4N}\right)\right\}$$

$$\times\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right]$$

$$= A\left(\frac{2N}{L}\right)\sin\left(\frac{\pi}{4N}\right)\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right] .$$

The integrated flux is obtained as the sum

$$\int\phi\,dx \simeq A\sum_n \phi(n,j,i)\left[\frac{L}{N}\right]$$

$$= A\left(\frac{L}{N}\right)\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right]\sum_{n=1}^{N}\cos\left[\frac{\pi}{4N}(2n-1)\right]$$

$$= A\left(\frac{L}{N}\right)\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right]\frac{\cos\left(\frac{\pi}{4}\right)\sin\left(\frac{\pi}{4}\right)}{\sin\left(\frac{\pi}{4N}\right)}$$

$$= A\left(\frac{L}{2N}\right)\frac{\cos\left[\frac{\pi}{4N}(2j-1)\right]\cos\left[\frac{\pi}{4N}(2i-1)\right]}{\sin\left(\frac{\pi}{4N}\right)} ;$$

$$B_N^2 = \frac{3\left(\frac{2N}{L}\right)\left[\sin\left(\frac{\pi}{4N}\right)\right]^2}{\left(\frac{L}{2N}\right)} ,$$

$$B_N^2 = 3\left\{\left(\frac{2N}{L}\right)\sin\left(\frac{\pi}{4N}\right)\right\}^2 .$$

Note that for large N, $\sin(\pi/4N) \to \pi/4N$, $B_\infty^2 \to 3(\pi/2L)^2$, the precise result.

The more general solution for a different number of mesh points along each coordinate follows directly,

$$B^2_{N,J,I} = \left\{\frac{2N}{L}\sin\left(\frac{\pi}{4N}\right)\right\}^2 + \left\{\frac{2J}{L}\sin\left(\frac{\pi}{4J}\right)\right\}^2 + \left\{\frac{2I}{L}\sin\left(\frac{\pi}{4I}\right)\right\}^2 .$$

Comparing the finite-difference solution to the precise one, the expressions for the flux are identical except for normalization. This aspect limits the generality of this assessment.

The error associated with any point flux value is given by comparing normalized results. Normalizing to the same loss rate, absorption plus leakage, yields

$$\int\int\int [\Sigma_a + DB_e^2] \quad \phi(x,y,z)\, dx\, dy\, dz$$

$$\simeq \sum_{n,j,i} \left[\Sigma_a + DB^2_{N,J,I}\right]\left[\frac{L^3}{NJI}\right] \phi(n,j,i) ,$$

and the right-hand side is easily obtained by the product of averages along each coordinate. This leads to the relative error

$$\frac{\phi(n,j,i) - \phi(x,y,z)}{\phi(x,y,z)} = \left(\frac{4}{\pi}\right)^3 NJI \sin\left(\frac{\pi}{4N}\right) \sin\left(\frac{\pi}{4J}\right) \sin\left(\frac{\pi}{4I}\right)$$

$$\times \left[\frac{1 + \frac{D}{\Sigma_a} B_e^2}{1 + \frac{D}{\Sigma_a} B^2_{N,J,I}}\right] - 1$$

$$\simeq \frac{-\frac{1}{6}\left[1 + \frac{D}{\Sigma_a}\left(\frac{\pi}{2L}\right)^2\right]\left[\left(\frac{\pi}{4N}\right)^2 + \left(\frac{\pi}{4J}\right)^2 + \left(\frac{\pi}{4I}\right)^2\right]}{1 + \frac{D}{\Sigma_a}\left(\frac{\pi}{2L}\right)^2\left[3 - \frac{1}{3}\left\{\left(\frac{\pi}{4N}\right)^2 + \left(\frac{\pi}{4J}\right)^2 + \left(\frac{\pi}{4I}\right)^2\right\}\right]} .$$

Thus the error in a point flux value depends on the problem, and it depends on the mesh, each coordinate making an independent contribution. Except for a small number of points, the error decreases as the sum of the reciprocals of the squares of the numbers of mesh points along each coordinate. Doubling the number of points along each of the coordinates would be expected to reduce the error by a factor of 4.

Consider the error in an integral quantity, namely the multiplication factor. Since

$$k_{N,J,I} = \frac{\nu\Sigma_f}{\Sigma_a + DB^2_{N,J,I}} ,$$

the error is given by

$$\frac{k_{N,J,I} - k_e}{k_e} = \frac{\frac{D}{\Sigma_a}\left(B_e^2 - B^2_{N,J,I}\right)}{1 + \frac{D}{\Sigma_a} B^2_{N,J,I}}$$

$$\simeq \frac{\frac{D}{3\Sigma_a}\left[\left(\frac{\pi}{4N}\right)^2 + \left(\frac{\pi}{4J}\right)^2 + \left(\frac{\pi}{4I}\right)^2\right]}{1 + \frac{D}{\Sigma}\left(\frac{\pi}{2L}\right)^2\left[3 - \frac{1}{3}\left\{\left(\frac{\pi}{4N}\right)^2 + \left(\frac{\pi}{4J}\right)^2 + \left(\frac{\pi}{4I}\right)^2\right\}\right]} ,$$

a similar dependence to that obtained above for the flux error.

The Leakage Operator Error

Consider the finite-difference approximation to the leakage operator. If the flux and derivatives were known at a point, the flux at a neighboring point is given by a Taylor expansion as

$$\phi(\Delta) = \phi(0) + \Delta \left.\frac{\partial\phi}{\partial x}\right|_0 + \frac{\Delta^2}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_0 + \frac{\Delta^3}{6}\left.\frac{\partial^3\phi}{\partial x^3}\right|_0 + \frac{\Delta^4}{24}\left.\frac{\partial^4\phi}{\partial x^4}\right|_0 + \ldots ,$$

$$\phi(-\Delta) = \phi(0) - \Delta \left.\frac{\partial\phi}{\partial x}\right|_0 + \frac{\Delta^2}{2}\left.\frac{\partial^2\phi}{\partial x^2}\right|_0 - \frac{\Delta^3}{6}\left.\frac{\partial^3\phi}{\partial x^3}\right|_0 + \frac{\Delta^4}{24}\left.\frac{\partial^4\phi}{\partial x^4}\right|_0 - \ldots ,$$

where Δ is the mesh spacing. Summing these gives the central difference approximation for the Laplace operator,

$$\frac{\partial^2\phi}{\partial x^2} = \frac{\phi(\Delta) + \phi(-\Delta) - 2\phi(0)}{\Delta^2} - \frac{\Delta^2}{12}\left.\frac{\partial^4\phi}{\partial x^4}\right|_0 + \ldots .$$

Thus the error from dropping the higher terms is to the order of the mesh spacing squared, so the error is expected to vary inversely as the square of the number of mesh points. This difference error is strictly true only for mesh-edge point location, and only with adequate points to make the higher order terms insignificance; however, a similar dependence is found from application experience given enough mesh-centered points.

Another approach to error estimation is the formulation of the neutron balance for a discrete element. The use of $\frac{1}{\Delta}\{\phi_i - \phi_{i-1}\}$ for the surface leakage is accurate to the order of the mesh spacing and the relative error in the balance proportional to the mesh spacing squared.

Application

Consider that a calculation produced a result V_1 with a mesh of N_1, J_1, and I_1 points. A second result is obtained with N_2, J_2, and I_2 points. We expect that

$$\frac{V_1 - V_\infty}{V_2 - V_\infty} = \frac{\alpha_1}{\alpha_2} ; \qquad V_\infty = \frac{\alpha_1 V_2 - \alpha_2 V_1}{\alpha_1 - \alpha_2} ,$$

where

$$\alpha_n = \left[\frac{1}{N_n^2} + \frac{1}{J_n^2} + \frac{1}{I_n^2} \right] ,$$

applicable to one, two or three dimensions (drop terms not applicable).

These results show that the errors in the point flux values and in the multiplication factor are inversely proportional to the square of the number of mesh points along each coordinate. Given two solutions,

$$\frac{V(N) - V(\infty)}{V(M) - V(\infty)} = \left(\frac{M}{N}\right)^2 ;$$

$$V(\infty) = \frac{V(N) - \left(\frac{M}{N}\right)^2 V(M)}{1 - \left(\frac{M}{N}\right)^2} ,$$

where $V(N)$ is the result with N mesh points, $V(\infty)$ is the extrapolation to approximate the result for a continuum. Note that N and M are the number of points along one coordinate, not the total points. The equations apply to one, two, or three dimensional problems.

Changes made locally or to less than all coordinates treated should not be expected to produce reliable extrapolation and error assessment, nor is error assessment of a coarse mesh result reliable. The reliability of such extrapolation in application to the general multi-group, complicated geometry problem is unknown. Extrapolation of integral quantities should be more reliable than of point properties; the points may be at different locations and an extreme (such as the maximum power density) may move from one location to another. For reliable assessment, it is recommended that a uniform increase in mesh points be made along all coordinate directions in each zone.

An illustration of application is given here. Explicit solutions are known for bare homogeneous problems. The results from extrapolation of answers for successive meshes are shown below for a particular seven-group three-dimensional case:

Space Mesh (M)	K(M)	$\left(\frac{M}{N}\right)^2$	k (∞)
6 × 2 × 4	0.7400339	-	-
12 × 4 × 8	0.7280397	4	0.7240416
24 × 8 × 16	0.7250360	4	0.7240348
48 × 16 × 32	0.7242847	4	0.7240343
96 × 32 × 64	0.7240969	4	0.7240343
144 × 48 × 96	0.7240621	2.25	0.7240343
∞ (continuum)	0.7240343		

Of course the problems solved in analysis usually have geometric and composition complexities; an integral quantity such as the multiplication factor may be monotonic with increasing mesh only above some mesh size, and extrapolation of coarse results is unreliable due to higher order error contamination.

END OF SECTION

Section 704: Calculation of Macroscopic Cross Sections, Normalization and Edits

This code is designed to use microscopic data for individual nuclides to take into account changes in the concentrations of the nuclides. It may be practical in some situations to use a pseudo nondepleting nuclide concentration of relative density and associated macroscopic cross sections.

The basic equations used for calculation of macroscopic cross sections are shown below. For subzone concentrations, the effective zone concentration of each nuclide is taken as the subzone concentration times the ratio of the subzone volume to the zone volume. It is assumed that nuclide densities are in atoms/barn-cm and microscopic cross sections in barns in calculating reaction rates, depletion, and determining mass balances.

Consider some zone within which each nuclide has a uniform, smeared concentration N. The usual cross sections are calculated as follows with indexes a-absorption, f-fission, tr-transport, s-scattering, and g and k-energy groups, z-zone, and n-nuclide.

$$\Sigma_{a,g,z} = \sum_n N_{n,z}\ \sigma_{a,n,g}\ ,$$

$$\Sigma_{f,g,z} = \sum_n N_{n,z}\ \sigma_{f,n,g}\ ,$$

$$\nu\Sigma_{f,g,z} = \sum_n N_{n,z}\ \nu\ \sigma_{f,n,g}\ ,$$

$$\Sigma_{tr,g,z} = \sum_n N_{n,z}\ \sigma_{tr,n,g}\ ,$$

where

$$\nu\ \sigma_{f,n,g} = \nu_{n,g}\ \sigma_{f,n,g}\ ,$$

and

$$N_{n,z} = M_{n,z} q_z + \sum_{sz} M_{n,sz} \frac{V_{sz}}{V_z} ,$$

where $M_{n,z}$ is the concentration of nuclide n in zone z, q_z is the volume fraction, $M_{n,sz}$ is a subzone concentration and V_{sz} and V_z are the subzone and zone volumes respectively;

$$D_{g,z} = \frac{1}{3\ \Sigma_{tr,g,z}} ,$$

$$\Sigma_{s,g\to k} = \sum_n N_{n,z}\ \sigma_{s,g\to k} . \qquad (704\text{-}1)$$

For the diffusion-approximation calculations, each $\Sigma_{s,g\to g}$ is set to zero to avoid slowing the rate of convergence of the iterative process.

The equations used to determine reaction rates are as follows. The reactor thermal pwoer level, P, is determined by

$$P = \frac{C_1}{C_2} \sum_z V_z \sum_n N_{n,z} \left\{ X_n \sum_g \bar{\phi}_{g,z}\ \sigma_{f,n,g} + Y_n \sum_g \bar{\phi}_{g,z}\ \sigma_{c,n,g} \right\} , \qquad (704\text{-}2)$$

where X_n is the nuclide thermal energy watt-sec per fission, Y_n is per capture, C_1 is the specified fraction useful power, C_2 is the specified fraction of the core treated and the flux level is adjusted such that the calculated P is that value specified in watts. The values of $\bar{\phi}_{g,z}$ are simply volume weighted over zones at each energy,

$$\bar{\phi}_{g,z} = \frac{\sum_{i\ \varepsilon\ z} \phi_{i,g}\ V_i}{\sum_{i\varepsilon z} V_i} , \qquad (704\text{-}3)$$

where i refers to a mesh point (and its associated elemental volume).

Given the microscopic type of energy data, not group dependent,

$$W_{g,z} = \sum_n N_{n,z} (X_n \sigma_{f,n,g} + Y_n \sigma_{c,n,g}) , \qquad (704\text{-}4)$$

then

$$P = \frac{C_1}{C_2} \sum_t V_z \sum_g W_{g,z} \bar{\phi}_{g,z} . \qquad (704\text{-}5)$$

That is, the normalization of the results of a calculation is to a desired power level. Point flux and zone average flux values are discussed above. Lacking energy data, X_n values are set to 3.2×10^{-11} watt-sec/Fiss. Edited results are based on the flux level required to satisfy the desired power level.

The local power density is given by

$$H_i = \sum_g W_{g,z} \phi_{i,g} , \qquad (704\text{-}6)$$

where i is contained in z. For traverses, the maximum value of H_i is found and values along each of the coordinate directions through this point are edited.

The local neutron density is given by

$$N_i = \sum_g \frac{1}{v_{g,z}} \phi_{i,g} , \qquad (704\text{-}7)$$

where $v_{g,z}$ is the group neutron velocity associated with point i.

When an edit of the "Primitive Fissile Conversion Ratio" is found, it is the ratio of the rate of capture (n,γ) in the defined fertile nuclides divided by the rate of absorption in the defined fissile nuclides using volume integrals of reaction rates summed over groups. It is

desirable to define such intermediate nuclides as Pa^{233} and Np^{239} as fissile for accounting purposes.

Edits of point values are for the locations of the mesh points (volume element centered), not interpolations to material boundary intersections.

END OF SECTION

Section 705: Types of Problems Solved

The procedures implemented in the VENTURE code block are oriented at resolution of any of a wide variety of basic problem types. These are described in this section with the equations cast in matrix form. We start with the usual neutron flux eigenvalue problem (see Eq. 701-2).

The Usual Eigenvalue Problem

The usual neutron flux eigenvalue problem may be cast in the form

$$A\,\phi = \frac{1}{k_e}\,\chi F\,\phi\ , \tag{705-1}$$

where A is the transport, scattering coupling, and loss operator; F is the fission source, a row operator; χ is the source distribution function, a column operator[a]; ϕ is the neutron flux vector; and k_e is the multiplication factor to be determined which effects a pseudo steady state condition.

Eq. (705-1) has the solution

$$\phi = \frac{1}{k_e}\,A^{-1}\,\chi F\,\phi \tag{705-2}$$

where A^{-1} is the inverse of A, $A^{-1}A = I$. For many problems of interest it is not practical to invert A. Given n space-energy points, A is an nxn square matrix containing n^2 entries. So an iterative procedure is used which takes advantage of the sparseness of both A and F.

Eq. (705-2) may also be expressed as

$$(A^{-1}\chi F - k_e\,I)\,\phi = 0\ , \tag{705-3}$$

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[a] χF could be a matrix, not separable.

indicating that k_e is an eigenvalue of $A^{-1}\chi F$. We hope that any flux eigenvalue problem to be treated has a unique, most positive eigenvalue in the set of all of them, $k_e = k_1 > k_2 > \ldots$. The requirements under which this is the situation have been studied.[a,b] Physically, it is required that each point in the space-energy system be coupled to every other point through the coupling coefficients (in both A and χF). Further, the solution vector ϕ is unique and each component ≥ 0, but only if χF is all positive and the diagonal terms of A dominate along columns; it is sufficient that all macroscopic cross sections be positive given the necessary coupling, but not absolutely necessary.

The Fixed Source Problem

The fixed source problem is expressed as

$$A\,\phi = \chi F\,\phi + S\ , \tag{705-4}$$

not an eigenvalue problem. Occasionally F = 0, as for deep penetration shielding problems, especially applicable to extending a solution for a fueled region to a remote location by an auxiliary calculation. In reactor core analysis, fixed source problems have been used mostly to play computation games. However, there are special situations which require this formulation, as for analysis of the start-up condition with a source inserted in the reactor.

For usual situations there is a neutron density distribution associated with a fixed source problem, and the level of this density is higher the larger the magnitude of the source. A prime objective of a

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[a] G. Birkhoff and R. S. Varga, "Reactor Criticality and Nonnegative Matrices," J. Soc. Ind. App. Math 6, p. 354 (1958).

[b] R. Froehlich, "Positivity Theorems for the Discrete Form of the Multigroup Diffusion Equations," NS&E 34, p. 57 (1968).

fixed source calculation is to determine the neutron flux level associated with the source.

When F is nonzero, there is a sensible solution to Eq. (705-4) only if the related problem

$$A\ \phi = \frac{1}{k_e}\ \chi F\ \phi$$

is subcritical, $k_e < 1$, when $S = 0$. Otherwise; the flux level would keep increasing, even without the fixed source, and the usual procedures for resolving fixed source problems generally fail.

The Adjoint Flux Problem

The adjoint flux eigenvalue problem is expressed as

$$A^t\phi^* = \frac{1}{k_e}(\chi F)^t\phi^* \ , \qquad (705\text{-}5)$$

where the superscript t refers to the transpose of elements about the diagonal (interchange of rows and columns). In diffusion-theory representation, transposing A involves

(1) no changes in the total removal (absorption + outscattering + DB^2) terms on the diagonal,

(2) no change in the diffusion coupling due to symmetry about the diagonal, but

(3) change in the group-to-group transfer or scattering terms, $\Sigma(g\to n)$ to $\Sigma(n\to g)$; inscattering no longer cancels removal if the equations are summed.

Transposing χF causes the contribution to group g by the distribution function $\chi(g)$ of neutrons produced in fission in group n from the reaction due to cross section $\nu\Sigma_f(n)$, namely $\chi(g)\nu\Sigma_f(n)$, for the usual

problem, to be reversed for the adjoint problem, namely $\nu\Sigma(g)\chi(n)$, or $F^t\chi^t$, if (χF) is separable.

The eigenvalue of the adjoint problem is the same as that of the regular problem, k_e. Thus it is common practice to use the result from the regular problem in the process of solution of the adjoint problem when they are treated in succession. However, it sometimes is of more interest to solve the perturbed adjoint problem for more precise analysis of perturbations when a specific perturbation is of interest. In this case the perturbation changes k_e requiring that it be determined as an unknown.

The adjoint fixed source problem is of special utility in analysis of the effect of perturbations to the system on some specific local effect. The problem to be solved is

$$A^t\phi^* = \frac{1}{k_e} F^t\chi^t\phi^* + S^* \quad , \tag{705-6}$$

and the appropriate source, S^* must be supplied for this adjoint problem.

When an adjoint problem is of the eigenvalue type and directly follows a regular problem, in the same code block access, then the result for k_e from the regular problem is used. It is thus assumed that these eigenvalue problems are for the same system. When an adjoint eigenvalue problem is of the eigenvalue type and directly follows a regular problem in which a criticality search was done, it is again assumed that these eigenvalue problems are for the same system, namely the result of the criticality search. This is true even for the 1/v search and the 1/v loss terms are included in the adjoint problem.

When an adjoint problem is of the fixed source type, it is assumed to be for the system initially presented, except when a regular problem is run first and adjustments are made in nuclide concentrations or dimensions.

An adjoint problem may be solved in an access to the code block without first solving a regular problem. This problem may be an eigenvalue problem, or a fixed source problem for which there may or may not be a transposed fission source.

Criticality Searches

The primary application of a code block designed to solve neutronics eigenvalue problems is analysis of reactor core conditions. To hold a reactor at a desired power level, it must be maintained at a near critical condition. Therefore, it is incumbent on analysis effort to determine representative conditions near this required state of operation. The type of problem to be solved has been named the "criticality search"; adjustments are to be made in certain parameters of the problem to establish a desired state of criticality.

Establishing the positions of individual control rods represented discretely in a finite-difference mesh which satisfy the critical condition and minimize the peak power density is one of the most difficult problems formulated in reactor analysis. This problem has only been solved by indirect methods when a fine scale flux distribution is included in the requirements to be satisfied.

The criticality search problem may be expressed in a general formulation as

$$(A - \frac{1}{k_e} \chi F)\phi = B\phi \ , \qquad (705\text{-}7)$$

where k_e is the multiplication factor to be satisfied, a specified number often unity, and B is the search operator. This problem is to be solved given a specified way in which the components of B are to be changed to effect the solution.

There may be constraints on acceptable solutions; a mathematical solution may not have a realistic physical interpretation. A system containing no fissile material cannot be made critical unless fissile material is added to it. A mathematical solution which involves negative nuclide concentrations or ones which exceed physical limitations is usually not acceptable.

A unique solution to the general search problem is not assured. There are often two different mixtures of D_2O and H_2O which will satisfy critical conditions in a wide lattice thermal reactor. There are often three different concentrations of the same mixture of plutonium isotopes which will satisfy critical conditions (mathematically) in a water-cooled core. The analyst is often seeking only one of these possible solutions. He is cautioned about the difficulties associated with the general criticality search problem. The automated procedures seek a mathematical solution, try to determine those situations where such a solution does not exist, and make key tests on a solution to determine if it is realistic in a physical sense, and discontinue further calculation if it is not. Quite generally, it is assumed that the initial state of the system is relatively close to the desired solution. When it is so, many of the difficulties are avoided. Beware the results when large changes to the initial conditions were required to effect a solution.

The sophistication of the treatment in a code such as VENTURE increases with development. Basic capability programmed in the code is

discussed here which includes extensions over simple procedures. Consider that concentrations of nuclides have been adjusted in accordance to specifications, but the problem solution is found to be unacceptable. Let us say it took more of the described fuel as makeup than is available. Adding the allotted amount of this fuel, and then searching on a secondary fuel mixture is possible. Thus some limiting constraint may be satisfied and the calculation continued to apply a second type of search, and then a third, etc.

For the basic criticality search problems treated in the VENTURE code, Eq. (705-7) is recast in the form

$$(A - \frac{1}{k_e}\chi F)\,\phi = \lambda(\frac{1}{k_e}\chi P - Q)\phi \;, \qquad (705\text{-}8)$$

where χP is the neutron source operator generally associated with search on fissile nuclide concentrations, similar to but often more sparse than χF, Q is a diagonal matrix representing loss only, and λ is the eigenvalue of the search problem to be determined. A procedure is available which iterates directly toward a solution.

The Direct Buckling Search

In Eq. (705-8), P = 0, and Q contains the contributions from buckling loss terms as specified, $DB_\perp^2V$. The local value of the diffusion coefficient D is used, the local volume V, and the buckling $B_\perp$ which may be energy group and position dependent. The value of λ, an eigenvalue, is to be determined; it is a relative magnitude of the buckling. That is, all the values of $B_\perp$ are adjusted proportionally ($\lambda B_\perp$) to effect a solution. As programmed, $\lambda - 1$ is determined during the iterative procedure, that is the change from the initial problem description.

The Direct Reciprocal Velocity Search

For this problem, P = 0, and only the diagonal elements of Q contain the product of the reciprocal of the velocity and the local volume, loss terms. The eigenvalue λ is a multiplier on the reciprocal velocity sink term which effects a solution. If λ is negative, a distributed source has been added to the system.

This calculation determines the prompt mode time constant. The dynamic neutron balance is considered in the form

$$\frac{\partial N}{\partial t} = \frac{1}{v}\frac{\partial \phi}{\partial t} = \text{sources} - \text{losses} \ , \tag{705-9}$$

where N is the neutron density and v is the neutron velocity. The asymptotic neutron flux mode is formulated by assuming that

$$\phi = Ce^{-\alpha t} \ ,$$

$$\frac{\partial \phi}{\partial t} = -\alpha Ce^{-\alpha t} \ .$$

Substitution of these into Eq. (705-9) leads to the form of Eq. (705-8), P = 0, with λ identified as α, a time constant usually associated with a prompt neutron mode (no contribution from delayed neutrons), and Q is v^{-1}. A suitable value of k_e must be specified and the results properly interpreted, but coverage of these important details is beyond the scope of this document. It is often necessary to solve another problem first to obtain the desired results, either to establish suitable conditions, as by adjusting some of the parameters, or to establish the value of k_e for the system.

The Direct Nuclide Concentration Search

The direct search technique may often be usefully applied to problems of determining nuclide concentration changes, the nuclide concentration search. Desired conditions may often be satisfied with little more calculational effort than required to solve the corresponding usual eigenvalue problem. It is assumed that the nuclides for which concentration changes are to be made will make a primary contribution to the macroscopic absorption and production cross sections, and only secondarily affect the scattering and transport terms. Thus application is to heavy metals or control absorber, not to moderator nor reflector.

The concentrations of certain nuclides are to be changed in the system as necessary to satisfy a desired value of k_e. Given specifications for these concentration changes, a common multiplier is desired such that at solution the actual change made in the concentration of nuclide n at location r is given by

$$\Delta N_r(k_e) = \lambda \, \Delta N_r(0), \tag{705-10}$$

where the argument (0) refers to the initial specification, and λ is a common multiplier, an eigenvalue to be determined. Consider the following which are effectively macroscopic properties:

$$\Sigma_{p,r,g} = \sum_n \Delta N_{n,r}(0) \, \sigma_{a,n} \, ,$$

$$\Sigma_{q,r,g} = \sum_n \Delta N_{n,r}(0) \, \nu \, \sigma_{f,n} \, ,$$

where sums are over the search nuclides.[a] Given an iterate estimate of

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[a]Account for volume fractions, and for volume ratios in the case of subzone search, is not shown.

the neutron flux, an overall neutron balance may be formulated as

$$\frac{1}{k_e} P_t - A_t - L_t = \lambda\left[A_s - \frac{1}{k_e} P_s\right] ,$$

where P_t is the summed neutron production rate for the system; A_t is the summed loss rate, absorption and buckling, for the system; L_t is the surface leakage, and

$$A_s = \sum_r V_r \sum_g \Sigma_{p,r,g} \phi_{r,g} ,$$

$$P_s = \sum_r V_r \sum_g \Sigma_{q,r,g} \phi_{r,g} ,$$

V_r being the region volume, and $\phi_{r,g}$ is region average neutron flux in group g.

Solving the above equation for the unknown eigenvalue gives

$$\lambda = \frac{\frac{1}{k_e} P_t - A_t - L_t}{A_s - \frac{1}{k_e} P_s} . \qquad (705\text{-}11)$$

Thus from an overall neutron balance, an estimate is made of the eigenvalue of the nuclide concentration search problem. With this estimate, the usual iterative procedure may be applied; account is taken of the contributions from the search nuclides using the macroscopic absorption and production cross sections associated with the changes.

To account for small changes in the scattering and transport properties, the nuclide concentrations are updated at convenient points in the iteration cycle, (after asymptotic extrapolation or prior to restart of the Chebyshev acceleration process), and the macroscopic cross sections and equation constants are recalculated at this point in the calculation.

The Indirect Search

The conventional way that the nuclide search problem has been solved is by solution of a series of usual eigenvalue problems with estimates of the required changes to the search nuclide concentrations introduced after each eigenvalue problem. First the usual eigenvalue problem is solved (for k_e) for the conditions presented. A change is made in the nuclide concentrations according to user specifications, and this new eigenvalue problem is solved. Based on these results, the nuclide concentrations are further adjusted, and the process continued to an apparent solution, subject to acceptance by the analyst.

The dimension search problem is done in the same manner. Changes are made in the geometric mesh spacing to effect a desired solution.

END OF SECTION

Section 716: The Iteration Procedures

Introduction

This section documents the iterative procedures implemented in the VENTURE code. An attempt is made to provide the user with the information he needs for practical use of the code and to choose between the programmed options available, for experimentation or selective application.

The procedures of calculation must be considered rather complicated when viewed by the analyst wanting results and not much concerned about how they are obtained. In solving large problems, computation cost is an important consideration; there is incentive to reduce the cost by applying an effective procedure. The overall strategy involves:

1. Initialization (see Section 718),
2. Inner iteration with overrelaxation to accelerate the fixed source problem at each energy,
3. Outer iteration with acceleration,
4. Convergence tests, and
5. Reliability checks (see Section 720).

The following discussion addresses the individual procedures. Introductory material is given first to orient the reader.

Inner iteration involves successive recalculation of the flux values. Given the fission and inscattering source, the coupling (neutron balance) equations are solved by an ordered sweep through the space mesh at one energy. This is expressed in matrix form as

$$\phi_{t,n} = T\,\phi_{t-1,n} + US_n,$$

a set of coupled linear equations where $\phi_{t,n}$ represents the point flux

values for inner iteration t, outer iteration n, T and U are the operators (coupling terms) and S_n represents the point source terms. Latest point values of the fluxes are used as they become available and new values are obtained for a block of points simultaneously. The newly calculated values are driven by overrelaxation which involves using the changes in the point flux values to drive the fluxes in the directions of individual changes from the previous iterate values. Thus, T above is appreciably altered from just a simple coupling operator; it may depend on n and t. The number of inner iterations carried out on one space problem each outer iteration is a key variable.

Outer iteration on an eigenvalue problem may be viewed as solving the matrix equation

$$\phi_n = \left(E + \frac{1}{k_{n-1}} \chi F\right) \phi_{n-1} ,$$

a set of coupled equations where ϕ_n represents the point flux values for outer iteration n, E is a space, energy coupling operator, F contains the terms for neutron production from fission and χ is the into-group distribution function, and k_{n-1} is the estimate of the multiplication factor. It is noted that inner iteration causes E to have a complicated form.

Each outer iteration there is full sweep yielding latest estimates of the point flux values ϕ_n, and a new estimate of the eigenvalue of the problem, k_n, is obtained. The calculation starts with the first or highest energy group for usual problems and proceeds downward, following the primary direction of neutron scattering. For adjoint problems, the sweep is reversed.

The same steps are carried out within each outer iteration. This is necessary to permit effective acceleration of the outer iteration process. Two acceleration schemes are used, Chebyshev acceleration applied repeatedly and asymptotic extrapolation done only occasionally.

The Chebyshev acceleration process involves acceleration each outer iteration of the calculated flux values given the iterate estimates for the two previous outer iterations. The objective is to beat down the contributions from all the error vectors having eigenvalues over a specific range. Practical considerations include selection of the stage of the calculation to initiate the process, identifying the eigenvalue spectrum range, identifying when the procedure is not effective and when it can be expected to not be effective.

Asymptotic single-error-mode extrapolation is based on the assumption that a single error vector dominates asymptotically, the others having decayed away. Two of the outer iteration sets of flux values are extrapolated to an apparent solution. An asymptotic double-error-mode extrapolation procedure is also implemented which uses three succeeding iterate sets of the flux values. Practical considerations include identifying when the iterative behavior indicates extrapolation will be effective and estimating suitable extrapolation factors. Extrapolation may be done when the Chebyshev process is being applied.

The primary criteria selected to identify that an iterative process is convergent is decrease in the maximum relative flux change with continued iteration. This quantity is used in the implemented procedure to evaluate the behaviors of the inner iteration and the outer iteration

processes. Also the sum of the absolute values of the flux changes relative to that for the previous iteration is used on outer iterations.

Remarks on Optimum Strategy

If the optimum number of inner iterations is very few, perhaps even one, a relatively straightforward and effective procedure can be identified and applied. If the optimum number of inner iterations is large, a different relatively straightforward and effective procedure can be identified. The two procedures are quite different and there is no smooth transition from one to the other which is needed when a modest number of inner iterations should be the optimum. Furthermore, an initial commitment to set data handling procedures makes it very difficult to shift the strategy during the calculation as information becomes available about the iterative behavior. Also, for a limited class of problems for which modest convergence criteria would be adequate in a specific application, a particular procedure could be chosen which would not be adequate for other applications nor for generating benchmark quality solutions in a general purpose code.

The objective is effecting an acceptable solution to a problem at a minimum cost of computation to the project. Considering the large number of variables involved, preselection of an optimum strategy is simply not possible. The subject is addressed in Section 717.

The procedures implemented admit selection between a number of alternatives. A strategy is selected which depends on the particular problem to be solved and this strategy undergoes modest changes as information about the iterative behavior becomes available. The

automatic selection of a strategy allows application with minimum burden to the user; however, it involves compromises and can hardly be expected to be a precise optimum in any given situation for a particular problem. Principal alternatives for basic selection between procedures are under the control of user-input options. For those problems for which the iterative behavior is predictable from past experience, input control is available and exercising this control is desirable. However, a note of caution is in order. Only a limited background of experience with the actual procedures implemented is available to the authors; it takes time to accumulate experience. Past experience with similar procedures but yet different in detail, may not be applicable nor trustworthy. Further, the overhead of handling the large amount of data for the larger problems and associated penalty must be considered in applying the procedures or attempting to modify them.

Before discussing the details of the procedures, an overview of the iteration strategy is presented.

An Overview of the Iteration Strategy

The general procedure of solution employed is one of iteration. For the usual eigenvalue problem, the equation to be solved is

$$A\phi = \frac{1}{k_e} \chi F \phi. \tag{716-1}$$

With special partitioning of the matrix A,

$$[D - J - L - U] \phi = \left[S + T + \frac{1}{k_e} \chi F\right]\phi \quad , \tag{716-2}$$

where

D = the main diagonal term (loss due to absorption, buckling, outscatter),

J contains the coupling terms for a block of points (as along a row in space at one energy) for which the flux values are determined simultaneously precisely given the current values of the other fluxes,

L = the lower triangular matrix containing coupling terms in space,

U = the upper triangular matrix containing coupling terms in space (excluding any appearing in J),

S = the downscattering source matrix (group-to-group scattering terms at a point),

T = the upscattering source matrix (group-to-group scattering terms at a point),

F = the fission source component (from all groups at a space point contributing to the total at that point, a row matrix operator),

χ = the source distribution (from the total to each group at a point, a column matrix operator), and

k_e = the unknown multiplication factor, a constant for any problem to be determined.

To illustrate how an iterative procedure is formulated, let us put the term $D\phi$ on one side of the equation, Eq. (716-2), and the remaining on the other, giving

$$D\phi = \left[J + L + U + S + T + \frac{1}{k_e}\chi F\right]\phi.$$

If a set of fluxes is available for iterate n, namely ϕ_n, then a simple iterative scheme is expressed as

$$\phi_{n+1} = D^{-1}\left[J + L + U + S + T + \frac{1}{k_n}\chi F\right] \phi_n \ , \tag{716-3}$$

where the inverse D^{-1} is of a diagonal, the reciprocals of terms in D. An estimate of k_e is required, k_n, and a continuing iterative process may proceed. The above with all positive entries and $\phi_n > 0$ produces $\phi_{n+1} > 0$; only with $\phi > 0$ can a unique and most positive value of k be assured. Eq. (716-3) does not even admit the use of newly calculated ϕ values, so it represents a rather crude procedure.

With downward sweep in energy and simple sweeps carrying the simultaneous solution for rows across the space problem, use of newly calculated fluxes causes them to contribute through the matrices J, L, and S, or

$$[D - J - L - S]\ \phi_{n+1} = \left[U + T + \frac{1}{k_n}\chi F\right] \phi_n \ ;$$

$$\phi_{n+1} = [D - J - L - S]^{-1} \left[U + T + \frac{1}{k_n}\chi F\right] \phi_n \ . \tag{716-4}$$

The inverse shown would generally be impractical to obtain. It is not needed, however, but rather is a consequence of the process and the partitioning of the coupling terms.

Overrelaxation is used as discussed later in detail. The basic equation is

$$X_{i,n} = X_{i,n-1} + \beta(X^*_{i,n} - X_{i,n-1}) \ , \tag{716-5}$$

where $X_{i,n-1}$ is a component of ϕ_{n-1} obtained from iteration n-1, $X^*_{i,n}$

is the newly calculated value for iterative sweep n, β is the overrelaxation factor, and $X_{i,n}$ is the overrelaxed value used thereafter for this sweep of the equations. Note that $\beta = 1$ causes the newly calculated value to be used; overrelaxation is done for $1 < \beta < 2$. A fixed value of β may be used, or a different overrelaxation coefficient may be used for the space problem at each energy. Also, the value of β used may be iteration dependent. This flexibility is shown in the equations by representing the overrelaxation process with a matrix B_n containing only the values of β on the main diagonal, the subscript n indicating the values may be changed during the iterative history. Overrelaxation changes Eq. (716-4) to

$$\phi_{n+1} = \left\{D - B_n[J + L + S]\right\}^{-1}\left\{(I - B_n)D + B_n\left[U + T + \frac{1}{k_n}\chi F\right]\right\} \phi_n \quad . \qquad (716\text{-}6)$$

Inner iteration may be done. For many types of problems, additional calculational effort shows advantage to reduce the error associated with the space problem at each energy. Thus, several sweeps may be made of the space problem at each energy. Considering a fixed number of inner iterations, Eq. (716-6) becomes

$$\phi_n = \left\{X_n^t - \sum_{i=1}^{t} X_n^{t-i} Y_n^{i-1} B_n S\right\}^{-1}\left\{\sum_{i=1}^{t} X_n^{i-1} Y_n^{t-i} B_n \left(T + \frac{\chi F}{k_{n-1}}\right) + Y_n^t\right\}\phi_{n-1} \quad , \qquad (716\text{-}7)$$

where

$$X_n = D - B_n(J + L) \ ,$$

$$Y_n = (I - B_n)D + B_n U \ ,$$

and t refers to the number of inner iterations. Eq. (716-7) would have to be altered if either the number of inner iterations is different for the space problems at each energy or if B_n is varied during inner iteration.

Equation (716-7) also applies to the direct search problem with rearrangement of the terms and inclusion of the estimate of the eigenvalue of the search problem. Acceleration on outer iteration adds further complexity not shown.

Regarding Rebalancing

We are well aware of the fact that one of the possible rebalancing schemes can be used to accelerate the rate of convergence of a specific class of problems. Indeed some experimenting has been done with this code. We find that in general for the class of problems of primary interest, the cost of effective rebalancing calculations can not be justified, especially for the problems which are too big for the space problem at one group to be stored in memory, problems typical of current application. We had hoped that it would be possible to suppress the contribution from the dominant error vector with simple and infrequent rebalancing, but have not found this to be the case. Such experimenting does continue and may allow a superior procedure to be identified which then can be used routinely.

Latest Iterate Estimates of the Flux Values

New values of the fluxes are obtained each inner iteration by applying the basic finite-difference neutron balance equations for the volume elements. Substitution of the leakage terms of Eq. (702-3) into Eq. (701-4) yields an equation for each point equating the loss rate with the source rate in the form.

$$a_i X_{i,t} = S_{i,t} + b_i X_{i-1,t} + b_{i+1} X_{i+1,t} , \qquad (716\text{-}8)$$

where i refers to a mesh point along a row, t refers to inner

iteration, S_i is the summed fission and scattering source plus the contributions from nearest neighbor points on adjacent rows, a_i is the loss constant, and b_i is the coupling coefficient between nearest neighbors along the row.

Line relaxation involves a forward, backward sweep to solve the tri-diagonal matrix yielding new flux values simultaneously for all the points along the row. To satisfy the recursion for the backward sweep

$$X_{i,t} = g_i \left\{ X_{i+1,t} + \frac{f_i}{b_{i+1}} \right\}, \tag{716-9}$$

requires a forward sweep

$$f_i = s_{i,t} + g_{i-1} f_{i-1} ,$$

and a previously done forward sweep,

$$g_i = b_{i+1} \left[\frac{1}{a_i - b_i g_{i-1}} \right] ,$$

with the amount of division minimized.

An alternative procedure[a] is attractive to reduce the amount of computation during iteration. To solve the system of equations

$$A\phi = S$$

a new set of operators is desired such that

$$CV^T VC\phi = S .$$

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[a]Cuthill, E. H. and Varga, R. S., "A Method of Normalized Block Iteration," J. Assoc. Comput. Mach., 6 (1959).

The elements of these operators are obtained as follows. Let a_i be the diagonal terms of A and b_i the off-diagonal terms, coupling point i with i-1. Then, an initial calculation is done giving

$$f_1 = a_1^{\frac{1}{2}}$$

$$f_i = \left[a_i - \left(\frac{b_i}{f_{i-1}}\right)^2\right]^{\frac{1}{2}} , \quad 1 < i \leq I$$

$$v_i = \frac{b_{i+1}}{f_i f_{i+1}} , \text{ elements of V, } 1 \leq i \leq I - 1$$

$$c_i = \frac{1}{f_i} , \text{ elements of C .}$$

The forward-backward sweep equations solved during iteration are:

$$\begin{aligned} x_i &= c_i s_i \\ y_1 &= x_1 \\ y_i &= x_i - v_{i-1} y_{i-1} \\ z_I &= y_I \\ z_i &= y_i - v_i z_{i+1} \\ \phi_i &= c_i z_i \ . \end{aligned} \tag{716-10}$$

It may be noted that the new values c_i and v_i must be made available, but that the original elements a_i and b_i and intermediate values f_i are not later required. This scheme is not applicable when the direct criticality search procedure is used (unless the new values of a_i are used each outer iteration and the precalculation of c and v is redone).

The direct inversion scheme requires ten arithmetic operations including two divisions, while the modified procedure involves at most six with no divisions during iteration. The reduction is a smaller fraction of the total calculation involving overrelaxation and summing the individual source terms which increases as the number of dimensions is increased.

For the repeating boundary condition, leakage from one end feeds back to the other end, and a term must be added to Eq. (716-9),

$$X_{i,t} = \left(\frac{f_i}{b_{i+1}} + X_{i+1,t} + h_i \, X_{I,t-1} \, g_i \right) , \qquad (716\text{-}11)$$

where I refers to one of the flux values. The unknowns are obtained from this recursion relationship.

The calculations are done in such a way that a zero value of $X_{i,t}$ indicates that the associated point lies in a black absorber region.

Clearly the whole point of solving for several point fluxes simultaneously is to invest calculational effort where it will accelerate the iterative process. We seek ways of resolving more points or different blocks of points which will accelerate problems.

A special situation is presented by rotational symmetry boundary conditions: a point on one row couples with a point on another row. The newest iterate value of the flux is used in this coupling, but half of the time this is a previous iteration value. Thus, the rate of convergence might be expected to be slower than without this coupling.

Sweep Order

By "normal ordering" is meant that new flux values are obtained at each point each inner iteration by a sweep across the space mesh at one energy. This sweep starts on the first plane at the first row, then the next row on the plane is done, and so on across the plane, then the first row on the second plane, and so on across the planes. With I inner iterations, the flux at each point is calculated I times with I successive sweeps.

With σ_1 ordering, new values are first obtained for alternate points or along alternate rows, then for the others. Consider the two-dimensional problem with simultaneous solution for point values along each row. Looking at the ends of the rows,

. x . x . x . x . x

the odd ones shown as a dot would be treated first (in any order) and then those shown as an x would be treated. Spacial coupling by the finite-difference equations relates only nearest neighbors, so there are no direct couplings between any . rows or between x rows. The neutron leakage contribution (space coupling) is calculated from the nearest x values when a . point is treated; therefore, this leakage contribution is obtained from the same iterate nearest neighbors. (With normal ordering, the adjacent points have values one iteration apart for the sweep row.)

In three dimensions, we look again at the ends of the rows and find

. x . x . x

x . x . x .

. x . x . x

Again with coupling only between nearest neighbors, the . points do not couple and are swept first in any order, then the x points. This ordering applies to all coordinate systems treated.

The σ_1 order of sweeping the mesh imposes rather severe data handling requirements for large problems. Thus it is not done in those modes having severe data handling burdens, and is done only on planes in the multi-plane stored mode.

Inner Iteration and Overrelaxation

Overrelaxation is a simple but powerful scheme for accelerating the rate of convergence of the iterative process. The theory is not well developed for optimizing the overall strategy to maximize the rate of convergence of a multigroup eigenvalue problem. However, the behavior of the fixed source problem involving the simple coupled finite difference equations, the space problem at one energy, is well known; the following discussion is directed at this inner iteration process.

Consider calculation of new values of the fluxes each inner iteration using only the old values. If we examine the eigenvalues of the iteration matrix, there is the same number of them as points or flux values to be determined, all less than unity. These contribute to the error in the sense of the difference between the answer and the current estimate of the flux at each point for iteration t,

$$X_{i,\infty} - X_{i,t} = \sum_j A_{i,j} \rho_j^t \ . \qquad (716\text{-}12)$$

Thus, there is a contribution to the error from each error vector having an associated eigenvalue ρ_j which depends on the value of $A_{i,j}$ and the iteration number. The values of ρ_j depend only on the equation constants, not on the source values. The values of $A_{i,j}$ depend on the

initial state of the problem, both the fixed source values and the initial flux values. Since $\rho_j^t \to 0$ as $t \to \infty$, $\rho_j < 1.0$, each contribution to the error dies away; the smaller the value of ρ_j, the more rapid its contribution decays.

Asymptotically as $t \to \infty$, the contribution from the largest ρ_j dominates. Eliminating the constant $A_{i,j}$ from the recursion equations yields information about the asymptotic behavior,

$$\frac{X_{i,\infty} - X_{i,t}}{X_{i,\infty} - X_{i,t-1}} = \rho = \frac{X_{i,t} - X_{i,t-1}}{X_{i,t-1} - X_{i,t-2}} ;$$

$$\frac{X_{i,\infty} - X_{i,t}}{X_{i,t} - X_{i,t-1}} = \frac{\rho}{1.0 - \rho} .$$

That is, asymptotically, the absolute error is reduced by ρ each iteration as is the iterate change. However, the ratio of the absolute error to the iterate change depends on the reciprocal of $1.0 - \rho$.

Quite generally the more unknowns in a given problem (the more space points used), the larger the value of ρ, the slower the rate of convergence, and the larger the ratio of the absolute error to the iterate change.

Use of the latest values as they become available in a consistently ordered process accelerates the rate of convergence. The effect is squaring the eigenvalues giving the asymptotic behavior

$$\frac{X_{i,\infty} - X_{i,t}}{X_{i,\infty} - X_{i,t-1}} = \rho^2 ;$$

$$\frac{X_{i,\infty} - X_{i,t}}{X_{i,t} - X_{i,t-1}} = \frac{\rho^2}{1.0 - \rho^2} .$$

Note that for $\rho = 0.9$, $\rho^2 = 0.81$, a significant improvement. The ratio of absolute error to iterative change decreases from 9 to 4.3. Of primary concern here is not this situation, but rather that where ρ approaches unity, having a value of 0.99 or even larger.

For certain problems, the value of ρ is larger than usual; one of these is the situation involving rotational symmetry for which old values of the fluxes along the coupled boundary are used since new ones are not yet available.

With overrelaxation, the iterate flux estimates are driven in the direction of the calculated change by the equation

$$X_{i,t} = X_{i,t-1} + \beta_t (X^*_{i,t} - X_{i,t-1}) \ . \tag{716-13}$$

Here $X^*_{i,t}$ is the newly calculated value and β_t is the overrelaxation coefficient. For the fixed source problem, there is an optimum value of β_t, given by[a]

$$\beta_{opt} = \frac{2.0}{1.0 + \sqrt{1.0 - \rho^2}} \ . \tag{716-14}$$

The eigenvalues of the overrelaxation process occur in pairs. Shown in Fig. (716-1) is the dependence of the dominating eigenvalues of the overrelaxation process on the value of β_t, $1 < \beta_t < 2$, for the situation where ρ^2 is 0.99. Considering only this fixed source problem (not the overall eigenvalue problem), the objective is to effect the minimum dominating eigenvalue of the process. This occurs when the optimum value of β_t is used. For $\beta_t < \beta_{opt}$, the pair of eigenvalues are real, one relatively large, the other small. For $\beta_t > \beta_{opt}$, the pair of

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[a]S. P. Frankel, Convergence Rates of Iterative Treatments of Partial Differential Equations, Math. Tables Other Aid Comp. 4 (1950).

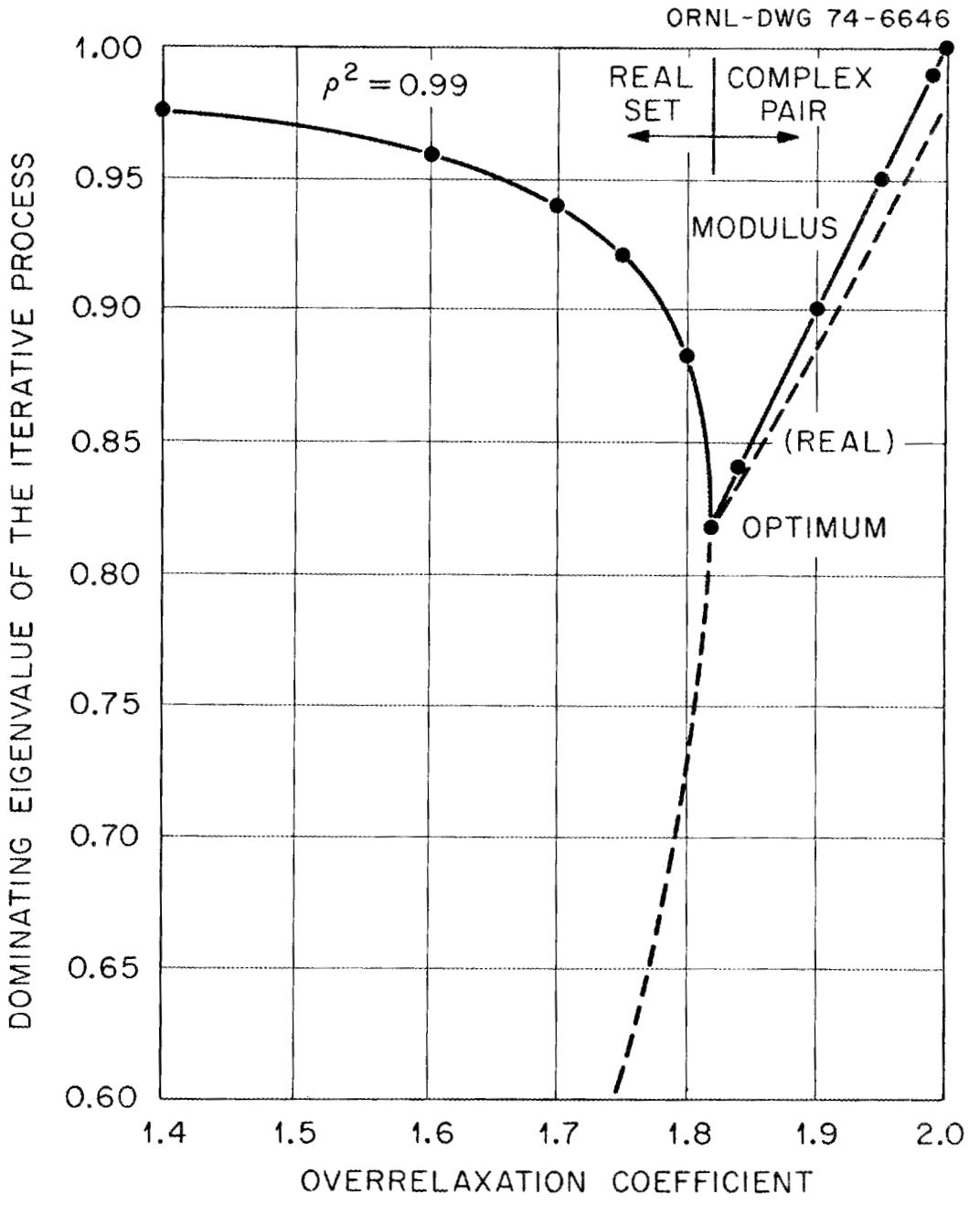

Fig. 716-1. Dominating Eigenvalue Dependence on the Overrelaxation Coefficient.

eigenvalues are complex conjugate. The error vectors associated with these eigenvalues are not independent, but have a rather complicated dependence on the iteration number.

The importance of the use of an overrelaxation coefficient near the optimum is evident from Fig. (716-1). Indeed, it is preferable that the value used be too large rather than too small because the convergence property is not degraded as much. It should be noted that asymptotically, the absolute error reduction is a factor of 0.82 each iteration with optimum overrelaxation compared with 0.99 without overrelaxation.[a] Each iteration done with optimum overrelaxation is the equivalent of 20 iterations without it. Clearly, the amount of calculation required to do overrelaxation returns a large dividend justifying its use, and a reasonable amount of calculation can be justified to determine near optimum requirements. However, a convergent process is indicated for $1 < \beta < 2$.

New values can be obtained of the fluxes for a block of points simultaneously. Thus, when line relaxation is done as discussed previously, these values are overrelaxed simultaneously.

It is of interest to compare asymptotic rates of convergence for a reference problem. For the two-dimensional square mesh with even mesh point spacing, homogeneous, and no sink term, the asymptotic rates of convergence for various schemes are shown below as dependent on the number of mesh points on one side. Line overrelaxation changes the spectral radius from ρ to $\rho/(2-\rho)$ for the separable square mesh.

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[a]The actual gain is somewhat less than indicated by this simplistic view; see Section 717.

Mesh Points	β	Asymptotic Rate of Convergence			
		Use Old Values	Use New Values	Point Overrelax	Line Overrelax[a]
10	1.560	0.041	0.081	0.58	0.82
50	1.884	0.0019	0.0038	0.12	0.17
100	1.940	0.00048	0.00097	0.062	0.088

[a]The scheme is the only one implemented; β is different for line overrelaxation.

During the early iterative progress of a problem, large changes in the flux values are associated with initial error vectors which may cause Eq. (716-13) to produce unacceptable negative values. We restrain the process by restricting the result in a manner which dampens out excessive driving, requiring

$$\left|X_{i,t} - X^*_{i,t}\right| \leq \min\left[0.5\ \left|X^*_{i,t}\right|,\ \left|X_{i,t-1}\right|\right] \tag{716-15}$$

$X^*_{i,t}$ is the newly calculated value and $X_{i,t}$ is the restrained overrelaxed value. The nature of restrained overrelaxation is shown in Fig. (716-2). When the iterative progress reaches a stage where the calculated changes are small, no restraint is required. Therefore, the restraint applies only during the early history when bad initial error vectors dominate ($|\varepsilon_n| > 0.01$, see later discussion).

Equation (716-15) is programmed to account for negative flux values when they occur and changes in sign of the flux values.

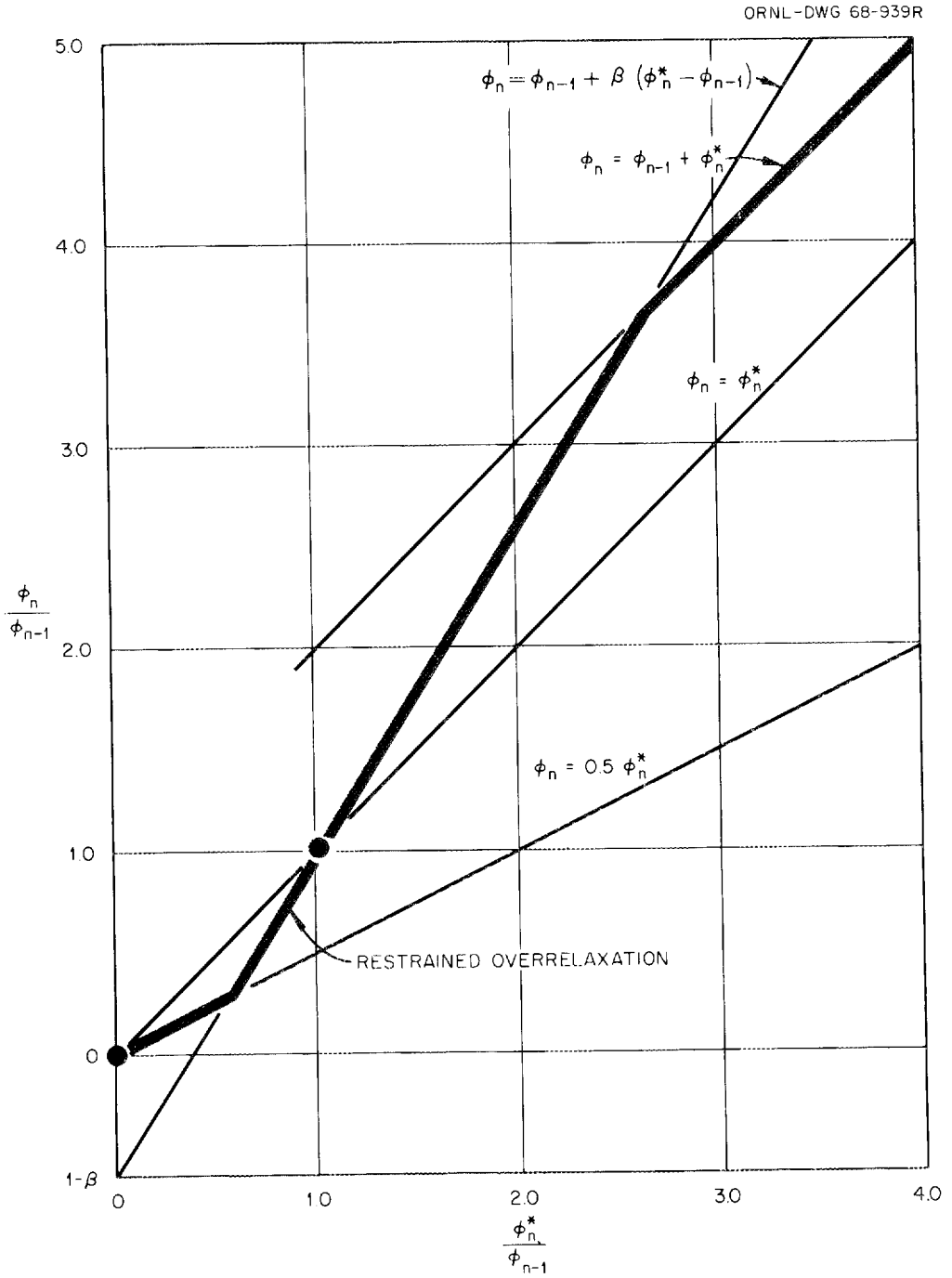

Fig. 716-2. Restrained Overrelaxation.

Inner Iteration Strategy

The procedure adopted is as follows where t is the inner iteration count, T the maximum, and n the outer iteration; this procedure is applied independently at each group and the default may be overridden by user control:

$$T < 4, \quad \beta_{t,n}(g) = \begin{cases} X(g), \text{ all } t,\ n = 1, \\ Y_{n-1}(g), \text{ all } t,\ n > 1, \\ \text{except as noted;} \end{cases}$$

$$T \geq 4, \quad \beta_{t,n(g)} = \begin{cases} X(g), \ t = 1, \text{ all } n, \\ Y_{t-1}(g), \ t > 1, \text{ all } n; \end{cases} \tag{716-16}$$

$$X(g) = \frac{1}{2.0}\left[\frac{2.0}{2.0-\rho^2(g)} + \frac{2.0}{1.0+\sqrt{1.0-\rho^2(g)}}\right];$$

$$Y_{m-1}(g) = \frac{1.0}{1.0 - \frac{1}{4.0}\rho^2(g)\ \beta_{m-1}(g)}.$$

Thus the Chebyshev polynominal relationship is used, but large values and the initial unity value at the beginning of the series are thrown away. In addition, if T < 4 and there are more than 5 groups or Chebyshev of the flux values on outer iterations has been specified, β_o is used rather than apply the Chebyshev polynominals. Note that the spectral radius $\rho(g)$ must account for line relaxation.

When the overrelaxation coefficient is larger than the optimum, the iterative behavior has a marked difference than when it is less. A direct measure of the behavior is obtained from the iterate values of the maximum relative flux change. Let $a_{i,t} = \frac{X_{i,t}}{X_{i,t-1}}$ where $X_{i,t}$ is the flux value at location i after overrelaxation is done at iteration t, and

$r_t = \max(a_{i,t})$,

$s_t = \min(a_{i,t})$,

over the space problem of interest. The maximum relative flux change is determined from this information with the sign retained to indicate if the flux at that location is rising (positive) or falling (negative),

$$\varepsilon_t = |\max| \ (r_t - 1.0, \ s_t - 1.0) \ . \tag{716-17}$$

Thus, $\varepsilon_t = |\max| \dfrac{X_{i,t} - X_{i,t-1}}{X_{i,t-1}}$, retaining the negative sign if descending.

A special condition exists when the changes in the flux values are so small that they lose significance. In this situation, arbitrarily if $|\varepsilon_t| < 10^{-10}$, the number of inner iterations is adjusted to

$$I_{n+1}(g) = \frac{4.0 + I_n(g)}{2.0} \ ,$$

reducing it, but not to less than 4. In the multirow or multiplane modes of data handling, the number of inner iterations being done may be a multiple of the rows or planes stored greater than one; in this case, the number of inner iterations is arbitrarily reduced when $|\varepsilon_t| < 10^{-10}$ by the number of rows or planes stored, down to a minimum of the number of planes stored, to take advantage of the associated reduction in data transfer.

Estimates are made of the dominating eigenvalue of the process from the maximum and minimum flux ratios. We assume that asymptotically,

$$\lambda_t = \frac{X_{i,t} - X_{i,t-1}}{X_{i,t-1} - X_{i,t-2}} = \frac{\dfrac{X_{i,t}}{X_{i,t-1}} - 1}{\dfrac{X_{i,t-1}}{X_{i,t-2}} - 1} \left(\frac{X_{i,t-1}}{X_{i,t-2}}\right) \ . \tag{716-18}$$

The data is deemed insignificant if for either m = t or t-1,

$$s_n \frac{(r_n - 1.0)}{(1.0 - s_n)} > 10, \text{ or } \frac{r_n (1.0 - s_n)}{(r_n - 1.0)} > 10.$$

Assuming the flux values tend to rise or fall together we take half the extreme relative change as an average and set

$$\lambda_t = \left|\frac{\varepsilon_t}{\varepsilon_{t-1}}\right| (1.0 + \frac{\varepsilon_{t-1}}{2.0}). \tag{716-19}$$

Otherwise the eigenvalue is estimated from the data for the extreme increases and decreases using

$$\lambda_{t,r} = \left[\frac{r_t - 1.0}{r_{t-1} - 1.0}\right] r_{t-1}, \qquad \lambda_{t,s} = \left[\frac{s_t - 1.0}{s_{t-1} - 1.0}\right] s_{t-1} ;$$

$$\lambda_t \doteq \sqrt{\lambda_{t,r} \lambda_{t,s}} , \tag{716-20}$$

which is essentially the average of the two values when they are not greatly different. In the event that all flux values are falling, both r_t and s_t will have values less than unity, or if they are all rising, they will both be greater than unity.

The crucial need to accelerate at near the optimum presents a challenge. In some programs in use, the implemented procedure is such that initially no acceleration is done, or at least it is done with parameters less than optimum, and these are increased using a scheme to predict the dominant error vector eigenvalue which generally produces an underestimate. It is generally more important not to accelerate above the optimum when Chebyshev acceleration is done on outer iterations than

when this procedure is not used, to avoid contamination of the outer iteration error vectors. We are not attracted to schemes of doing a large number of inner iterations initially without acceleration to produce accurate eigenvalue estimates, nor to iteration on zero source problems, especially when the space problem at one group cannot be contained in memory and a large amount of data transfer would be necessary.

We use a scheme to identify acceleration above the optimum. If

$$|\varepsilon_t| < |\varepsilon_{t-1}|$$

for all iterations, there is assurance that the process is convergent. Indeed failure of this criterion has generally been useful to identify acceleration above the optimum, used in several local codes in the past. Unfortunately, there are situations where acceleration is below the optimum but the criteria is violated. Such is the case in the early history using σ_1 ordering. Generally, this criterion is violated the next iteration after full propagation of each boundary condition to the most remote point, when the iteration count (total inner iterations from the start) is one more than the number of rows in a two-dimensional problem with normal ordered line relaxation on rows.

A less stringent but apparently adequate criteria is that

$$|\varepsilon_t| < |\varepsilon_{t-2}| \ .$$

We use two failures of this test for either $t = T$ or $t = T - 1$ to indicate that the acceleration is above the optimum but require $|\varepsilon_n| > |\varepsilon_{n-1}|$ on outer iteration or non convergence on outer iteration to be indicated, $|\varepsilon_n| > |\varepsilon_{n-2}|$. If this criterion is satisfied, an adequate measure of the asymptotic mode is deemed to establish when

$$\lambda_{T,n} < 0.99999,$$

$$0.975 < \left(\frac{1.0 - \lambda_{T,n}}{1.0 - \lambda_{T,n-1}}\right) \quad \frac{\lambda_{T,n-1}}{\lambda_{T,n}} < 1.025,$$

$$0.95 < \left(\frac{1.0 - \lambda_{T,n}}{1.0 - \lambda_{T-1,n}}\right) \quad \frac{\lambda_{T-1,n}}{\lambda_{T,n}} < 1.05,$$

where T refers to the last inner iteration for outer iteration n. When these criteria are satisfied, a new estimate is made of the spectral radius[a], using

$$\beta(g) = \frac{2.0}{1.0 + \sqrt{1.0 - \rho^2_{n-1}(g)}},$$

$$\rho^2_n(g) = \frac{1.0}{\lambda_{T,n}} \left[1.0 - \left(\frac{1.0 - \lambda_{T,n}}{\beta(g)}\right)\right]^2 . \tag{716-21}$$

The overrelaxation coefficient is recalculated with Eq. (716-4), but only if the asymptotic single error mode extrapolation criteria discussed later are satisfied, indicating that an asymptotic behavior of the outer iteration process has established, and only if $\beta_{T,n}(g) - 1.0 < \gamma_{T,n}$, and the adjusted value is constrained to

$$\beta_{T,n+1}(g) \leq \frac{10.\beta_{T,n}(g)}{8. + \beta_{T,n}(g)} . \tag{716-22}$$

If the inner iteration process is deemed to be nonconvergent, the overrelaxation coefficient is arbitrarily decreased

$$\beta_{T,n+1}(g) = \max\left[0.9\beta_{T,n}(g), \beta_{T,n}(g) - \left|\left(\frac{\beta_{T,n}(g) - 1}{3\beta_{T,n}(g)^3}\right)\right|\right] . \tag{716-23}$$

When $\beta(g)$ is changed, the associated value of $\beta(g)$ is recalculated to make them consistent. If any $\beta(g)$ is decreased, this coefficient is not

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[a]D. M. Young, "Iterative Methods for Solving Partial Difference Equations of Elliptic Type," Harvard University Dissertation (1950).

permitted to be increased later. Reduction in $\beta(g)$ is allowed no more frequently than every other outer iteration, and when in use, the application of Chebyshev polynominals in reinitiated, and any $\beta(g) < \max \beta(g) - 0.2$ is not reduced. When fewer than 4 inner iterations are done, inner iteration behavior is not tested and thus the overrelaxation coefficients are not increased nor are they reduced based on inner iteration behavior.

On demand by user option, at a point preselected in the initialization procedures, or when the code is so disposed to, at some outer iteration the regular iterative procedure is interrupted. Twenty iterations are done without overrelaxation on the space problem at each energy without a source, having the solution $\phi = 0$. (The calculated flux values are not used as the normal procedure resumes.) New values for the overrelaxation coefficients are obtained from the L_1 norm estimate of the dominant error vector eigenvalue, see Eq. (716-31) and the discussion about initialization. Procedures in use, such as the Chebyshev acceleration, are restarted, and iteration delays are reinitialized.

Re-Calculation of Overrelaxation Coefficients

The number of outer iterations required for the boundary fluxes to propagate through the mesh is given by

$$T = \frac{N\ (\text{planes}) + M\ (\text{rows})}{(\text{min inners})}$$

where

$N = \frac{1}{2}$, $M = \frac{1}{2}$ for full σ_1 ordering, or

$N = 1$, $M = \frac{1}{2}$ for partial σ_1 ordering, or

$N = 1$, $M = 1$ for normal ordering.

At outer iteration T (or optionally at an outer iteration number specified by input) the overrelaxation coefficients are re-calculated with Eq. (716-14) using an L_1 norm estimate of the dominating eigenvalue of the inner iteration process (ρ^2) with no source and no overrelaxation at each energy group.

Considering the L_1 norm definition of $\lambda_t \simeq \rho^2$, the procedure is as follows for t inner iterations with the definitions:

$$\lambda_t = \frac{\sum_i \left|\phi_{i,t} - \phi_{i,t-1}\right|}{\sum_i \left|\phi_{i,t-1} - \phi_{i,t-2}\right|} ,$$

$$\mu_t = \frac{\lambda_t - \lambda_{t-1}}{\lambda_{t-1} - \lambda_{t-2}} ,$$

$$F = \min\left(75.0, \frac{\mu_t}{1-\mu_t}\right) ,$$

$$X = \left(\frac{\mu_t}{\mu_{t-1}}\right)\left(\frac{1 - \mu_{t-1}}{1 - \mu_t}\right) , \text{ and}$$

$$Y = \left(\frac{\lambda_t}{\lambda_{t-1}}\right)\left(\frac{1 - \lambda_{t-1}}{1 - \lambda_t}\right) ,$$

an attempt is made to extrapolate the eigenvalue estimate. The extrapolated value

$$\lambda_\infty = \lambda_t + F\left(\lambda_t - \lambda_{t-1}\right)$$

is used provided

$$\mu_t < 0.999 ,$$

$$0.95 < X < 1.05 ,$$

$$\lambda_\infty < 0.999 , \text{ and}$$

$$\frac{1 - \lambda_t}{1 - \lambda_\infty} < 3.0 .$$

Otherwise $\lambda_\infty = \lambda_t$

provided $\lambda_t < 0.9999$,

$\lambda_{t-1} < 0.9999$, and

$0.9 < Y < 1.1$.

Failing these tests, the overrelaxation coefficient is left unchanged unless $\lambda_t > \lambda_{t-1} > \lambda_{t-2}$, in which case the new overrelaxation coefficient is the average of the one in use and that calculated with λ_t.

Outer Iteration Strategy

Here we discuss assessment of the behavior of the outer iteration process and delays imposed on adjusting the parameters of the individual procedures. When the flux values for successive iterations are available at the same time (as when the Chebyshev process is applied), behavior of the outer iteration process is assessed directly.

Let $a_{i,n} = \dfrac{X_{i,n}}{X_{i,n-1}}$

where $X_{i,n}$ is one of the flux values (component of ϕ_n), and

$$r_n = \max\ (a_{i,n})$$

$$s_n = \min\ (a_{i,n}). \tag{716-24}$$

$$\varepsilon_n = \left|\max\right|\ (r_n - 1.0,\ s_n - 1.0). \tag{716-25}$$

To judge the behavior of the outer iteration process, if $\left|\varepsilon_n\right| > \left|\varepsilon_{n-2}\right|$, the process is deemed to be not convergent, requiring that the acceleration parameters be reduced to effect a convergent process, after allowing a reasonable delay in iteration count from the start, or after any

action such as extrapolation or the start of Chebyshev acceleration which would be expected to require a delay. (We have used $|\varepsilon_n| > |\varepsilon_{n-1}|$ as the criteria in the past.) One failure of this test is allowed.

When succeeding outer iterate flux values are not readily available, the maximum relative flux change is estimated by a bound. Given the values of r_t and s_t for the inner iteration, at each energy group, the estimate is

$$r_n = \max \prod_{t=1}^{n} r_t$$
$$s_n = \min \prod_{t=1}^{n} s_t \qquad (716\text{-}26)$$

over the individual energy groups. Quite generally the values obtained from Eq. (716-26) are wider bounds than the values from Eq. (716-25).

The dominating eigenvalue of the outer iteration process is estimated. We assume that

$$\mu = \frac{X_{i,n} - X_{i,n-1}}{X_{i,n-1} - X_{i,n-2}} \, . \qquad (716\text{-}27)$$

We judge the data insignificant if for m = n and n-1,

$$s_m \frac{(r_m - 1.0)}{(1.0 - s_m)} > 10, \text{ or } r_m \frac{(1.0 - s_m)}{(r_m - 1.0)} > 10, \text{ and set}$$

$$\mu_{n,o} = \left|\frac{\varepsilon_n}{\varepsilon_{n-1}}\right| (1.0 + \frac{\varepsilon_{n-1}}{2.0}); \qquad (716\text{-}28)$$

otherwise using

$$\mu_{n,r} = \left(\frac{r_n - 1.0}{r_{n-1} - 1.0}\right) r_{n-1} \text{ , and } \mu_{n,s} = \left(\frac{1.0 - s_n}{1.0 - s_{n-1}}\right) s_{n-1},$$

the estimate of this dominant eigenvalue is

$$\mu_{n,o} = \sqrt{\mu_{n,r}\ \mu_{n,s}} \tag{716-29}$$

Other estimates of μ have also been used, for example the L_2 norm,

$$\mu_{n,2} = \sqrt{\frac{\sum_i (X_{i,n} - X_{i,n-1})^2}{\sum_i (X_{i,n-1} - X_{i,n-2})^2}} \text{ ,} \tag{716-30}$$

or the L_1 norm estimate,

$$\mu_{n,1} = \frac{\sum_i \left|X_{i,n} - X_{i,n-1}\right|}{\sum_i \left|X_{i,n-1} - X_{i,n-2}\right|} \text{ .} \tag{716-31}$$

It is not practical to obtain $\mu_{n,2}$ in this code which allows the source and flux values to float to an arbitrary level making it likely that the numbers would exceed machine range. The L_1 norm estimate $\mu_{n,1}$ is used and reported when easily calculated without data access, as when Chebyshev acceleration is done and for the forced extrapolation discussed later.

Together, the individual procedures act in a complicated way on the overall process which displays interaction effects. Certain delays and cycles are incorporated as found desirable from the behavior of representative test problems. These are discussed here. With line relaxation on rows, for a problem containing R rows and P planes, R + P - 1 sweeps are required for the most remote boundary condition to propagate across the space problem. Typically, there is a change in the iterative behavior when this number of inner iterations have been done. However, it has been found that the behavior should be assessed earlier.

Let R = Number of rows

P = Number of planes

T = Number of inner iterations (minimum)

$$a = \sqrt{\frac{R + P - 1}{T}}$$

$$J = \max\left[\frac{21a - 9}{a + 1}, 5\right] \qquad (716\text{-}32)$$

$$L = \max\left[\frac{R + P}{T} + 1.99, 10\right]$$

$$K = \min\,[L, 2J]$$

$$M = \max\,[J + 2, K]$$

where

J is the initial delay in accessing convergence behavior,

M is the initial delay in applying extrapolation arbitrarily, and

K is the delay between arbitrary extrapolations.

Initiation of the Chebyshev acceleration procedure is normally delayed until after the overrelaxation coefficients have been reevaluated (after propogation), or 5 outer iterations for one-dimensional problems.

Asymptotic extrapolation is delayed 5 iterations whenever any action is taken which would disrupt the outer iteration process preventing an

approach to an asymptotic error mode. Extrapolation itself or adjustment of the acceleration parameters cause such delay.

When Chebyshev acceleration is initiated or restarted after asymptotic extrapolation or after the estimated eigenvalue spectrum range has been decreased, start of the process is delayed one iteration.

Testing to reduce the overrelaxation coefficients is permitted only 5 iterations following restart of the Chebyshev acceleration process or 4 iterations following asymptotic extrapolation when inner iteration behavior is examined (requires $\geq$ 4 inner iterations), or 5 iterations after these events otherwise, and 5 iterations after any prior reduction has been done.

When the minimum number of inner iterations done at any group is less than 4, nonconvergence of the outer iteration process is used as criterion for reducing the overrelaxation factors. However, if the number of inner iterations done at any group is 4 or more and this inner iteration process is deemed convergent, that overrelaxation coefficient is not reduced the first time reduction of these coefficients is done based on outer iteration behavior.

When the minimum number of inner iterations is 4 or more and Chebyshev acceleration is not being done and after the outer iteration count satisfies the set delays, if the outer iteration process is deemed to be not convergent, all of the overrelaxation coefficients are arbitrarily reduced using Eq. (716-23). This can occur no more frequently than every other outer iteration. Note that once reduced, an overrelaxation coefficient will not be increased later, except if they were all reduced simultaneously.

The continuing discussion addresses acceleration of the outer iteration process.

Chebyshev Acceleration on Outer Iterations

We have experimented with procedures for acceleration of the iteration process on outer iteration. The simple scheme of driving the point fission source values is practical in some situations, but generally has been found to be inferior to driving the point flux values, so we justify the added processing cost for the latter. We tested acceleration of the point flux values before calculation of the inscattering source and found this to be quite effective; unfortunately there is a complicated relationship between the dominant eigenvalue, the driving factors and the eigenvalues spectrum range for which an explicit formulation has not been found. With this procedure the eigenvalue spectrum range is smaller, or at least the factors must be smaller than for acceleration on outer iterations, the more so the larger the number of energy groups treated, a cascade effect. In early implementations we relied on an estimate of the multiplication factor from the ratio of integrated fission source between successive iterations, normalization to effect the same source to establish the pseudo steady state condition. The procedure now in use applies a scheme of dampening the estimates from the source ratios which has been found effective. Also, asymptotic extrapolation is used when Chebyshev acceleration is done to attempt to force the point flux values to a solution when the behavior indicates this can be done. Either single or double error mode extrapolation is done simultaneously with Chebyshev acceleration, as discussed later, and

then the Chebyshev acceleration is restarted.

We note that regardless of how acceleration is done, the dominant error vector eigenvalue must be estimated. In many situations we find that this error vector is highly suppressed; it may not surface before an adequate convergence level is attained and estimates of the eigenvalue may be hopelessly contaminated. We do rely on a continuing assessment of behavior and continuing estimation of the dominant error vector eigenvalue of the overall iteration process in progress.

There are unfortunate characteristics of the Chebyshev acceleration process on outer iteration. The eigenvalue spectrum range must be underestimated because the process is not convergent using driving factors which are too large. The incentive is to minimize the number of inner iterations done at each group to reduce the amount of calculation; however, with an inadequate number of inner iterations or use of overrelaxation coefficients too large or too small, severe contamination results which is hard to overcome. This complication causes us to adopt a procedure of stopping the acceleration periodically and restarting it. Quite generally the identification of a nonconvergent process is difficult; large iterate flux changes can mean a divergent process or effective acceleration. Thus a rather complicated procedure is in use for evaluation. The details of this procedure have been worked out in study of the behavior of many small problems and as many problems typical of application as could be justified. We have relied on the experience of others, some of which has been published,[a] and only

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[a]E. L. Wachspress, Iterative Solution of Elliptic Equations, Prentice-Hall, Inc., N. J. (1966).

selectively apply the procedure when deemed to be worth its cost. A discussion is presented here about the implemented procedure.

When Chebyshev acceleration is initiated the equation applied (pointwise) is

$$\phi_N = \phi_N^* + f_N\,(\phi_N^* - \phi_{N-1}) \;, \tag{716-33}$$

and each outer iteration after this one,

$$\phi_n = \phi_n^* + f_n(\phi_n^* - \phi_{n-1}) + g_n(\phi_{n-1} - \phi_{n-2}) \;. \tag{716-34}$$

But the value of the driven point flux value is restrained to

$$\left|\phi_n - \phi_n^*\right| \leq \min\left[0.5\,\left|\phi_n^*\right|,\ \left|\phi_{n-1}\right|\right]$$

with account taken of negative flux values when calculated. Here n refers to outer iteration, N is the outer iteration when the process is initiated, ϕ_n^* is the newly calculated flux, ϕ_n the accelerated flux, and f_n and g_n are acceleration parameters. The latter are determined as follows. The Chebyshev polynominal recursion is used in the form

$$T_{N-1}(b) = 1.0$$

$$T_N(b) = b$$

$$T_n(b) = 2.0\ b\ T_{n-1}(b) - T_{n-2}(b),\ n > 1,\ \text{or}$$

$$\frac{T_{n-1}(b)}{T_n(b)} = \frac{1}{2.0\ b - \left[\dfrac{T_{n-2}(b)}{T_{n-1}(b)}\right]} \tag{716-35}$$

Note that $\dfrac{T_{n-1}(b)}{T_n(b)} \to b - \sqrt{b^2 - 1}$ as $n \to \infty$,

where

$$b = \frac{2.0 - (\mu_2 + \mu_1)}{(\mu_2 - \mu_1)} , \tag{716-36}$$

and μ_1 and μ_2 are the lower and upper bounds of the eigenvalue spectrum, respectively. Given the above recursion, the acceleration parameters are determined for the early iterative history as

$$f_N = \frac{\mu_2 + \mu_1}{2.0 - (\mu_2 + \mu_1)} \tag{716-37}$$

$$f_n = \frac{4.0}{(\mu_2 - \mu_1)} \left[\frac{T_{n-1}(b)}{T_n(b)} \right] - 1.0 ,$$

$$g_n = 2.0b \left[\frac{T_{n-1}(b)}{T_n(b)} \right] - 1.0; \text{ or} \tag{716-38}$$

$$f_n = \left(\frac{4.0}{\mu_2 - \mu_1} \right)^2 \left[\frac{1.0}{\left(\frac{8.0b}{\mu_2 - \mu_1} \right) - 1.0 - f_{n-1}} \right] - 1.0 , \; n > N + 2 ,$$

$$g_n = (1.0 + f_n)[1.0 - 0.5 \; (\mu_2 + \mu_1)] - 1.0 , \; n > N . \tag{716-39}$$

Whenever the Chebyshev process is restarted, f_N above is used but thereafter asymptotic values of f_n and g_n are used.

Consider the acceleration Eq. (716-34). The new estimate of the flux is obtained by applying the iteration matrix

$$\phi_n^* = M\phi_{n-1} ,$$

$$\phi_n = [(1 + f_n) \; M - f_n] \; \phi_{n-1} + g_n \; (\phi_{n-1} - \phi_{n-2}) .$$

Define the error $E_n = \phi_n - \phi_\infty$, and since $M\phi_\infty$ returns ϕ_∞

$$E_n = [(1 + f_n) M - f_n] E_{n-1} + g_n (E_{n-1} - E_{n-2}) .$$

Consider that asymptotically f_n and g_n become constants, and assume that an error vector dominates, each component having the form

$$\sum_i A_i \mu_i^n \to A\mu^n \text{ for n large,}$$

and that this error vector must be driven by the dominant one of the iteration matrix,

$$M \to \lambda .$$

These assumptions lead to

$$\mu^2 - [(1 + f_n)\lambda - f_n] \mu + g_n(1 - \mu) = 0 .$$

Given an estimate for μ when the Chebyshev process is in use, an estimate of the dominant eigenvalue of the iteration matrix (and hence the upper limit of the spectrum of eigenvalues needed to select the Chebyshev parameters) is given by

$$\lambda = \frac{\mu^2 + \mu f_n + g_n(1 - \mu)}{\mu(1 + f_n)} . \tag{716-40}$$

We seek the smallest value of μ for maximum acceleration,

$$\mu = \frac{1}{2}\{[(1 + f)\lambda - f + g] \pm \sqrt{[(1 + f)\lambda - f + g]^2 - 4g}\} .$$

Note that for $f = g = 0$, $\mu = \lambda$ as it should with no acceleration.

The values of f and g are related through the polynominal equations for Chebyshev acceleration by

$$g_n = f_n - \left(\frac{\lambda + a}{2}\right)\left(1 + f_n\right) ,$$

where a is the lower limit of the spectrum. Assuming that λ is known,

$$\mu = \frac{1}{2}\left\{\left(\frac{\lambda - a}{2}\right)(1 + f) \pm \sqrt{\left[\left(\frac{\lambda - a}{2}\right)(1 + f)\right]^2 - 4f + 2(\lambda + a)(1 + f)}\right\} .$$

The largest value of μ can be reduced to a point by increasing f, but further increase in f causes it to have an imaginary component. This occurs when

$$\left[\left(\frac{\lambda - a}{2}\right)(1 + f)\right]^2 - 4f + 2(\lambda + a)(1 + f) = 0 \text{ , and}$$

$$\mu = \left(\frac{\lambda - a}{4}\right)(1 + f) \text{ , or from above,}$$

$$1 + f = \frac{4}{(\lambda - a)^2}\left[2 - (\lambda + a) - 2\sqrt{(1 - a)(1 - \lambda)}\right] ,$$

the smallest value selected, and

$$\mu = \frac{1}{(\lambda - a)}\left[2 - (\lambda + a) - 2\sqrt{(1 - a)(1 - \lambda)}\right] . \tag{716-41}$$

Asymptotically, we expect optimum Chebyshev acceleration of an iterative process having a dominant eigenvalue λ to have a dominant eigenvalue μ. An estimate of μ from the behavior of a problem may be compared with this value to assess effectiveness. These eigenvalues are simply related when the lower limit of the eigenvalue spectrum range is zero by

$$\lambda = \frac{4\mu}{(1 + \mu)^2} . \tag{716-42}$$

It is of interest to examine the gain in the rate of error reduction with Chebyshev acceleration (asymptotic optimum). Values of μ and λ are compared on the following page (a = 0).

No Acceleration (λ)	Optimum Acceleration (μ)
0.25	0.0718
0.50	0.1716
0.75	0.3333
0.85	0.4417
0.95	0.6345
0.99	0.8182

If the basic iterative process reduces the absolute error by 5 percent each outer iteration, the Chebyshev process optimally reduces this absolute error 36.5 percent each outer iteration asymptotically, an impressive gain. In practice such gain is not realized; there is smaller gain in the early history, contamination later, and it is necessary to operate below the top of the eigenvalue spectrum band. A better estimate of actual behavior we have used is λ^2.

The automated procedure for selection of the Chebyshev acceleration process involves estimating the dominant error vector eigenvalue for a selected one-dimensional problem (Sec. 718). An exception is the one-dimensional problem for which the procedure is automatically applied. Occasionally we find that there is a small negative error vector eigenvalue, which causes serious impact if ignored, so μ_1 is initially set at -0.1 and left at this value; this may be altered with input data.

After starting or restarting the process, a set minimum delay is imposed before the behavior is evaluated. Then if the outer iteration behavior does not satisfy the criteria for a convergent process, the procedure is restarted with a reduced value for the estimate of the eigenvalue spectrum limit,

$$\mu_{2,n} = \min\,[0.98,\ \max\,(\mu_{2,n-1}{}^2,\ 0.75\ \mu_{2,n-1})], \qquad (716.43)$$

where $\mu_{2,n-1}$ refers to the value in current use. Equation (716-43) is applied only twice, and then Chebyshev acceleration is discontinued if the behavior is still apparently not convergent. The process will later be restarted if the single-error-mode extrapolation criteria are satisfied. Whenever the upper limit of the eigenvalue spectrum μ_2 is reduced, a new upper limit of 0.9 times the old value plus 0.1 times the new value is used which is then gradually increased one percent of the difference from unity each iteration.

The maximum relative flux change, ε_m for iteration m, is saved whenever the procedure is restarted. After the set delay, if $|\varepsilon_n| > 1.5\ |\varepsilon_m|$, the process is deemed to be ineffective even if the process is judged to be convergent, Eq. (716-43) is used, and the procedure restarted, but only if $|\varepsilon_n| > \mu_2\ |\varepsilon_{n-1}|$.

Given a convergent process when Chebyshev acceleration is in use, the behavior is examined after the set delay in iteration count, or if $f_n/f_{n-1} < 0.999$. Asymptotic extrapolation may then be done as discussed later, and then the process is restarted after a delay of one outer iteration. When the asymptotic single-error-mode extrapolation criteria are satisfied, μ_2 is reset to λ from Eq. (716-40), extrapolation is done, and the Chebyshev acceleration process is restarted after a delay of one iteration.

The value of μ_2 used for restart is limited to

$\mu_{2,n} < \dfrac{B - 1.0 + \mu_{2,n-1}}{B}$, where $B = \max[1.4,\ \ln\,(2 + \sqrt{I})]$ and I is the minimum number of inner iterations done, except that B is defaulted to

2.0 for one-dimensional problems.

When the iteration count from the beginning of the Chebyshev process in this cycle exceeds the limit, the process (cycle) is restarted unless $|\varepsilon_n| < |\varepsilon_{n-1}| < |\varepsilon_{n-2}|$ and $\mu_{n,o} < \mu_{n,1}$, where $\mu_{n,1}$ is the L_1 norm estimate of the dominant eigenvalue of the process.

Asymptotic Extrapolation

Asymptotic extrapolation is used here to mean the attempt to eliminate one or two dominating error vectors by driving the flux values toward an apparent solution as indicated by the iterative behavior. This scheme has proven to be very effective over a wide range of problems. To be effective it is necessary that the contribution dominates over that from other error vectors. This can be due to a large separation in the values of the eigenvalues of the error vectors or to large differences in their coefficients. Indeed that error vector which will dominate asymptotically may have such low coefficients that it does not surface before an acceptable solution is obtained, but another with a smaller eigenvalue will.

When the iterative behavior of a problem indicates that an asymptotic mode has established, an extrapolation is done on sets of the outer iteration flux values.

Consider the outer iteration problem in the form

$$\phi_{n+1} = (G_n + \frac{1}{k_n} \chi F)\phi_n , \tag{716-44}$$

or in the alternative form

$$\phi_{n+1} = (G_n + \frac{1}{k_e} \chi F)\phi_n + \left(\frac{k_e - k_n}{k_n k_e}\right)\chi F\phi_n . \tag{716-45}$$

Note that an error from the estimated value of the multiplication factor enters the problem directly since the true value k_e is not known.

This iterative process may be expressed as

$$\phi_{n+1} = M_n \phi_n \ , \tag{716-46}$$

where M_n is the iteration matrix. M_n depends on the latest estimate of the problem eigenvalue, the multiplication factor for the usual type of eigenvalue problem or the eigenvalue of the direct search problem. For a process which converges to a solution, the largest eigenvalue of M must tend to unity; the operation $M_\infty \phi_\infty$ must return ϕ_∞.

It is assumed that the outer iteration flux vector can be expanded into a set of linearly independent error vectors,

$$\phi_n - \phi_\infty = Q_n E_o + O_n, \tag{716-47}$$

where Q_n has diagonal entries $\prod_{\ell=m}^{n} \mu_{\ell,j}$, and O_n is a residual error (associated with the eigenvalue estimate), hopefully small and decreasing as n increases. E_o is the initial error vector, and the $\mu_{\ell,j}$ represent eigenvalues of the error vectors, eigenvalues of the iteration matrix M_n.

The single error mode extrapolation procedure is based on one error vector dominating asymptotically at each space energy point

$$X_{i,n} - X_{i,\infty} = a_i \mu^n \ , \tag{716-48}$$

where a_i is a constant and μ the eigenvalue of the dominating error vector. This recursion relationship yields the expression for the eigenvalue

$$\mu = \frac{X_{i,n} - X_{i,n-1}}{X_{i,n-1} - X_{i,n-2}} , \tag{716-49}$$

and the extrapolation equation to be applied is

$$X_{i,\infty} = X_{i,n} + b(X_{i,n} - X_{i,n-1}) . \tag{716-50}$$

where

$$b = \frac{\mu}{1 - \mu} .$$

Alternatively, iterate values spaced two iterations apart may be used by properly determining the extrapolation factor. At the time this is written, we use

$$X_{i,\infty} = X_{i,n} + p(X_{i,n} - X_{i,n-2}) , \tag{716-51}$$

where

$$p = \frac{\mu^2}{1 - \mu^2} .$$

The dependence of the extrapolation factor [for Eq. (716-50)] is shown in Fig. (716-3).

Thus, the asymptotic single-error mode extrapolation procedure uses information from three succeeding outer iteration flux values to give a single factor applied to the most recent flux values and those from two outer iterations back to drive the iterate estimates toward an apparent solution. The scheme is used to eliminate an error vector which dominates asymptotically, or one which dominates at any stage of the calculation.

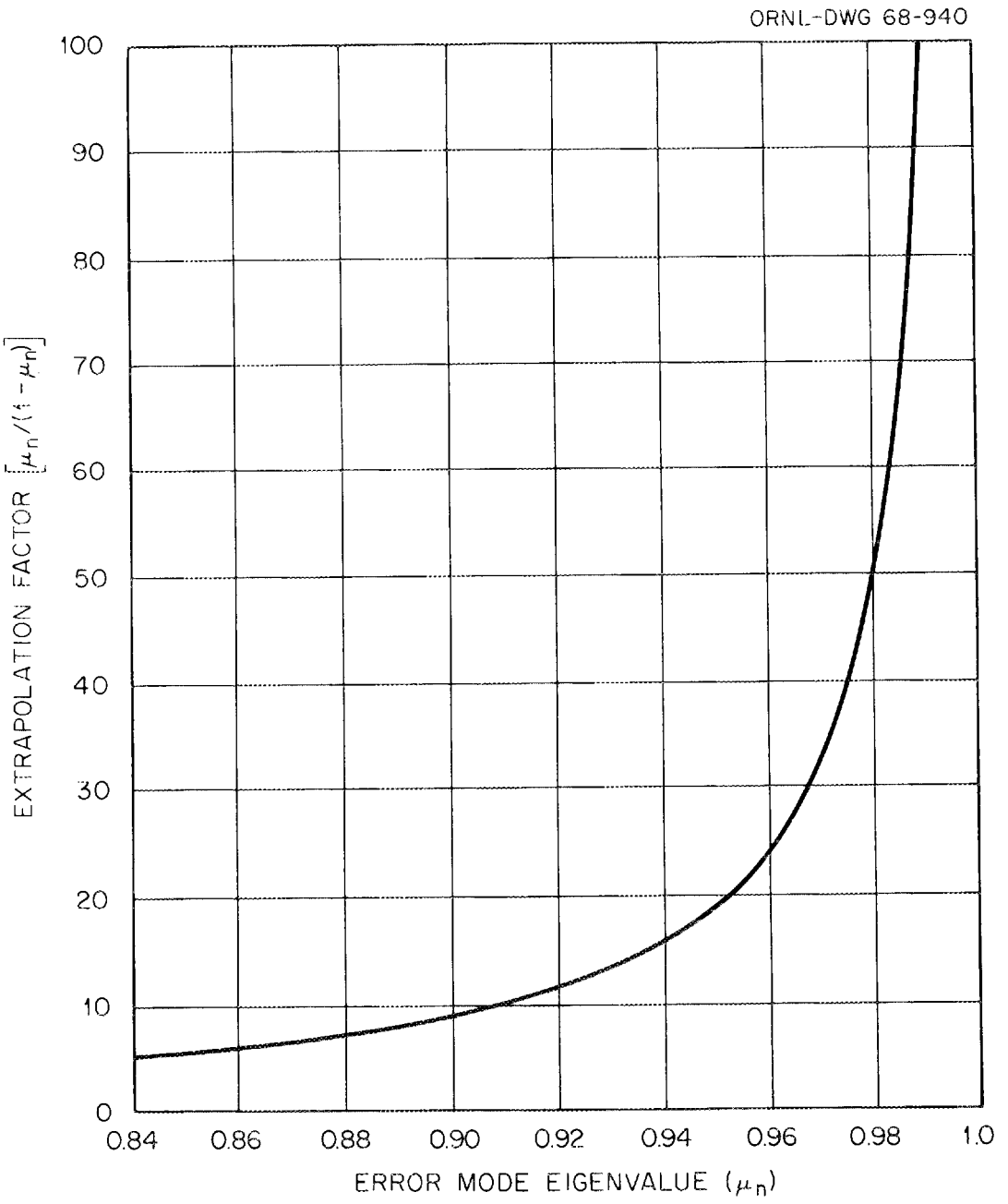

Fig. 716-3. Dependence of the Extrapolation Factor on the Single Error Eigenvalue.

Of critical importance are (1) determining when one error vector dominates, and (2) producing a good estimate of the eigenvalue of the dominating error vector.

The single-error mode process is restrained. A maximum value for b of 75 is used. A restraint is imposed which prevents the calculation of negative flux values if all iterate values are positive and also limits the increase in value from the extrapolations,

$$\left|\phi_\infty - \phi_n\right| \leq \min\left[0.9\ \left|\phi_n^*\right|,\ \left|\phi_{n-1}\right|\right] \tag{716-52}$$

The equations are programmed to account for negative flux values when calculated and any change in sign of the value of a flux at a point.

The asymptotic two-error-mode extrapolation procedure is less clearly defined. Basically, it is assumed that the composite error vector is given by

$$\phi_\infty - \phi_n = b_n(\phi_n - \phi_{n-1}) + q_n\ (\phi_{n-1} - \phi_{n-2}).$$

This recursion relationship leads to the equation

$$\mu_n(1.0 + b_n + \frac{q_n}{\mu_n}) = b_{n-1} + \frac{q_{n-1}}{\mu_{n-1}}\ , \tag{716-53}$$

where μ_n is defined above. At some stage in the calculation, it is assumed that the individual error vectors contribute in such a way that the values of b_n and q_n are nearly independent of the outer iteration n.

When so independent,

$$q_n = \frac{\mu_{n-1}\mu_{n-2}(\mu_n - \mu_{n-1})}{\mu_{n-2}(1.0 - \mu_{n-1})^2 - \mu_{n-1}(1.0 - \mu_n)(1.0 - \mu_{n-2})} ;$$

$$b_n = \frac{\mu_n - q_n\left[\frac{1.0 - \mu_{n-1}}{\mu_{n-1}}\right]}{1.0 - \mu_n} . \qquad (716\text{-}54)$$

Note that a test for significance can be made on the denominator of the equation for q_n. In any event, $q_n = 0$ defaults the equations to those for the single-error mode.

The asymptotic two-error-mode extrapolation equation is

$$X_{i,\infty} = X_{i,n} + b_n(X_{i,n} - X_{i,n-1}) + q_n(X_{i,n-1} - X_{i,n-2}) , \qquad (716\text{-}55)$$

applied to each flux value. An attractive feature of this procedure is that the eigenvalues of the two dominating error vectors may be a complex conjugate set. The rather indefinite state of the contributions from the individual error vectors which are required for the procedure to be effective is a distinct disadvantage.

The criteria which are used to assess error vector dominance include that the outer iteration process be convergent. Using the eigenvalue estimate $\mu_{n,o}$, or $\mu_{n,1}$ if Chebyshev acceleration is done, we require

$|\varepsilon_n| < 10,$

$|\varepsilon_n| < |\varepsilon_{n-1}| < |\varepsilon_{n-2}|,$

$\mu_n < 0.99999,$

$0.975 < \left[\frac{1.0 - \mu_m}{1.0 - \mu_{m-1}}\right] \frac{\mu_{m-1}}{\mu_m} < 1.025,$ for $m = n$ and $n-1$,

and if Chebyshev acceleration is done on outer iteration, we also require the value of μ_n calculated from the max, min flux ratios on outer iterations to be < 1.0. If $\mu_n < 1.0$ and the other criteria are satisfied, the outer iteration process is judged to be not convergent, over-accelerated after allowing the delays in assessment.

First priority is given to the double-error-mode procedure, applied when the following criteria are satisfied, using values from Eq. (716-54),

$$\mu_n < 0.99999$$

$$b_n + q_n > 0 \ ,$$

$$0.8 < \frac{b_n + q_n}{b_{n-1} + q_{n-1}} < 1.2 \ ,$$

$$|b_n| < 1000 \ ,$$

$$b_n b_{n-1} > 0 \ ,$$

$$q_n q_{n-1} > 0 \ ,$$

$$|q_{n-1}| < |b_n| \ ,$$

$$|q_n| < |b_n| \ ,$$

$$q_n < 0 \ .$$

In addition, a new value for b_n is obtained from

$$b'_n = \frac{1}{\mu_n}\left\{b_{n-1} + \frac{q_{n-1}}{\mu_{n-1}} - q_n - \mu_n\right\} \tag{716-56}$$

and the extrapolation is done only if

$$0.5 < \frac{b'_n}{b_n} < 1.5 \ .$$

The b'_n is used instead of b_n. Default is to the single-error-mode procedure, applied when its criteria are satisfied.

The same restraints are applied to the flux values as for the single-error-mode process.

Extrapolation is allowed only after the initial set delay in outer iteration count, and after the set delay following any major change in the process, as when extrapolation is done, or parameters are changed as discussed earlier. Otherwise, the procedure involves a continuous check on the iterative behavior for conditions allowing extrapolation. After extrapolation, the overrelaxation coefficients are not permitted to be adjusted for the set delay of 5 outer iterations; when the Chebyshev acceleration process is used, it is restarted whenever extrapolation is done.

When the minimum number of inner iterations ≥ 4, the selection of the number of inner iterations at each group is reassessed only when forced extrapolation, discussed below, is done:

$$I_{n+1}(g) = \frac{XI_n(g)}{\ell n\mu_n(g)} + 0.5 \ , \tag{716-57}$$

restrained to

$$\max\,[4, \min I_n(g)] \leq I_{n+1}(g) \leq \max I_n(g)$$

where

$$X = \max\left[I_n(g)\right]\ell n\left[\max\left\{\mu_n(g)^{\frac{1}{I_n(g)}}\right\}\right]$$

and $\mu_n(g)$ is determined at each group by Eq. (716-30).

If any $\mu_n(g) > 0.99999$, extrapolation is not done and the overrelaxation coefficient for that group is reduced.

It is possible to do simultaneous Chebyshev acceleration and extrapolation, by redefining the Chebyshev acceleration parameters to $f'_n = b + (1.0 + b)\ f_n$, $g'_n = (1.0 + b)\ g_n + q$, for double error mode (or single error mode on successive sets), or

$f'_n = (1.0 + p)\ f_n + p$; $g'_n = (1.0 + p)\ g_n + p$,

for single error mode extrapolation on alternate sets, and this is done with one iteration delay after the parameters satisfy criteria for asymptotic behavior.

Forced Extrapolation

A scheme of forced extrapolation is used in the event that the criteria for other schemes of acceleration on outer iteration have not been satisfied. After the set delay, outer iteration convergence criteria must be satisfied, and these are tested again five iterations later if the tests fail. Estimates are made of the error vector eigenvalues at each group and overall based on the L_1 norm, Eq. (716-30), using three successive outer iterate flux values. If a $\mu_n(g) > 0.99999$, the associated overrelaxation coefficient is reduced by Eq. (716-23), and if the overall estimate of $\mu_n < 0.99999$, single error mode extrapolation is done. The estimate of the outer iteration error vector eigenvalue is used to initialize the Chebyshev acceleration procedure when no estimate of the top of the spectrum is available, as from the initialization one-dimensional problem. Forced extrapolation may again be done after the set delay following any extrapolation, but not if Chebyshev acceleration is in progress.

Estimating the Eigenvalue

After each outer iteration, each full sweep of the mesh points, the eigenvalue is estimated from an overall neutron balance. If the point neutron balance equations are summed, the scattering and internal leakage terms cancel leaving only production, surface leakage and absorption (plus buckling and internal black absorber loss) terms. Therefore, for the usual eigenvalue problem,

$$k_n = \frac{P_n}{L_n} , \tag{716-58}$$

where P_n refers to the total neutron production rate, and L_n to the neutron absorption rate plus the surface leakage rate, each determined for outer iteration n. This estimate of the multiplication factor is used the next outer iteration except when outer iteration acceleration is done, or Chebyshev acceleration is done, or in the early history.

In the event that the sum of the distribution function for source neutrons is not unity for one or more zones, then the totals must be applied to the total production rate,

$$P_n = \sum_z V_z \left(\sum_g \nu\Sigma_{f,z,g} \overline{\phi}_{z,g}\right) \sum_{g'} \chi_{z,g'} . \tag{716-59}$$

Calculations of the losses to internal black absorber regions, inleakage from adjacent regions, presents a bit of a problem. To avoid a significant cost in computer time, this contribution to the overall neutron balance is approximated as a calculation proceeds, which involves use of all the latest point flux values available, but some point flux values have not yet been recalculated for the last inner

iteration. The effect of this approximation has been found to be insignificant for usual situations where the total black absorber contribution is a small part of the total neutron losses.

For the first iteration, the estimate of k is set to unity (lacking other data, as from a preceding case), and for the subsequent iterations it held at the initial value until

$$\frac{k_n - k_{n-1}}{k_0 - k_n} < 0.05 \text{ , or}$$

$|\varepsilon_\phi| < 8$ times required convergence,

where k_0 is the value used for the first iteration and k_n is the value calculated for iteration n. The first iteration that the initial value is not used, $\frac{1}{2}(k_0 + k_n)$ is used.

The estimate of k_n used when Chebyshev acceleration is done is from the source ratio shown below but modified to dampen oscillation. Considering

$$X = \frac{1}{k_{n-1}} - \frac{1}{k_{n-2}} ,$$

nothing is done if $X < 10^{-8}$;

let $\alpha = \frac{1}{X}\left(\frac{1}{k_n} - \frac{1}{k_{n-1}}\right)$

if $\alpha > 1.0$, set to -1.0

if $\alpha > 0$, set to 0.

if $\alpha < -1.0$, set to -1.0

then the adjusted value is

$$k_n' = \frac{1}{\frac{1}{k_n} + \left(\frac{\alpha}{1-\alpha}\right)\left(\frac{1}{k_n} - \frac{1}{k_{n-1}}\right)} .$$

For the adjoint eigenvalue problem, the outscattering and removal terms do not cancel. Therefore, the overall neutron balance equation is complicated, and it would be expensive in computer time to apply an overall neutron balance. So when the associated adjoint problem is solved after a regular problem, the available estimate of k_e from the latter is used. When the adjoint problem is done alone, or whenever Chebyshev acceleration is done, the source ratio estimate is used except in the early history,

$$k_n = \frac{k_{n-1} \; P_n}{P_{n-1}} \; . \tag{716-60}$$

This formulation is also used when solving the consistent P_1 equations or on user option.

We have also experimented with other schemes to estimate the eigenvalue of the problem. An attractive formulation is the estimate

$$k_n = k_{n-1} \frac{(\phi_n, \phi_n)}{(\phi_n, \phi_{n-1})} \; , \tag{716-61}$$

when special access of the flux values is not required, which is the case when Chebyshev acceleration is done on outer iterations; here, a matrix form is used to indicate sums of the pointwise products. Another scheme we have tested amounts to the assumption that the first energy group flux values are a reasonable approximation of an adjoint weighting factor. Saving these by zone from the previous iteration and applying the weighting,

$$k_n = k_{n-1} \frac{\sum_z P_n(z) \; \overline{\phi}_{n-1}(1,z)}{\sum_z P_{n-1}(z) \; \overline{\phi}_{n-1}(1,z)} . \tag{716-62}$$

Some weighting of two or more values obtained by different ways might prove to be superior, or one of them in a specific application area, but such has not been established. (Oh for more complete theoretical analysis!)

For other types of eigenvalue problems, the direct searches, the overall neutron balance yields an estimate of the eigenvalue,

$$\lambda_n = \frac{L_n - \frac{1}{k_e} P_n}{\left[\frac{1}{k_e} \Delta P_n - \Delta A_n\right]} \quad , \qquad (716\text{-}63)$$

where the new terms ΔP_n and ΔA_n are productions and losses associated with the changes introduced through the search parameter. Generally a λ of zero means none of the material to be adjusted is added to the system; the exception is the buckling search where the specified buckling term is initially included in the equation constants, so the search is done on the changes to it, zero λ meaning no change.

To avoid trouble with initial error modes, a change which is less than indicated by Eq. (716-63) is introduced during the early iterations. Let λ^* be the value calculated from Eq. (716-60) and λ_{n-1} be the value used the previous iteration; the formulation used is

$$\lambda_n = \lambda_{n-1} + C_n(\lambda^* - \lambda_{n-1}) \quad , \qquad (716\text{-}64)$$

where C_n is initialized at a small value, say 0.1, and is doubled after each time it is used until it exceeds unity, after which the estimate of λ given by Eq. (716-61) is used directly. In the event that the system has a very low multiplication factor, Eq. (716-63) tends to be an overestimate; therefore, if $k_n/k_e < 0.5$, where k_n is determined from Eq. (716-58), the factor C_n of Eq. (716-64) is not increased, nor is it

increased during the first few iterations if $0.95 < k_n/k_e < 1.05$. Other techniques have been used, as to dampen oscillatory behavior. However, it is quite important that asymptotic extrapolation be allowed; this requires that the detailed treatment of each iteration be identical, after the early history, or extraneous error vectors will be introduced.

Special care must often be taken when the iterate estimate of the search problem eigenvalue is negative. This causes a negative contribution to be added to the absorption at a point, decreasing the diagonal dominance. Thus, for a subcritical system, one having an associated k_e considerably less than unity, the solution for a desired k_e of unity of a reciprocal velocity search involves a negative value of λ. At solution the negative absorption contribution from the $\lambda(1/v)$ term may exceed that from the sum of outscatter and absorption, even at solution. During the iterative process, if not controlled, negative point flux values could be obtained. The technique used for control is to determine those values of λ which cause the total removal term with and without the diffusion coupling terms to be zero. Then the iterate estimate of λ is allowed to move only slowly from one value to the other, and no negative point flux can be obtained.

The Indirect Search

Consider that the results are available for two succeeding problems, namely, the multiplication factors associated with two conditions representing different contributions from the search parameters. Then use is made of the formulation

$$\lambda = \frac{C_1 k}{C_2 - k} \tag{716-65}$$

where C_1 and C_2 are constants to evaluate, k is the multiplication factor, and λ is the search problem eigenvalue. Equation (716-65) is assumed to fail if $|C_2| > 10^4$ as calculated, or if the estimated search eigenvalue exceeds either of the first two values. In this event, a linear approximation is used which gives the new estimate,

$$\lambda_{i+1} = \lambda_i + (k_e - k_i) \Big/ \left[\frac{k_i - k_{i-1}}{\lambda_i - \lambda_{i-1}}\right] , \tag{716-66}$$

where k_e is the desired value of the multiplication factor, often unity, and i refers to the index on the eigenvalue problem loop.

A third eigenvalue problem is then solved. Given three states and the associated values for the multiplication factors, the formulation used is

$$\lambda = C_3 + \frac{C_1 k}{C_2 - k} , \tag{716-67}$$

where C_1, C_2, and C_3 are constants to evaluate. Again significant results are required, or Eq. (716-66) is used in default.

To allow old results to be used, an estimate is made of the change in multiplication factor with change in the search eigenvalue

$$\lambda \frac{\partial k}{\partial \lambda} \simeq \lambda_i \left(\frac{k_i - k_{i-1}}{\lambda_i - \lambda_{i-1}}\right) , \tag{716-68}$$

and the last significant value of this derivative (calculated during the process of an indirect search) could be made available if another search problem of the same type were solved.

The Fixed Source Problem

A special aspect must be considered if the procedure for solving fixed source problems is to be effective. Given a fixed source, there is an associated neutron flux level, provided there is a solution. This solution may be far away from the conditions used to initialize the problem. Quite generally, that error contribution which is hardest to remove is associated with the flux level being far from solution.

To remove this major error contribution, the source is scaled during the iterative calculation. After each outer iteration, an overall neutron balance is used to estimate the required level of the fixed source,

$$P_n + h_n S_o = L_n \ ,$$
$$h_n = \frac{L_n - P_n}{S_o} \ , \tag{716-69}$$

where P_n is the fission source rate, L_n is the loss rate, and S_o is the total fixed source. The factor h_n determined above is a multiplier on the total source,

$$S_{n+1} = \begin{cases} S_o, & n = 0 \\ h_n S_o, & n > 0 \end{cases} \tag{716-70}$$

and therefore on the individual components of it.

Upon completion of the problem, the solution flux values are scaled to give the solution associated with the specified fixed source. This procedure applies in any situation where there is no feedback into the problem. Note that the procedure allows the source to go negative if so

calculated as necessary. The result of a calculation may be that a negative source is required for the situation presented, and this is generally deemed not acceptable.

When there are negative fixed source values, the factor is held fixed for 10 iterations at

$$h_n = 1.0 \ , \tag{716-71}$$

and once near convergence is again held fixed ($h_n = h_{n-1}$ if the calculated relative change is $< 10^{-4}$).

Also for fixed source problems which have negative source terms, the point flux values are allowed to go negative and scaling of the source is constrained to a positive factor, $h_n > 0$. Note the special initialization of the flux for these problems, Sec. 718.

Extrapolated Eigenvalue

When extrapolation is done of the flux values some outer iteration n, a new estimate is made of the problem eigenvalue. If the flux values have been driven with the extrapolation factors b and q, then the summed neutron production and external loss terms for the asymptotic situation are

$$P_\infty = P_n + b(P_n - P_{n-1}) + q(P_{n-1} - P_{n-2}) \ ,$$

$$L_\infty = L_n + b(L_n - L_{n-1}) + q(L_{n-1} - L_{n-2}) \ , \tag{716-72}$$

and the eigenvalue estimated from this extrapolated data. When the flux values are driven with alternate iterate values, the appropriate equations are

$$P_\infty = P_n + p(P_n - P_{n-2}) \ ,$$

$$L_\infty = L_n + p(L_n - L_{n-2}) \ . \tag{716-73}$$

The latter procedure is especially useful when the behavior is oscillatory. If the maximum relative flux change for the last iteration exceeded 10 percent, only half of the changes in P and in L from the extrapolation are used.

END OF SECTION

Section 717: Optimum Number of Inner Iterations

The calculational procedure involves inner iteration on the fixed source problem at each discrete neutron energy (each group). From among a large number of possibilities, we seek an optimum in the sense of minimizing the cost of solving a problem with emphasis on those types of problems most representative of application. These include rather large three-dimensional problems and also reactor core problems of modest size treating one, two or three dimensions, cell problems, and criticality search problems, treating from a few to many energy groups. Usually the solution is far from the initial estimate of the flux distribution. Also of considerable interest is the class of problems where there are relatively small changes from one problem to the next, as in long-time exposure (depletion) application, and a relatively good solution is available for a succeeding flux, eigenvalue problem.

Minimizing computer cost may well require assessment of the algorithm for allocating charges and performance characteristics of the particular computer in use. Here we grant that the cost associated with data transfer must quite generally be kept down, which requires that an effective procedure be used for data transfer, that an effective mode be used to balance computer memory and data transfer, which may well depend on the rates of computation and data transfer, and that the data transfer be efficient.

The major concerns are the use of an effective inner iteration procedure, which is addressed next, and selection of an optimum number of inner iterations which is then addressed considering iteration behavior and costs.

Regarding an Optimum Inner Iteration Procedure

It is of interest to examine the theoretical basis for optimizing the inner iteration process in more depth. When the eigenvalues of linearly independent error vectors are real, it has been shown that a linear combination may be taken of the iterate error vectors, a characteristic polynominal results which yields the solution, given sufficient iterations, and the Chebyshev polynominal is appropriate for adjusting the overrelaxation coefficients.[a]

There are two basic difficulties which limit the utility of the information now available from theoretical analysis of the reactor problem inner iteration process at one group. First, consider the problem

$$\phi_n = T\phi_{n-1} + US$$

in the sense of an error vector behavior,

$$\phi_{n-1} = T\phi_{n-2} + US,$$

$$\phi_n - \phi_{n-1} = T\ (\phi_{n-1} - \phi_{n-2});$$

$$E_n = \phi_n - \phi_\infty = M^n E_o,$$

$$E_n - E_{n-1} = \phi_n - \phi_{n-1} = M\ (\phi_{n-1} - \phi_{n-2}),$$

where the eigenvalues of the iteration matrix T lie on the main diagonal of M. The influence of the start of inner iterations each outer iteration, and the early behavior is of most interest, not the asymptotic behavior for n large. Further there is the basic problem that an asymptotic

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[a] L. F. Richardson, Philos, Trans. Roy. Soc. London, AZIO (1910).

error behavior can not establish until sufficient iterations have been done to establish full communication, to sweep in the boundary conditions, which requires essentially as many iterations as rows of points with normal ordered line relaxation. The impact of this delay on the early process, and of other aspects which affect the coefficients of the error vectors, the initial error vector itself, can not simply be assessed.

The second difficulty is that with this form of error representation, overrelaxation of the difference equations results in error vectors which are not linearly independent. If we consider the matrix M, it contains pairs of eigenvalues. Without overrelaxation and using only last iterate flux values, there are pairs of eigenvalues $\pm \mu_j$. Using newly calculated values as they become available, the pair becomes $(\mu_j^2, 0)$. With overrelaxation, for $\beta = 1$, the pair is still $(\mu_j^2, 0)$, and increasing β causes the two values to move together and be equal at the optimum for a fixed value of β_o, (λ_o, λ_o). Increasing β causes these to become a complex pair $(a + ib,\ a - ib)$. At the optimum, the submatrix of M associated with this pair requires an off-diagonal term[a]

$$\begin{bmatrix} \lambda_j & 1 \\ 0 & \lambda_j \end{bmatrix}$$

and the process goes as

$$M^2 = \begin{bmatrix} \lambda_j^2 & 2\lambda_j \\ 0 & \lambda_j^2 \end{bmatrix}, \quad M^3 = \begin{bmatrix} \lambda_j^3 & 3\lambda_j^2 \\ 0 & \lambda_j^3 \end{bmatrix};$$

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[a] D. M. Young, Trans. Amer. Math. Soc. 76 (1954).

or the contribution to the error for iteration n is

$$h_n = 2\lambda^n + n\lambda^{n-1}. \tag{717-1}$$

Of course there is not an anomaly at $\beta = \beta_o$; application results show that error reduction is a smooth function through the optimum. Thus in general the eigenvalue deficiency must be made up and the submatrix of M has the form

$$\begin{bmatrix} \lambda_1 & 1 \\ 0 & \lambda_2 \end{bmatrix}$$

over the range. (In what follows, everything should probably be multiplied by a leading $\frac{1}{2}$, or associate a factor of 2 multiplied onto the initial error vector.) For two real values, $\beta < \beta_o$, the general result is,

$$h_n = \lambda_1^n + \lambda_2^n + \sum_{k=1}^{n} \lambda_1^{n-k} \lambda_2^{k-1}, \text{ or}$$

$$h_n = \lambda_1^n + \lambda_2^n + \lambda_1^{n-1} \left[\frac{1-\rho^n}{1-\rho}\right], \tag{717-2}$$

where $\rho = \lambda_2/\lambda_1$. For two imaginary values, $\beta > \beta_o$, we have the submatrix

$$\begin{bmatrix} a + ib & 1 \\ 0 & a - ib \end{bmatrix} = \begin{bmatrix} \lambda e^{i\theta} & 1 \\ 0 & \lambda e^{-i\theta} \end{bmatrix},$$

where $\theta = \tan^{-1}(b/a)$, $\lambda = \sqrt{a^2+b^2}$.

successive contributions are

$$h_o = 2$$

$$h_1 = 2a + 1 = 2\lambda \cos\theta + 1$$

$$h_2 = 2(a^2 - b^2) + 2a = 2\lambda^2 \cos 2\theta + 2\lambda\cos\theta,$$

or in general

$$h_n = 2\lambda^n \cos(n\theta) + \lambda^{n-1} \left\{ 1-k + 2\sum_{j=1}^{\left[\frac{n}{2}\right]} \cos\ (2j-k)\ \theta \right\}, \qquad (717\text{-}3)$$

where k = 1 if n is even, 0 if odd, and $\left[\frac{n}{2}\right]$ truncates down. Note that if $\beta = \beta_o$ for max λ_j, for all other λ_j, $\beta > \beta_o$, so all the other error vectors should behave in this complicated fashion. An interesting aspect of the off-diagonal contribution when $\beta > \beta_o$ is that the individual terms involving increasing angles have positive and negative signs and hence tend to cancel out, except for very small θ or n, or as n takes on very large values. As λ_j decreases, θ increases. Thus if for some λ_j, β is the optimum, for all other $\lambda_m < \lambda_j$,

$$h_n(m) = 2(\beta-1)^{n-1} \left[\beta + f(\theta,n)\right],$$

where $f(\theta,n)$ is a symbolic function, and

$h_n(m) < h_n(j)$, n larger than some rather small value. The contributions from the error vectors associated with all λ_m continue to make a contribution, but this decreases relative to that from max λ_j. If this were not so, it would be practical to occasionally make a sweep without overrelaxation to cause the contribution from those error vectors having small eigenvalues to be suppressed. Application testing also

For $\beta < \beta_o$, as n increases, $h_n \to \lambda_1^{n-1} [\lambda_1 + \frac{1}{1-\rho}] + \lambda_2^n \to \lambda_1^{n-1} [\lambda_1 + \frac{1}{1-\rho}]$, but for $\beta = \beta_o$,

$$h_n = (\beta - 1)^{n-1} [2(\beta - 1) + n],$$

and the off-diagonal term dominates for n large.

If we consider the ratio of the error contribution at one iteration to the previous one,

$$g_n = \frac{h_n}{h_{n-1}},$$

The equations and behavior for n large but not too large are:

$$g_n = \begin{cases} \dfrac{\lambda_1^n + \lambda_2^n + \lambda_1^{n-1}\left[\dfrac{1-\rho^n}{1-\rho}\right]}{\lambda_1^{n-1} + \lambda_2^{n-1} + \lambda_1^{n-2}\left[\dfrac{1-\rho^{n-1}}{1-\rho}\right]} & \to \lambda_1, \ \beta<\beta_o \\ (\beta-1)\left[\dfrac{2(\beta-1)+n}{2(\beta-1)+n-1}\right] & \to (\beta-1), \ \beta=\beta_o, \\ (\beta-1)\left[\dfrac{\beta + f(\theta,n)}{\beta + f(\theta,n-1)}\right] & \to <(\beta-1), \ \beta>\beta_o. \end{cases} \tag{717-4}$$

If the eigenvalue pair were real and equal, having the values (λ_j, λ_j) for $j > 0$ and $\lambda_o = 1$, successive operations by,

$$\begin{bmatrix} \lambda_j & 1 \\ 0 & \lambda_j \end{bmatrix}$$

yields

$$h_n = 2 \prod_{j=o}^{n} \lambda_j + \sum_{k=1}^{n} \prod_{\substack{j=o \\ j\neq k}}^{n} \lambda_j .$$

This expression properly simplifies when all λ_j are equal. However, an acceptable result is not produced when the pair is complex conjugate because the operation

$$\begin{bmatrix} a_j + ib_j & 1 \\ 0 & a_j - ib_j \end{bmatrix}$$

produces a dangling imaginary component. A resolution of the discrepancy is not known.

The Chebyshev polynominals are appropriate to minimize the error contribution when the error vectors are independent, if real,

$$h_n = \prod_{j=o}^{n} \lambda_j,$$ or if imaginary with the operation

$$\begin{bmatrix} a_j + ib_j & 0 \\ 0 & a_j - ib_j \end{bmatrix},$$

if account is taken of the situation.[a] The optiumum for the actual situation of the inner iteration process of interest is not known due to complexity from the vector deficiency.

A simple fixed source, homogeneous, no sink, uniform mesh problem was solved by σ_1 ordered line overrelaxtion. Error level was measured as the sum of the absolute relative differences from the results for a well converged solution divided by the number of unknowns, an average absolute relative error. Results are shown in Table 717-1. For these cases the flux values were set equal at a reasonable level considering the solution; the initial average absolute relative error was 2.96 for the 10 x 10 mesh and decreased to 1.05 for the 100 x 100 mesh. These predicted number of iterations were obtained by determining the additional number of iterations required to reduce the error from 0.01 to 0.0001 (or to 0.001 lacking significance) assuming error decay as max λ^n for N, normally $\lambda = (\beta-1)$, and as $(\beta-1)^n$ $(\beta-1 + n/2)$ for L.

The behavior is substantially as expected, excepting the anomaly in the vicinity of 3,000 meshpoints, which is associated with initial suppression of the error vector having the largest eigenvalue, and the behavior of the larger problems using β slightly larger than β_o, which we address later. For $\beta < \beta_o$, relatively rapid reduction of the contribution from most of the error vectors appears to cloud the picture of how those with the larger eigenvalues behave.

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[a] L. A. Hageman, "The Estimation of Acceleration Parameters for the Chebyshev Polynominal and the Successive Overrelaxation Iteration Methods," Atomic Energy Commission Report (June 1972). WARD-TM-1038

Table 717-1. Behavior of the Inner Iteration Process

Mesh Points	Max μ_j^2	β_o	β used	Number of Iterations to Reduce the Error to 0.1	0.01	0.001	0.0001	Predicted N	L
$10^2 = 100$	.85034	1.4421	1.0	13	27	42		41.2	
			1.05	12	25	37	50	50.5	
			1.4421	4	8	11	15	13.6	14.3
			1.87	14	30	47		46.5	
			1.8844[a]	16	33	51		51.7	
			1.9	17	38	58		59.9	
$19^2 = 361$	.95194	1.6404	1.6404	7	15	19	26	25.3	26.6
$20^2 = 400$	.95631	1.6542	1.5772[b]	10	22	33	45	44.7	
			1.6542	7	15	20	27	25.8	27.1
$21^2 = 441$	.96010	1.6670	1.6670	8	16	21	28	27.3	28.7
$30^2 = 900$	.97969	1.7505	1.7505	9	21	28	38	37.0	39.1
$40^2 = 1600$	.98833	1.8050	1.8050	9	25	35	48	46.2	49.2
$50^2 = 2500$	.99244	1.8400	1.8400	9	25	39	52	51.4	55.8
$60^2 = 3600$	.99471	1.8644	1.6864[b]	18	69	150		146.6	
			1.8644	10	30	45	63	61.6	66.9
$70^2 = 4900$	.99609	1.8823	1.8823	14	38	59	80	74.8	80.6
$80^2 = 6400$	.99700	1.8961	1.8691	21	46	72	94	88.2	94.4
			1.9	20	44	63	82	87.7	
$81^2 = 6591$	.99707	1.8973	1.8973	21	47	73	96	89.5	95.6
$82^2 = 6724$	.99714	1.8985	1.8985	22	48	74	97	91.0	97.4
$90^2 = 8100$	.99762	1.9070	1.9070	26	55	83	108	102.2	109.0
			1.915	25	48	63	104	99.8	
			1.92	24	47	77	102	102.2	
$100^2 = 10000$	.99807	1.9158	1.9158	31	63	94	122	115.3	122.8
			1.85	56	145	227		234.	

[a]Real and imaginary components equal in magnitude.

[b]Largest eigenvalue twice the smallest one

We consider a reasonable measure of convergence level to be the maximum relative iterate flux change. Data for the reference cases (using β_o) are given in Table 717-2 which shows the average absolute relative flux error to be about a factor of five less than the iterate maximum relative flux change, but decreasing significantly for the larger and more slowly converging problems. The maximum error would be expected to be considerably larger than the average.

Applying the Chebyshev polynominals to the overrelaxation coefficients involves the formulation:

$$\beta_t(g) = \begin{cases} 1.0, \ t = 1 \\ \dfrac{2.0}{2.0 - \rho^2(g)}, \ t = 2 \\ \dfrac{4.0}{4.0 - \rho^2(g) \ \beta_{t-1}(g)}, \ t > 2 \ . \end{cases} \tag{717-5}$$

Here t refers to inner iteration with normal sweeps. With σ_1 ordering, t refers to each sweep on alternate points so the overrelaxation coefficient is adjusted at the start of and midway through the inner iteration sweep, the so-called cyclic Chebyshev procedure.[a]

The 50 x 50 meshpoint problem was solved with application of the Chebyshev polynominals, and without these, varying a fixed overrelaxation coefficient in the neighborhood of β_o. Results are shown in Table 717-3 for three different methods of absolute error level measurement and with the level of the initial flux values varied. Note that the apparent optimum value of β is near β_o and that use of a larger value does not

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[a]R. S. Varga, Matrix Iterative Analysis, Prentice-Hall (1960)

Table 717-2. Comparison of Flux Change with Absolute Convergence

Meshpoints	Maximum Iteration Relative Flux Change at Average Absolute Relative Error Levels		
	0.01	0.001	0.0001
10^2	.052	.0037	.00019
20^2	.038	.0094	.00034
30^2	.035	.0061	.00026
40^2	.047	.0076	.00042
50^2	.10	.0098	.0015
60^2	.10	.0056	.00094
70^2	.15	.0037	.00038
80^2	.037	.0024	.00024
90^2	.018	.0014	.00015
100^2	.013	.0011	.00010
Arithmetic Average	.059	.0051	.00045
Average, ℓn basis	.046	.0041	.00033

Table 717-3. Effects of the Variables on the Behavior of the 50 x 50 Meshpoint Problem

β_o	Relative Initial Flux	Iterations to Effect Error Level Reduction					
		$\frac{1}{I_i}\sum_i \left\lvert \frac{X_{i,n}}{X_{i,\infty}} - 1 \right\rvert$		$\left\{ \frac{1}{I_i}\sum_i \left[\frac{X_{i,n}}{X_{i,\infty}} - 1 \right]^2 \right\}^{1/2}$		$\left\{ \frac{1}{I_i}\sum_i (X_{i,n} - X_{i,\infty})^2 \right\}^{1/2}$	
		.01	.0001	.01	.0001	.01	.0001
				Fixed Overrelaxation Coefficient			
1.81005	4	15	63	15	61	27	75
1.82005	4	15	57	15	57	26	69
1.83005	4	15	50	16	49	25	61
1.83505	4	17	48	17	49	25	57
1.84005[a]	4	19	49	19	50	25	54
1.84505	4	20	50	20	52	25	52
1.85005	4	21	50	20	52	27	55
1.85505	4	21	52	21	55	29	59
1.86005	4	21	56	22	56	31	61
1.84005[a]	1	38	67	39	69	35	65
1.84005[a]	15	30	61	34	64	34	64
				Chebyshev Polynominals Applied			
1.84005[a]	1	33	58	34	59	27	54
1.84005[a]	4	21	50	31	57	31	58
1.84005[a]	15	25	56	28	57	30	58

[a] $\beta = \beta_o$

effect improvement for the reference initialization. This behavior is associated with initial suppression of one or perhaps several of the error vectors having the larger eigenvalues. The other initialization conditions show a gain from use of a value of $\beta > \beta_o$.

Although the error reduction effected depends on how and when it is measured, these results indicate a gain from applying the Chebyshev polynominals except for that case where the initialization appears to suppress the error vector having the largest eigenvalue (eigenvalue pair). When so suppressed, the optimum is a smaller value rather than the value β_o causing the eigenvalue pair to coalesce, or than the even larger values which result from application of the Chebyshev polynominals.

Shown below are results for the 80 x 80 meshpoint problem as dependent on the value of a fixed overrelaxation coefficient; only slightly different results were obtained using different measures of absolute error level.

Fixed Overrelaxation Coefficient	Iterations Required to Reduce Error Level to .01	.0001	Apparent Decay Rate
1.894	48	101	.9168
1.8961[a]	46	94	.9085
1.898	45	87	.8962
1.90	44	82	.8859
1.901	43	80	.8830
1.902	43	83	.8913
1.904	42	89	.9067
1.906	42	91	.9103
1.91	42	91	.9103
1.92	49	104	.9197

[a] $\beta = \beta_o$

The optimum is apparently above the coalescing value β_o. It appears that the form of the error contribution shown above admits an optimum slightly larger than β_o; a small increase in β causes a relatively large increase in θ. It is noteworthy that application testing usually indicates that a large coefficient is effective in the early iterative history for bringing down the error level, but the optimum fixed value decreases as the desired error level is decreased, entirely consistent with the application of the Chebyshev polynominals.

Some of the problems treated above were solved in several ways adjusting the overrelaxation coefficient each iteration applying the Chebyshev polynominals. Of special interest here is application when only a few inner iterations are used between new source calculations. We have become suspect of the use of a value of unity the first iteration and then a relative large value, so testing was done omitting the usual first two terms; we found that this caused a little decrease in the effectiveness, but far less than omitting only the first term. Simple upper bounds on the first value of the coefficient were tested which caused initialization well down the series. Except for the anomaly in the neighborhood of 3,000 meshpoints, a gain was quite generally found with application of the Chebyshev polynominals. Restarting the cycle becomes less efficient as the value of β_o increases. Constraining the maximum value may not be the optimum, but if the procedure applied involves restarting within the inner-outer iteration procedure for solving reactor problems, it may be prove desirable as found to be true in these tests.

Quite inferior results were obtained when only the first term of the series using Chebyshev polynominals, $\beta = 1$, was dropped; it is practical to drop two terms but not one. Testing was also done alternating between two values of the coefficient without significant gain; it was noted that the error levels were independent of the order of use of two values.

Results are shown below for problems slightly different from those treated above which show the number of iterations required to effect an absolute error level, line relaxing along the first dimension:

	Iterations Required			
Scheme/Mesh Size (Points)	40×40	40×80	80×40	80×80
Normal Ordering	60	86	73	122
Normal Ordering, Chebyshev	55	87	72	120
σ_1 Ordering	47	60	60	98
σ_1 Ordering, Chebyshev	41	52	53	81

The advantage from the σ_1 ordering is clearly demonstrated; it shows the largest gain for the rectangular mesh with line relaxation along the short rows. A primary reason for this gain is believed to be propagation. For normal ordered sweep, R iterations are required for the first row to feel the influence of the remote boundary condition, where R is the number of rows of unknowns; full propagation occurs with σ_1 ordering at R/2 iterations in two dimensions with relaxation on rows.

We note that there can be considerable gain from suppression of the error vectors having the larger eigenvalues. Full advantage of this gain can not be taken when a procedure is used which determines the largest eigenvalue whether or not the associated error vector makes significant contribution. Suppression of those error vectors having large eigenvalues is a challenging subject, to practice and theory. The classical situation often found in application is that when control rods are repositioned, the problem converges more slowly starting from the result for the initial position than if a flat flux were used. Note that one selected procedure may prove superior to another one for a particular problem but inferior for another problem, severely impacting evaluation of methods.

Inner Iteration Threshold

Acceleration is done on outer iteration, continuous application of the Chebyshev polynominals in accelerating iterate flux estimates, or occasional extrapolation to an apparent solution. The effectiveness of these schemes depends on effective error reduction during inner iteration and error vectors of the outer iteration process which are simple and linearly independent. Significant contamination of these error vectors can be expected to cause the acceleration schemes to be ineffective. This would result, for example, if the number of inner iterations at one energy were not held fixed. Thus there can be a threshold number of inner iterations required for effective acceleration on outer iteration. It is known that such threshold depends on

the problem, or at least on the class of problem, and on the procedures applied. For example, the single error mode extrapolation procedure is usually effective even with only one inner iteration, but there are some problems for which it is not.

When the procedure of calculation involves assessment of inner iteration behavior to make changes, as in the overrelaxation coefficient, some minimum number of inner iterations are required. This is necessary to obtain adequate information about the behavior and to cause stabilization of the process for the new source that outer iteration. If there were a single error vector dominating the iterative process

$$\phi_t = T\phi_{t-1} + US,$$

$$\phi_2 - \phi_1 = T\ (\phi_1 - \phi_0),$$

and one expects little useful information after one iteration, useful information after two iterations, and three iterations allow comparison of successive estimates of the eigenvalue of the dominating error vector. At least two inner iterations is a minimum if inner iteration behavior is to be assessed in any detail.

The Nature of Cost Optimization

The cost to solve a specific problem may be estimated by an approximation which is intended to allow for allocation of charges (cost C in equivalent processor time),

$$C = N\ (q + J) + r, \tag{717-6}$$

where N is the number of outer iterations, J the number of inner iterations, q the ratio of the special cost associated with each outer iteration relative to that associated with each inner iteration, and r allows

for overhead. For those modes of calculation where more inner iterations can be done without additional data transfer, data transfer cost is associated with outer iteration and q increases with increase in the cost of data transfer. This increase may be caused by increase in the amount of data, decreased efficiency, or by effects of aspects of the algorithm for allocating charges.

Quite generally the number of outer iterations decreases as the number of inner iterations is increased, N is sensitive to changes in J when J is small and should take on an asymptotic value for large J. For a specific problem a reasonable but simple correlation is

$$N = a + \frac{b}{J} , \tag{717-7}$$

where a and b are constants, undoubtedly problem dependent. Note that this correlation may well be adequate over a narrow range of the values of J. The cost is now given by

$$c = (aq + b + r) + \frac{bq}{J} + aJ.$$

Setting the first derivative equal to zero yields

$$J = \sqrt{\frac{bq}{a}} . \tag{717-8}$$

The optimum number of inner iterations increases as the outer iteration cost increases relative to inner iteration cost, and increases with increase in the sensitivity of the number of outer iterations to change in the number of inner iterations. Note that there may be some threshold value of J.

A problem was selected which needs large overrelaxation coefficients and which converges rapidly on outer iteration when a large number of inner iterations are done, has a small amount of data transfer but requires sufficient computer time to generate significant cost data. It is a two-dimensional two-group flux, eigenvalue cell problem for a water reactor, reflected on all sides. Results from application of a specific procedure for a mesh of 96 x 96 meshpoints (2 groups, 18,432 unknowns) are shown below for an overrelaxation coefficient of 1.93091 in the first group:

J	N	Processor Time for Iteration (min)	Local Job Cost ($)	
			Processor	Total
1	137	2.36	11.0	19.6
3	66	1.73	8.5	14.4
4	47	1.53	7.5	13.0
6	36	1.52	7.5	12.5
8	27	1.41	7.3	12.2
10	24	1.54	7.6	12.3
12	22	1.64	8.0	12.6
15	19	1.68	8.0	12.6
20	14	1.64	7.8	12.2
40	9	2.07	10.0	14.3
80	8	3.56	14.5	18.7

The dependence of N on J is relatively smooth with variation associated with effectiveness of the outer iteration acceleration procedure. Processor time allocated to a run depends on the work load

on the machine under multitasking, as does allocated cost.

Both processor time and cost are rather flat over a large range in the value of J. An estimated value for a q of 2.0 is obtained from processor time, 4.0 with cost data, but dependent on weighting of the data. Using an extrapolated value of 3.5 for a, b is about 200, and b/a = 57, which yields an optimum value of 11 for J from Eq. 717-8 for q = 2.

Contamination from Inner Iteration

Theory yet provides us with little information about contamination of the outer iteration process from truncation of the inner iterations. Thus we seek a correlation. To be reasonable, this must account for large contamination at small J and take on an asymptotic value for large J. Here we take the view that this contamination does not cause the outer iteration eigenvalues to take on imaginary components, but rather that the real values are increased.

Consider that a near optimum value of the overrelaxation coefficient will be used. The dominant error vector of the inner iteration process is expected to contribute in the amount

$$(\beta - 1)^{J-1} \quad [\beta - 1 + \frac{J}{2}] \ .$$

Note that for $\beta = 1.93091$, it requires J = 46 to reduce this contribution below its initial level. Experience tells us that it does not take this many inner iterations each outer iteration to effect error reduction; the optimum is many fewer. However, if this error vector makes significant contribution we can expect that the product of the number of inner and outer iterations must indeed reduce the contribution,

$$(\beta - 1)^{NJ-1} \quad [\beta - 1 + \frac{NJ}{2}] < 1.$$

For this problem, reduction from its initial level starts at NJ = 46, and reduction by a factor of 10 occurs at NJ = 86, and by a factor of 100 at NJ = 123.

We would not expect any outer iteration acceleration procedure to be effective before this error contribution starts to decrease unless the error vector were highly suppressed. The peak value of this error contribution occurs at

$$NJ = \frac{-1}{\ln (\beta-1)} - 2 \ (\beta-1),$$

or at NJ = 12 for the reference problem. We suspect from application experience that Chebyshev acceleration on outer iteration will not generally prove effective if started before this error contribution is less than unity.

If the new source each outer iteration caused re-excitation of the dominant inner iteration error vector, many more inner iterations would be required than found to be necessary or the optimum in usual application.

A reasonable approximation of the reduction in the contribution from all inner iteration error vectors each inner iteration is $(\beta-1)$. Given J inner iterations, we approximate the reduction in error contribution as $(\beta-1)^J$. A formulation for contamination which satisfies the endpoint values of $J = 0$ and $J \to \infty$, and includes a free parameter α

to allow adjustment for the effectiveness of iteration is

$$\gamma = \lambda + (1-\lambda)\ (\beta-1)^{\alpha J}. \qquad (717\text{-}9)$$

This equation was applied to the reference problem with a selected value for α of 1/3 and an estimated value of 0.231 for λ. Shown below are estimates of the dominating outer iteration error vector eigenvalue, estimates from Eq. (717-9), and the expected number of outer iterations required to reduce the associated error contribution to a relative level of 0.0005:

J	N	γ		Estimated Outer Iterations (no acceleration)
		Estimated from the behavior by the code	Eq. 717-9, α = 1/3	
1	137	.992	.982	418
3	66	.948	.947	140
4	47	.935	.930	105
6	36	.866	.897	70
8	27	.855	.866	53
10	24	.850	.837	43
12	22	.831	.810	36
15	19	.772	.769	27
20	14	.749	.708	22
40	9	.523	.527	12
80	8	.313	.345	7

The calculated number of outer iterations is interpreted as an estimate without outer iteration acceleration. The calculations applied

asymptotic extrapolation but not Chebyshev acceleration. The case applying 20 inner iterations was resolved not allowing extrapolation, and 20 outer iterations were required to satisfy the specified convergence. (The case applying 80 inner iterations also did not apply asymptotic extrapolation.) Note that if we seek an optimum value for J from the predicted behavior without acceleration at an outer to inner iteration relative cost of 2, the apparent optimum J is about 20, but with acceleration it is much less. More effective outer iteration acceleration could shift this value even lower.

Cases were run to test the dependence of the number of outer iterations required to effect an adequately converged solution, on the value of the overrelaxation coefficient. Recall that 27 outer iterations were required for the reference case above doing 8 inner iterations and using overrelaxation coefficients of 1.93091 in the first group and 1.89665 in the second group with application of Chebyshev polynominals to the coefficients starting well down the series. The results with a fixed coefficient, same value in each group, are:

β	Outer Iterations	γ
1.911	35	.895
1.931	30	.842
1.951	38	—

Shown below are selected results for coarse meshpoint arrangements. We estimate little dependence on λ of the mesh.

Space Points	β	J	N	Processor time (min)	γ Estimated from the behavior by the code	γ Eq. 717-9 ($\alpha = 1/3$)	Estimated Outer Iterations (no acceleration)
12^2	1.7050	4	10	.038	.30	.714	23
		10	8	.040	.20	.471	10
		20	7	.046	.20	.306	6
24^2	1.804	4	17	.093	.66	.806	35
		10	11	.085	.48	.602	15
		20	9	.112	.32	.41	9
48^2	1.882	4	33	.41	.85	.881	60
		20	13	.45	.59	.564	13

Although the values of γ are not in good agreement, the predictions of the required number of iterations are reasonable. For many inner iterations, the behavior does not stabilize to allow an accurate estimate of the eigenvalue and extrapolation, while for few, the gain from extrapolation about halves the required number of iterations for these small small problems. The code estimated value of $\gamma < \lambda$ is not explained.

Other approaches to correlation of outer iteration contamination from inner iteration truncation have not been successful. Unfortunately we find that the value of α in Eq. (717-9) has some dependence on problem type yet unpredictable, although it often is 1/4 to 1/3. The use of other free parameters does not appear useful in this form of correlation.

To seek an optimum with outer iteration acceleration, a revision is needed to Eq. (717-9) to account for its effect. Basically we expect there is an effective value of γ, $\gamma_e < \gamma$, which accounts for the behavior. This may be the next largest eigenvalue of the outer iteration error vectors, assuming they are real, etc., when asymptotic extrapolation is done, or some effective value when Chebyshev acceleration is applied. A number of considerations including the need for a simple minimum point lead to the form,

$$\gamma_e = \lambda_e + (1-\lambda_e)\ (\beta-1)^{\alpha_e J}, \qquad (717\text{-}10)$$

where α_e is an iteration effectiveness factor.

Using the cost formulation above, the apparent optimum number of inner iterations is given by satisfying

$$\frac{-dN}{NdJ} = \frac{1}{q_e+J} \quad .$$

Considering a fixed reduction in the error contribution,

$$\gamma_e^{\ N} = \text{constant}$$

$$\frac{1}{\gamma_e \ln\gamma_e} \quad \frac{d\gamma_e}{dJ} = \frac{1}{q_e+J} \ ;$$

$$\frac{d\gamma_e}{dJ} = (\gamma_e - \lambda)\ \alpha_e \ln\ (\beta-1);$$

$$(q_e + J)\ (\gamma_e - \lambda_e)\ \frac{\ln\ [(\beta-1)^{\alpha_e}]}{\gamma_e \ln\gamma_e} = 1, \qquad (717\text{-}11)$$

where γ_e is given by Eq. (717-10). These equations do not admit an explicit solution for J, but it may be determined by careful iteration. Note that we may be interested in the value of γ from Eq. (717-9) for preselection of the iteration procedures.

It may be noted that if Eq. (717-9) were applied to the individual

eigenvalues of a set of error vectors, these formulations apply with λ_e replaced in Eq. (717-10). However, this would predict that these eigenvalues move closer together as J decreases, λ_2/λ_1 decreases in the dominance ratio sense, which would tend to cause asymptotic extrapolation to be less effective, a behavior not usually found in application testing.

Representative values of γ_e as dependent on α_e and J are shown below for $\lambda_e = \lambda = 0.231$ and $\beta = 1.93091$ from Eq. (717-10).

α/J	5	10	20
2.0	.607	.415	.275
1.5	.681	.494	.321
1.0	.769	.607	.415
.75	.819	.681	.494
.5	.874	.769	.607
.25	.934	.874	.769

The apparent optimum value of J for the reference problem using $\alpha_e = 2.0$ is 8 inner iterations using $\lambda_e = \lambda$, compared with 23 for $\alpha_e = 1/3$. Quite generally both γ_e and the apparent optimum value of J decrease as α_e increases. If J is to be reduced, λ_e must be increased rather than decreased which would seem more realistic.

A few representative values of the apparent optimum J are

shown below for iteration effectiveness factor $\alpha_e = 2.0$ and cost factor $q_e = 2.0$:

β/λ_e	.2	.5	.8	.9
1.5	2.2	1.8	1.6	1.5
1.8	3.9	3.0	2.6	2.5
1.9	6.5	4.8	4.1	3.9
1.95	10.2	7.3	6.1	5.9

Reducing α_e to 1.0 and increasing q to 3.0 yields:

β/λ_e	.2	.5	.8	.9
1.6	4.1	3.2	2.8	2.7
1.8	7.1	5.4	4.7	4.5
1.9	11.6	8.5	7.2	6.9
1.95	18.2	13.0	10.8	10.3

Quite generally we find that the optimum number of inner iterations is small except when β is very large or when many iterations are required to effect propogation across the space mesh. The optimum with Chebyshev acceleration on outer iteration is apparently not well defined. Whereas in many instances of implementation a large number of inner iterations is automatically set to protect against contamination of the outer iteration process, we have chosen to adopt a procedure which generally is relatively effective when fewer inner iterations are done. It is true that the higher the cost of outer iteration relative to inner and the more the

effect of truncation of inner iteration, especially impact on effective acceleration, then the use of more inner iterations is best.

Inner Iteration Error Reduction

If the error contribution associated with inner iteration has the form

$$E(\beta,J) = A(\beta-1)^{\alpha J}, \tag{717-12}$$

where A and α are constants, then the number of inner iterations required to reduce this error from its initial value to a set, relative level, is given by proportionality with some factor X,

$$J = \frac{X}{\ln(\beta-1)} . \tag{717-13}$$

Other estimates of the contribution, as from the dominant inner iteration error vector, lead to other formulations.

Considering the contribution at any energy group, the reduction can be made the same as that at the group where the overrelaxation coefficient is the largest by requiring

$$J_g = J_{max} \frac{\ln(\beta_g-1)}{\ln(\beta_{max}-1)} . \tag{717-14}$$

Propogation

A reliable solution to a problem can not be assured unless the number of sweeps of the equations causes full propogation. Indeed we find that given L sweeps to effect propogation, from one to four times this number of sweeps are required. This places the minimum number of required sweeps at about

$$NJ \geq 2.5L, \tag{717-15}$$

where

$$L \simeq \begin{cases} R + P-1, \text{ normal ordered,} \\ \frac{R}{2} + P, \text{ partial } \sigma_1 \text{ ordered,} \\ \frac{1}{2}(R + P), \ \sigma_1 \text{ ordered.} \end{cases}$$

To reduce the contribution from only one error vector having an eigenvalue of γ by a factor of .01 in the sense of

$$\gamma^N = 0.01,$$

and set a minimum value on N of 15, then

$$J \geq \frac{2.5L}{\max\left[15, \frac{\ln .01}{\ln\gamma}\right]} \quad . \tag{717-16}$$

Note that γ must be an effective value which accounts for the gain from Chebyshev acceleration or asymptotic extrapolation, or the level of error contribution reduction be reduced accordingly. More iterations may be required to effect propogation than to reduce the error contribution, Eq. (717-16) vs Eq. (717-14).

It may be of interest that we have observed that sometimes changes which cause β to increase tend to reduce λ (or γ).

Concluding Remarks

The procedures in the VENTURE code tend to be most effective if 4 or more inner iterations are done, or if 1 inner iteration is done. We have sought evidence that an odd number of inner iterations would be more or less effective than an even number, but have found none. For a wide range of problem types representative of application, we have found that

the use of 4 inner iterations is more effective than 5 or more, unless there is a severe penalty from the cost of an outer iteration (high relative cost). This penalty tends to increase as the number of groups increases (more scattering calculation involved), and as the amount of data transfer increases, especially if relative cost of data transfer is high or the impact from the associated increase in clock time is a real penalty in application (increasing turn-around or limiting computer availability for such application).

END OF SECTION

Section 718: Initialization

This section discusses the procedures implemented to initialize a neutron flux eigenvalue problem. The objectives here are to

1. Provide a reasonable flux guess which hopefully has the error vectors with largest eigenvalues suppressed,
2. Select from the implemented procedures a set which appears the best considering computation cost, and
3. Initialize the iteration parameters at values expected to effect a rapid rate of convergence toward a solution.

An existing set of the flux values may be available for use. It could be the solution for a similar problem. Situations are known for which seemingly small changes in a system cause the solution for another problem to be a poor starting point, as when control rods are repositioned. However, considerable reduction in computation time is associated with use of the previous solution to start each problem for discrete step depletion calculations. The capability is incorporated to perform a linear interpolation of the flux values when a finer mesh point description is presented; this expansion from a coarse-mesh result is appropriate only if the number of mesh points has been increased regularly along any one coordinate (for example, doubled along each coordinate, or each two replaced by three).

On user or control module option, the flux values are recovered from an available flux file, initialized as described below, or set equal. Generally for an adjoint problem, the flux values in all groups are set equal to the available regular flux values for the first energy group. The one-dimensional procedure discussed below is not used when there is only one group. It is not used if there are less than 144 space points and the problem to be solved will be contained in memory,

but rather the overrelaxation coefficients are set with the default procedures and only one inner iteration is done at each group.

Also, for successive accesses of the neutronics code in the computation system after the first access, certain data is automatically saved and recovered which eliminates the need to apply the initialization calculations. Flux values are recovered from the appropriate interface file RTFLUX and overrelaxation coefficients and Chebyshev acceleration data are saved and recovered on the end of file RZFLUX.

Use of a One-Dimensional Problem

The recommended initialization procedure involves solution of a one-dimensional problem selected from the multidimensional mesh. A zone (of uniform nuclear properties) is selected on the basis of

$$\max V_z \sum_{g=\frac{G}{2},\min 2}^{G} \nu\Sigma_{f,g} \quad , \tag{718-1}$$

a dominant fuel zone. A mesh point is found which lies in this zone and on a row which is away from zero flux or nonreturn boundaries (near reflected boundaries or toward the middle). The multidimensional coupling coefficients are adjusted for this row to delete the coupling terms with points on neighbor rows. Complicated boundary conditions are replaced with simple ones (e.g., repeating with reflected). Black absorber points are eliminated simply by setting the coupling coefficients equal to that for the nearby point outside of the black absorber zone. (A sink here might be added to improve the flux solution.)

The procedure involves

1. A direct buckling search to effect a near critical situation,
2. Inner iteration on the space problem at each group with no source, point relaxation, to predict inner-iteration behavior, and
3. Continued outer iteration to produce data about the outer iteration process and a reasonable initial flux distribution.

The criticality search calculation is done with simultaneous solution of the flux values along the row at each iteration. An absorption cross section contribution is included in the total loss coefficient at each point after each outer iteration, as indicated to be necessary from an overall neutron balance with constraint applied during the first few iterations (see discussion about criticality searches). This iterative problem is terminated at a relatively low convergence level, 0.1 relative change in the search eigenvalue.

The first outer iteration of the direct buckling search procedure, inner iteration is done at each group with simple point relaxation using newly calculated values as available, σ_1 ordered to accelerate asymptotic behavior, with the source term set equal to zero. (Experiments using the actual source showed that estimates of the error vector eigenvalues were often unreliable when produced from an L_1 norm estimate, when the source problem is solved, often low as would be expected if the error vector dominating asymptotically has a small coefficient and is thereby suppressed.) The matrix formulation of the nonsource problem is

$$(D - L - U)\phi = 0 \ ,$$

where ϕ is the flux vector. With partitioning consistent with the process,

$$(D - L)\phi_n = U\phi_{n-1}$$
$$\phi_n = (D - L)^{-1}U\phi_{n-1} \;;$$
$$\phi_n = E\phi_{n-1} \;,$$

where ϕ_n is the flux vector at iteration n. (With σ_1 ordering, E has zero entries associated with the contribution from the odd ϕ_{n-1} values.) Assuming that independent error vectors contribute to selected point values (say the even points), since $\phi_n \to 0$ as $n \to \infty$, over these selected points,

$$\phi_{i,n} - \phi_{i,\infty} = \phi_{i,n} = \sum_j C_{i,j}\,\lambda_j^n$$

$$\phi_{i,n} = \lambda_{jmax}^n \sum_j C_{i,j}\left(\frac{\lambda_j}{\lambda_{jmax}}\right)^n \;, \qquad (718\text{-}2)$$

i being a mesh point, n the iteration count, and λ_{jmax} the largest eigenvalue of the error vectors. Thus at point i,

$$\frac{\phi_{i,n}}{\phi_{i,n-1}} = \lambda_{jmax}\,\frac{\sum_j C_{i,j}\left(\frac{\lambda_j}{\lambda_{jmax}}\right)^n}{\sum_j C_{i,j}\left(\frac{\lambda_j}{\lambda_{jmax}}\right)^{n-1}} \to \lambda_{jmax},\ \text{n large} \;;$$

$$\frac{\sum_i|\phi_{i,n} - \phi_{i,n-1}|}{\sum_i|\phi_{i,n-1} - \phi_{i,n-2}|} = \lambda_{jmax}\,\frac{\sum_i\left|\sum_j C_{i,j}\left(\frac{\lambda_j}{\lambda_{jmax}}\right)^n\left(1-\lambda_j^{-1}\right)\right|}{\sum_i\left|\sum_j C_{i,j}\left(\frac{\lambda_i}{\lambda_{jmax}}\right)^{n-1}\left(1-\lambda_j^{-1}\right)\right|} \to \lambda_{jmax},\ \text{n large; and}$$

$$\frac{\sum_i (\phi_{i,n})^2}{\sum_i (\phi_{i,n}\phi_{i,n-1})} = \lambda_{jmax} \frac{\sum_i \left[\sum_j C_{i,j} \left(\frac{\lambda_j}{\lambda_{jmax}}\right)\right]^2}{\sum_i \left[\sum_j C_{i,j} \left(\frac{\lambda_j}{\lambda_{jmax}}\right)^n\right]\left[\sum_j C_{i,j} \left(\frac{\lambda_j}{\lambda_{jmax}}\right)^{n-1}\right]} \to \lambda_{jmax}, \text{ n large.}$$

The following estimates of this largest eigenvalue are readily available:

$$\lambda_{1,n} = \min \frac{\phi_{i,n}}{\phi_{i,n-1}} ,$$

$$\lambda_{2,n} = \max \frac{\phi_{i,n}}{\phi_{i,n-1}} ,$$

$$\lambda_{3,n} = \frac{\sum_i |\phi_{i,n} - \phi_{i,n-1}|}{\sum_i |\phi_{i,n-1} - \phi_{i,n-2}|} , \text{ and}$$

$$\lambda_{4,n} = \frac{\sum_i \phi_{i,n}^2}{\sum_i \phi_{i,n}\, \phi_{i,n-1}} . \qquad (718\text{-}3)$$

Currently we estimate the eigenvalue from

$$\lambda_n = [\lambda_{2,n}\, \lambda_{3,n}\, \lambda_{4,n}]^{1/3} , \qquad (718\text{-}4)$$

not using the first estimate above because it typically is a gross underestimate. Convergence criteria is required to be satisfied,

$$\lambda_n < 0.9999 ,$$

$$0.995 < \frac{\lambda_n}{\lambda_{n-1}} < 1.005 ,$$

$$0.995 < \frac{\lambda_{n-1}}{\lambda_{n-2}} < 1.005 .$$

Often in the early iterative history there are many point values which do not change ($\lambda_{2,n} = 1$); there are no source terms at the first energy group for the points in a reflector. To force full propagation we require a miminum number of iterations equal to half the number of points on a row. Typically the asymptotic value is approached from above by $\lambda_{2,n}$ but from below by $\lambda_{3,n}$ and $\lambda_{4,n}$; since the latter two are generally more accurate estimates than the former, the weighting used is reasonable.

When convergence criteria are not satisfied, the process is terminated if the iteration count becomes four more than the number of points on a row or any $\phi_{i,n} < 10^{-30}$. The latest estimate of λ_n will then be used provided three successive values are approaching a solution monotonically,

$$\lambda_{n-2} < \lambda_{n-1} < \lambda_n \quad \text{or} \quad \lambda_n < \lambda_{n-1} < \lambda_{n-2} \text{ , and}$$

$$|\lambda_n - \lambda_{n-1}| < |\lambda_{n-1} - \lambda_{n-2}| \text{ .}$$

If acceptable estimates are not found for at least half of the space problems at each group, the default procedure discussed later is used. Otherwise an unacceptable value due to the iterative behavior is replaced by that obtained for the next lower numbered group. The overrelaxation coefficients are set initially to

$$\beta_o(g) = \frac{2}{1 + \sqrt{1 - \mu_L^2 (g)}} \text{ ,} \qquad (718\text{-}5)$$

where μ_L is determined as follows, independently at each group.

Let $\rho = \lambda_n$ from the one-dimensional calculation. Setting $X = \cos^{-1}\rho$, values of parameters are chosen,

$$\alpha_1 = \begin{cases} \dfrac{X}{1.2} \text{ if reflected on only one side,} \\ X \text{ otherwise,}^a \text{ and} \end{cases}$$

$$\alpha_2 = \begin{cases} 1.2\alpha_1 \text{ if reflected only top or bottom,} \\ \alpha_1 \text{ otherwise.}^a \end{cases}$$

In triagonal geometry if 1.5 times the number of rows < the number of columns, this value of α_2 is multiplied by 1.50, except when there is rotational symmetry.

For two dimensional problems the eigenvalue is estimated as

$$\mu_J = \frac{\cos \alpha_2}{2 - \cos \alpha_1}. \tag{718-6}$$

For three dimensional problems, a third parameter is chosen,

$$\alpha_3 = \begin{cases} 1.2\alpha_1 \text{ if reflected only front or back,} \\ \alpha_1 \text{ otherwise,} \end{cases}$$

and the associated eigenvalue estimated,

$$\mu_J = \max \left[0.74536, \frac{\cos \alpha_2 + \cos \alpha_3}{3 - \cos \alpha_1} \right]. \tag{718-7}$$

If the number of groups exceeds 5, the eigenvalue estimate used to calculate the overrelaxation coefficient is

$$\mu_L = \mu_J; \quad \text{otherwise } \mu_L = \frac{2\,\mu_J}{1 + \mu_J}.$$

Next, outer iteration is done on the usual eigenvalue problem normalizing the fission source each iteration to its value the previous one. Flux values are obtained at each group for the row simultaneously, and

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[a]Or if reflected on one side and there is rotational symmetry.

the eigenvalue of the dominating error vector is estimated by the L_1 norm,

$$\gamma_n = \frac{\sum_i |\phi_{i,n} - \phi_{i,n-1}|}{\sum_i |\phi_{i,n-1} - \phi_{i,n-2}|} \quad . \tag{718-8}$$

This eigenvalue is required to satisfy the same criteria as given above for the inner iteration process on λ_n.

The one-dimensional multigroup flux solution is used for initialization along rows. A separable flux distribution is assumed and the distribution for the row is normalized to unity at a selected point and adjusted to the mesh and boundary conditions for the second coordinate, the square roots of the values are taken for this second traverse, and the two-dimensional values calculated in the sense of $\phi(x,y) = \phi(x)\phi(y)$ at each energy. Normally a cosine distribution is used across planes for three-dimensional problems as discussed below with account of the boundary conditions.

In the event that a solution is not obtained for a selected one-dimensional problem as discussed above, cosine flux distributions are used as follows. The flux distribution is assumed to be separable in the sense of

$$\phi(g,r) = A(g)\ B(x)\ C(y)\ D(z) \ , \tag{718-9}$$

where $\phi(g,r)$ is the flux guess for energy group g and space location r, A(g) is determined by applying a neutron balance to a point selected in the dominant fuel zone,

$$T(g)\ A(g) = \chi(g) + \sum_{g'} S(g')\ A(g') \ , \tag{718-10}$$

where T(g) is the loss term for the group including a buckling loss arbitrarily with $B_\perp^2$ set to 0.01; $\chi(g)$ is the fission source distribution

(i.e., a unit source distributed), and S(g) is the inscattering cross section. B(x), C(y), and D(z) are determined for the individual coordinate directions by the relationship,

$$B(x) = \cos\left[\frac{0.8\pi\ (X - X_o)}{2L}\right], \tag{718-11}$$

where X is the distance from the boundary as follows:

Boundary Conditions (Left, Right)	L	X_o
Reflected, Reflected[a]	(Not used)	(Not used)
Reflected, Extrapolated[b]	width	0
Extrapolated, Reflected	width	width
Extrapolated, Extrapolated	half-width	half-width

[a]Or repeated.
[b]Nonreturn or zero flux.

When a fixed source contains negative terms, the above procedure is replaced. The flux values are set equal to the fixed source values except that where the source is zero, a small value is assigned to the flux to avoid conflict with the identification of internal black absorber points with zero flux values.

The Default Procedure for Initialization of Acceleration Parameters

On user option or under special conditions such as failure of the one-dimensional problem initialization procedure, a default initialization procedure is used. An estimate of the inner iteration problem spectral radius is needed for selection of an overrelaxation coefficient,

$$\beta_o(g) = \frac{2}{1.0 + \sqrt{1.0 - \mu(g)^2}} \ . \tag{718-12}$$

An eigenvalue is calculated for an ideal mesh along each coordinate for a uniform mesh homogeneous problem based on half of the mesh points to compensate for a sink term contribution,

$$\mu_j = \cos\left\{\frac{\pi}{\alpha_j N_j}\right\}, \tag{718-13}$$

where j refers to a coordinate direction; N_j is the number of mesh intervals; and α_j depends on the boundary conditions: 0.5 for zero flux or nonreturn (extrapolated) boundaries associated with this coordinate, 1.0 if one boundary is reflected, or 1.5 if both are reflected, but μ_j is then set max (μ_j, 0.995) except for the first coordinate direction.

For line overrelaxation along the first coordinate direction, the "ideal" eigenvalue is estimated as

$$\mu_L = \frac{\sum_{j=2}^{J} \rho_j}{J - \rho_1}, \tag{718-14}$$

where J is the number of coordinates, 2 or 3. Note that for the one-dimensional problem with line relaxation, $\mu_L = 0$, the optimum overrelaxation coefficient is unity, and overrelaxation is not done.

To allow for dependence on the relative magnitudes of the leakage constants and the total loss term in the finite-difference formulation, an internal mesh point location is selected where the product of the volume and $\nu\Sigma_f$ is largest, and the estimate of the eigenvalue is adjusted by

$$\rho(g) = \max \left[\lambda_G \left\{ \frac{1.0}{1.0 + \frac{C_{R,i}(g)}{\sum_s C_{s,i}(g)}} \right\}, 0.74536 \right] , \qquad (718\text{-}15)$$

where $C_{R,i}(g)$ is the total loss constant (the finite-difference-element volume times the total cross section for outscatter and absorption plus the buckling loss term, mesh point i), and $C_{s,i}(g)$ refers to the leakage constant associated with a surface of the element for that energy group. Equation (718-13) is not used if the overrelaxation coefficients are fixed at a single value.

The eigenvalue estimates obtained from Eq. (718-15) are arbitrarily adjusted as follows

$$a = \min \left\{ (g) \right\},$$

$$b = 1.0 - \sqrt{1.0 - \lambda_G} ,$$

$$c = \max \rho(g) ,$$

$$f = \begin{cases} c, & c > b , \\ \frac{1}{2}(\lambda_G + b), & c \leq b . \end{cases}$$

Then only if $a < b$,

$$\rho^1(g) = b + \left[\frac{f - b}{c - a} \right] \left[\rho(g) - a \right] . \qquad (718\text{-}16)$$

Setting the Number of Inner Iterations

Information was presented in the previous section regarding the dependence of the outer iteration eigenvalue on the difficulty of the inner iteration process. However, our testing has not produced

a generally acceptable optimizing formulation has not been found. We still find problems where the Chebyshev acceleration procedure on outer iteration causes the iteration process to be non-convergent even if many inner iterations are done, and the class of problems for which this is the situation has not been simply identified. Presented here is the procedure for selecting the number of inner iterations in use for the current release version of the code. We continue a study of the requirements and expect to improve this procedure given more experience with results from wide application. In the mode of data handling required to solve large three-dimensional problems, it is most desirable to preselect the number of inner iterations to be done. The impact of increasing the data transfer to do more inner iterations is not simply assessed. The user should be aware that this procedure causes the number of inner iterations to increase as the number of neutron groups increases, and more memory is needed to contain sufficient planes of data to minimize data transfer as the number of inner iterations is increased.

Unless overridden by input instructions, the number of inner iterations is set as follows:

$$\text{Let } I_{max} = \min\left[20, \frac{L_n}{4}\right] ,$$

$$I_{min} = \max\left[4, \frac{L}{10}\right] ,$$

where L_n is the number of inner iterations required to sweep the boundary conditions across the problem with normal ordering, and L is the number of inner iterations required to sweep the boundary conditions across the

problem with the ordering to be used (normal, partial σ_1 or σ_1, discussed earlier). Thus we seek propagation in 10 outer iterations except for the largest problems.

For that group having the largest overrelaxation coefficient, an initial estimate of the number of inner iterations is set at

$$I_1 = \min\left[I_{max}, \max\left(I_{min}, 1 - \frac{A}{\ln(\beta(g)-1)}\right)\right], \qquad (718\text{-}17)$$

Where A is assigned a value as follows:

Chebyshev acceleration to be done	No	Yes
No upscatter	0.8	1.5
With upscatter	0.48	0.9

Since the cost penalty of outer iteration relative to inner iteration generally increases as the number of groups increases, the reference initial inner iteration estimate is adjusted by the following formulation to approximate an economic optimum:

$$I_2 = \min\left(20, I_1\left[\max\left(1.0, \left\{\frac{B}{3}\right\}^{0.2}\right]\right)\right), \qquad (718\text{-}18)$$

where B is the maximum downscatter band in groups.

This value may be reduced by one if this significantly reduces the amount of data transfer.

Then at each group, the number of inner iterations is set at

$$J(g) = \min\left[\frac{I_{max}}{2}, \max\left(I_{min}, \frac{I_2 \ln(\beta_{max}-1)}{\ln(\beta(g)-1)}\right)\right], \qquad (718\text{-}19)$$

except that J is set to unity for one-dimensional problems, and also for all others for which the total number of space, energy mesh points < 144 provided that the problem will be solved in the all data stored mode.

Outer Iteration Limit

Generally the user is expected to supply a maximum number of outer iterations which causes termination of the iteration process when the iteration count reaches this value. When no value is supplied, an estimate is provided and used by the code. It is not usually a conservatively high estimate, but rather a reasonable estimate given the available information. The estimate is as follows which may be useful for estimating computation cost, especially given additional information from the requirements for a class of problems of interest:

$$N = \max\,(20,\ -A\,\ell n\varepsilon_\phi),$$

$$\text{where } A = \max\,(1.5,\ \frac{L}{5I},\ \frac{-1}{\ell n\mu}),\qquad (718\text{-}20)$$

$$\mu = \max\,\left[(\beta_{max}-1)^{J/4},\ \gamma\right],$$

$$\gamma = \begin{cases} \lambda \text{ without Chebyshev acceleration,} \\ \left[\frac{1}{\lambda}\,(2-\lambda-2\sqrt{1-\lambda}\,)\right]^{0.4} \text{ otherwise,} \end{cases}$$

N = maximum number of outer iterations,

J = maximum number of inner iterations,

I = minimum number of inner iterations,

L = number of iterations required to effect full propagation,

ε_ϕ = specified maximum relative flux change on outer iteration,

λ = estimated dominant outer iteration error vector eigenvalue with normal ordered sweeps, and

β_{max} = maximum overrelaxation coefficient.

Data not applicable or not available is dropped out (L/I is set to zero for one-dimensional problems). Note that the default to one inner iteration for small problems will cause more outer iterations to be required than if several inner iterations were done, perhaps requiring a larger maximum to be specified than typical. Also, the special input data processor for data for the VENTURE code yet sets the value of N = 50 if input 0.

END OF SECTION

Section 720: Reliability of Solution

A solution obtained by an iterative process is generally not entirely converged. It is uneconomical to satisfy tight convergence criteria. Therefore, the user relaxes the criteria to the extent possible which will still cause the result to satisfy the particular needs. Unfortunately, a simple measure of the reliability of a solution is not directly available from the iterative results. A satisfactory measure of reliability is, however, of critical importance.

If the inner iterations were continued enough times, the flux ϕ_{n+1} in Eq. (716-1) would satisfy the relationship in Eq. (720-1) provided there were no upscatter:

$$\phi_{n+1} = R\phi_{n+1} + \frac{1}{k_n} \chi F \phi_n \text{ , or} \tag{720-1}$$

$$(I - R)\ \phi_{n+1} = A\ \phi_{n+1} = \frac{1}{k_n} \chi F\ \phi_n \ .$$

The process could now be written as

$$\Psi_n = \chi F \phi_n \ ,$$

$$\Psi_{n+1} = \frac{1}{k_n} M\ \Psi_n \ .$$

Under this condition, bounds on k_e can be identified and calculated as simply the maximum and minimum ratios of the source, components of Ψ, between outer iterations, times k_n. Use has been made of these bounds, especially in the PDQ series of codes.[a] Unfortunately, the bounded range tends to be wide at low levels of convergence, and relaxation of the

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[a]W. R. Cadwell, WAPD-TM-179.

inner iteration convergence destroys the proof that the estimates are bounds. Only with a relatively large number of inner iterations does one have assurance that bounds have been identified. The optimum number of inner iterations for problem solution, considered here to minimize the computation cost, may be far fewer than are required to insure that bounds on the eigenvalue are established. Thus, we seek an alternative measure of reliability.

The Maximum Relative Flux Change

The iterative process, Eq. (716-1), may be described as

$$\phi_{n+1} = M_n \phi_n \ , \tag{720-2}$$

where the flux vector from outer iteration n is operated on by the iteration matrix M_n to generate the new estimate. The iteration matrix M is iteration dependent because it contains the latest estimate of k_e. Bounds on the largest eigenvalue or spectral radius of M can be calculated.[a] Consider the set of components of the flux vector ϕ to be X_i, and the elements of M to be a_{ij}. Now consider the new matrix formed of the elements

$$b_{ij} = a_{ij} \frac{X_j}{X_i} \ .$$

The new matrix is the result of performing the operation $P^{-1}MP$; therefore, it is similar to the matrix M and has the same eigenvalues. The spectral radius of this new matrix is bound by the maximum and the minimum of sums along columns or rows. The sum along a row is simply the ratio of flux values at one point between outer iterations.

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[a]Due to M. L. Tobias, unpublished.

Therefore

$$\min\left(\frac{X_{i,n}}{X_{i,n-1}}\right) \leq \rho(M_n) \leq \text{maximum}\left(\frac{X_{i,n}}{X_{i,n-1}}\right) . \tag{720-3}$$

Since $\rho(M_n)$ must tend to unity, an indication that the iterative process is convergent is that

$$|\varepsilon_{\phi,n}| < |\varepsilon_{\phi,n-1}| , \tag{720-4}$$

where

$$\varepsilon_{\phi,n} = |\max| \frac{X_{i,n} - X_{i,n-1}}{X_{i,n-1}} . \tag{720-5}$$

Further, $\rho(M_n)$ is bounded by $1 \pm |\varepsilon_{\phi,n}|$. There is not a one to one correspondence between bounds on k_n and on $\rho(M_n)$ because of the way k_n appears in M. However, a reasonable estimate of the probable uncertainty in k_n is

$$k_n\left(1 \pm |\varepsilon_{\phi,n}|\right) . \tag{720-6}$$

Occasionally, a result falls outside of this range, so it should be interpreted as an approximate bound, perhaps two standard deviations. Increasing the number of inner iterations generally increases the reliability of this bound, excluding the upscattering problem.

The VENTURE code tests $\varepsilon_{\phi,n}$ against a specified convergence criterion as the primary way an acceptable solution is identified and the iteration process is discontinued. Thus, if the estimated k is desired to within 0.01 percent, the criterion on the convergence of the point fluxes should be 0.0001. Quite generally a value of 0.00005 is

recommended for wide use, a smaller value when necessary, and a larger value for situations where a lower degree of convergence is acceptable.

At the time this is written, it appears that the penalty associated with reaccess and/or storing away a copy of the iterate flux set for each iteration as necessary to determine the maximum relative point flux change is not justified. As an alternative, each reevaluated point flux may be tested and the maximum for that inner iteration determined. Thus, at one energy g, outer iteration n and inner iteration m, we calculate

$$r_{g,n,m} = \max \left(\frac{X_{i,n,m}}{X_{i,n,m-1}} \right) , \text{ and}$$

$$S_{g,n,m} = \min \left(\frac{X_{i,n,m}}{X_{i,n,m-1}} \right) ;$$

by group g for outer iteration n, inner iteration m.

Then over the inner iterations, taking

$$p_{g,n} = \prod_m r_{g,n,m} \quad , \text{ and}$$

$$q_{g,n} = \prod_m s_{g,n,m} \quad ,$$

and finding the maximum over all g,

$$w_n = |\max|(p_{q,n} - 1,\ q_{g,n} - 1) \ ,$$

$$|w_n| \geq |\varepsilon_{\phi,n}| \ .$$

Thus the convergence property tested by $\varepsilon_{\phi,n}$ is also tested by w_n. Experience with its use indicates that $|w_n| >> |\varepsilon_{\phi,n}|$ during the early

iterative history, but usually approaches its value by that stage of the calculation when the convergence level is low enough to terminate the process.

It should be noted that the discussion above is directed at the reliability of a solution regarding the error due to lack of convergence of the iterative process, not the error associated with the finite-difference approximations, the use of diffusion theory, or the discrete energy group representation.

The Residues Estimate

An independent measure of reliability is also available unless overridden by user. The value of the multiplication factor is determined which minimizes the sum of the squares of the residues of the point neutron balance equations cast in the form of actual reaction rates. The residue R_i is defined as

$$R_i = \frac{1}{k_r} F_i + S_i - T_i \ , \tag{720-7}$$

where R_i is the residue which would be zero if the problem were completely converged, F_i is the associated fission source, S_i is the inscattering plus inleakage term, and T_i is the total removal and outleakage term. Each of the above terms is evaluated with the solution flux vector components. Summing equations and determining

$$\frac{\partial}{\partial k_r} \sum_i R_i^2 = 2 \sum_i R_i \frac{\partial R_i}{\partial k_r} = 0 \ ,$$

$$k_r = \frac{\sum_i F_i^2}{\sum_i F_i (T_i - S_i)} \ . \tag{720-8}$$

Experience has shown the residues estimate of the multiplication constant to be quite useful, especially when a problem solved has an unfamiliar iterative behavior. If the residues estimate differs markedly from the value used in the iterative process, then the problem is not converged.

The analyst wants to know the best estimate of the multiplication factor for a problem, especially of concern when convergence criteria has been relaxed. Results from a wide range of problems indicate that the residues estimate is often not superior to that from the neutron balance used in the calculation. We suggest simply averaging the two values.

In some situations, even the residues estimate of k_e will not reflect lack of convergence, one case being that where the flux is quite flat over much of the system. The point neutron balance equations are used at each space-energy point having fission source to yield independent bounds on k_e

$$\frac{1}{k_b} F_i + S_i = T_i$$

$$k_b = \frac{F_i}{T_i - S_i} , \qquad (720\text{-}9)$$

and maximum and minimum values of k_b are determined as bounds. Unfortunately, in most situations there are locations where the magnitude of F_i is small relative to S_i, due either to small values of the macroscopic production cross sections ($\nu\Sigma_f$) or a small distribution factor, causing the bound estimates to be uselessly wide. For more useful estimates we restrict the test to locations and energy groups

where $F_i/S_i > 0.0001$ if $S_i > 0$. Since S_i is zero for the first energy group, all of the first-group equations are always considered. A user must rely on experience in assessing the results of such tests.

Premature Termination

The iterative process may be terminated before an acceptable convergence level is achieved. The outer iteration count may reach the limit allowed. Continuation is generally not allowed in the event of machine error, as in data transfer, because an unreasonable amount of time may be required for recovery from such error. An attempt at division by zero or exponential underflow or overflow are deemed fatal errors in this program.

Another mode of automatic termination has recently been implemented. The number of block data transfers required for a full outer iteration is determined. The number yet allowed before termination by the operating system (as dependent on the job control instructions and past usage) is accessed and termination initiated if less than 4 outer iterations would cause system termination, or 12 if the perturbation integrals are to be done. The residues sweep of the equations is made and wrap-up procedures followed regarding the calculation of derived results and writing data on files. This procedure is also executed if the remaining processor time allowed for the job is inadequate for the same number of iterations, or if the user specified processor time limit for the problem (this access of the neutronics code) is exceeded.

The acceptability, reliability of results from an iterative procedure terminated prematurely must be questioned.

The Absolute Error

The responsible analyst must have some concern for the absolute error possible in a reported solution associated with lack of convergence of the iterative process. Certainly the iterative change in any integral quantity must be small if the absolute error is small. However, the multiplication factor calculated for two successive iterations may be nearly the same and yet differ considerably from a proper solution.

An indication of the absolute error is available from reported estimates of the eigenvalue of the overall iterative process which dominates asymptotic. See Section 716 for further discussion. When in this asymptotic mode, this eigenvalue μ is related to the iterate point flux values by

$$\mu = \frac{X_n - X_{n-1}}{X_{n-1} - X_{n-2}} , \tag{720-10}$$

where n refers to outer iteration, and

$$\mu = \frac{X_\infty - X_n}{X_\infty - X_{n-1}} . \tag{720-11}$$

Thus, μ is a direct measure of the absolute error reduction each iteration. Further

$$\frac{X_\infty - X_n}{X_n - X_{n-1}} = \frac{\mu}{1 - \mu} ; \tag{720-12}$$

that is, an estimate of the ratio of the absolute error to the iterative change is given directly. Given the maximum relative flux change, ε_n, the absolute error in the local flux is estimated and reported as

$$\frac{X_\infty - X_n}{X_\infty} \simeq \frac{X_\infty - X_n}{X_n} \simeq \left(\frac{\mu}{1-\mu}\right) \varepsilon_n \ , \qquad (720\text{-}13)$$

where the value of μ is that obtained the last time the single error mode extrapolation criteria was satisfied, or the upper bound estimate of the eigenvalue band when Chebyshev acceleration is done.

Since the procedure of calculation attempts to make use of this information and apply asymptotic extrapolation, reported values of μ each iteration have limited utility. However, asymptotic extrapolation is only done when it appears that an aysmptotic mode has developed. Thus, the estimate of μ at that point in the calculation is of interest, especially so if the extrapolation was effective as indicated by subsequent values of ε_n being considerably smaller than before extrapolation. In applying Eq. (720-13), the largest eigenvalue of the iterative process should be used, not a smaller one associated with the dominating error contribution at any stage of the calculation, nor any unusually large estimate of it. Note that we recommend use of the factor ε_n, which makes a primary contribution in Eq. (720-13), as the primary user control for termination of the iterative process. Tests on the iterate estimates of the eigenvalue of the problem (the multiplication factor or search problem eigenvalue) are unreliable at best, especially when acceleration schemes are used.

Finally we caution the users that full propagation of boundary conditions across a problem is essential for reliable results which requires a minimum product of the numbers of outer and inner iterations (see the discussion about sweep order in Section 716).

END OF SECTION

Section 721: Perturbation

Discussion

The equations used to estimate the effect of small changes are discussed here. First order perturbation theory is applied which is precise only in the limit of zero change. The adjoint flux is used which requires solution of this special problem. The fact that finite-difference equations must be dealt with rather than a continuum introduces complexity.

The following discussion contains an introduction cast in simple terms. This is intended to help the reader who desires to understand the subject from a practical standpoint. Then the actual equations used in the code are presented. A theoretical analysis has been presented.[a]

Consider a neutron balance associated with the finite-difference volume about a mesh point for a one-energy-group, one-dimensional slab geometry problem. With usual terminology,

Source = Removal + Leakage, or

$$\frac{1}{k}\,\nu\Sigma_{f,i}\,V_i\,\phi_i = \Sigma_i V_i \phi_i + D_i A_i \left[\left(\frac{\phi_i - \phi_{i-1}}{\Delta_{i/2}}\right) + \left(\frac{\phi_i - \phi_{i-1}}{\Delta_{i+1/2}}\right)\right] , \qquad (721\text{-}1)$$

where i refers to a location, V refers to volume, A to the leakage surface, and Δ to mesh spacing. Let $\Delta_{i+1} = \Delta_i$.

A change in the nuclear properties would change the flux distribution and also the multiplication factor. Let us neglect the change in flux and consider the partial derivative of terms of Eq. (721-1) with respect to Σ_i. This operation gives

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[a]Melvin Tobias, T. B. Fowler and D. R. Vondy, "First-Order Perturbation Theory as used in the Multigroup Diffusion Code EXTERMINATOR-2," USAEC Report, ORNL-TM-1741 (January 1967).

$$\nu \Sigma_{f,i} V_i \phi_i \frac{\partial(\frac{1}{k})}{\partial \Sigma_i} = V_i \phi_i .$$

Considering change in Σ_i only at certain points within some material m and summing equations gives

$$\frac{\partial(\frac{1}{k})}{\partial \Sigma_m} \sum_i \nu \Sigma_{f,i} V_i \phi_i = \sum_{j \varepsilon m} V_i \phi_i .$$

Since $\partial(\frac{1}{k}) = -\frac{1}{k^2} \partial k$,

$$\frac{1}{k} \frac{\partial k}{\partial \Sigma_m} = \frac{-\sum_{i \varepsilon m} V_i \phi_i}{\frac{1}{k} \sum_i \nu \Sigma_{f,i} V_i \phi_i} .$$

If we simply accept that Eq. (721-1) may be multiplied through by a weighting factor, namely the adjoint flux, ϕ_i^*, which will cause both $\phi_i \phi_i^*$ and the flux slope in the leakage terms to be invariant, increasing the accuracy, then the result becomes

$$\frac{1}{k} \frac{\partial k}{\partial \Sigma_m} = \frac{-\sum_{i \varepsilon m} V_i \phi_i \phi_i^*}{\frac{1}{k} \sum_i \nu \Sigma_{f,i} V_i \phi_i \phi_i^*} . \qquad (721\text{-}2)$$

This expresses the change in the multiplication factor associated with a unit change in the cross section. Similarly

$$\frac{1}{k} \frac{\partial k}{\partial D_m} = \frac{-\sum_{i \varepsilon m} \frac{2 A_i}{\Delta_i} \left[(\phi_i - \phi_{i-1}) + (\phi_i - \phi_{i+1}) \right] \phi_i^*}{\frac{1}{k} \sum_i \nu \Sigma_{f,i} V_i \phi_i \phi_i^*} . \qquad (721\text{-}3)$$

Also,

$$\frac{1}{k}\frac{\partial k}{\partial(\nu\ \Sigma_{f,m})} = \frac{-\sum_{i\varepsilon m} V_i\ \phi_i\ \phi_i^*}{\sum_i \nu\ \Sigma_{f,i}\ V_i\ \phi_i\ \phi_i^*}\ , \qquad (721\text{-}4)$$

where the region of interest m must be for $\nu\ \Sigma_{f,i} \neq 0$. Complications associated with material interfaces have been avoided here, and the equations must be extended to consider more than one group and other dimensions, and to treat the trans-group scattering.

Once the changes due to changes in macroscopic cross sections have been determined, the effects of nuclide density changes may be obtained, but not in the VENTURE code. Adding contributions gives

$$\frac{\partial k}{\partial N_b} = \sum_m \left\{ \left[\sum_j \frac{\partial k}{\partial \Sigma_{j,m}} \frac{d\ \Sigma_{j,m}}{d\ N_{b,m}} \right] + \frac{\partial k}{\partial D_m} \frac{d\ D_m}{d\ N_{b,m}} + \frac{\partial k}{\partial(\nu\ \Sigma_{f,m})} \frac{d(\nu\ \Sigma_{f,m})}{dN_{b,m}} \right\}\ , \qquad (721\text{-}5)$$

where $N_{b,m}$ is the density of a nuclide in region m and index j is over appropriate cross sections.

Since

$$\Sigma_{j,m} = \sum_b N_{b,m}\ \sigma_{j,b,m}\ ,\ \frac{d\ \Sigma_{j,m}}{d\ N_{b,m}} = \sigma_{j,b,m}\ ;$$

$$D_m = \frac{1}{\sum_b 3\ N_{b,m}\ \sigma_{tr,b,m}}\ ,\ \frac{d\ D_m}{d\ N_{b,m}} = -\ 3D_m^2\ \ \sigma_{tr,b,m}\ ;$$

$$\nu\ \Sigma_{f,m} = \sum_b N_{b,m}\ \nu\ \sigma_{f,b,m},\ \frac{d\ (\nu\ \Sigma_{f,m})}{d\ N_{b,m}} = \nu\ \sigma_{f,b,m}\ ;$$

$$\frac{\partial k}{k\partial N_b} = \sum_m \left\{ \left[\sum_j \left(\frac{\partial k}{k\partial \Sigma_{j,m}}\right) \sigma_{j,b,m} \right] + \left(\frac{\partial k}{k\partial D_m}\right) \left(- 3\ D_m^2\ \sigma_{tr,b,m}\right) \right.$$

$$\left. + \left[\frac{\partial k}{k\partial(\nu\ \Sigma_{f,m})}\right] \nu\ \sigma_{f,b,m} \right\} . \qquad (721\text{-}6)$$

This does assume consistent treatment over the individual zones of material. The estimate of the effect of an actual change, decreasing in accuracy as the amount of change increases, is then

$$\frac{\Delta k}{k\Delta N_b} \simeq \frac{\partial k}{k\partial N_b} . \qquad (721\text{-}7)$$

The Perturbation Equations

Within region m, the change in multiplication factor relative to change in a macroscopic property is calculated as

$$\frac{\partial k}{k\partial X_{m,n}} = \frac{\sum_{i\varepsilon m} G_i(n)}{\frac{1}{k} \sum_i V_i \sum_g \chi(m,g)\ \phi^*_{i,g} \sum_n \nu\ \Sigma_{f,n}\ \phi_{i,n}} , \qquad (721\text{-}8)$$

where $X_{m,n}$ refers to a macroscopic property in region m,i refers to a space point in geometric space and g and n to energy groups. G_i is defined below. It is assumed in this discussion that $\sum_g \chi(m,g) = 1$.

$X = \Sigma_a(n),\ \Sigma_r(n) = \sum_g \Sigma(n\to g)$, or $D(n)B^2(n)$

$$- G_i(n) = V_i\ \phi_{i,n}\ \phi^*_{i,n} \qquad (721\text{-}9)$$

$X = \Sigma(g\to n)$

$$G_i(n) = V_i\ \phi_{i,g}\ \phi^*_{i,n} \qquad (721\text{-}10)$$

$\underline{X = D(n)}$

$$G_i(n) = \sum_j A_j \begin{cases} \left[\dfrac{1}{\Delta_i + \Delta_j}\right] \phi^*_{i,n} \left[\phi_{i,n} - \phi_{j,n}\right] \text{ , internal ,} \\[2ex] \dfrac{1}{\Delta_i} \left[\dfrac{1}{1 + \dfrac{\Delta_j \; D_i(n)}{\Delta_i \; D_j(n)}}\right]^2 \left[\phi^*_{i,n} - \phi^*_{j,n}\right]\left[\phi_{i,n} - \phi_{j,n}\right] \text{ , at} \\[2ex] \text{material interfaces, or} \\[2ex] \dfrac{1}{\Delta_i}\left[\dfrac{1}{1 + \dfrac{D_i(n)}{\Delta_i C_s(n)}}\right] \phi^*_{i,n} \; \phi_{i,n} \text{ , adjacent to} \\[2ex] \text{any black boundary.} \end{cases} \tag{721-11}$$

Here j refers to each of the nearest neighboring mesh points, A_j is the normal leakage area, and Δ_i is the distance from a point to the appropriate interface between mesh points. $C_s(n)$ is the internal or external black boundary constant (see Section 702). At reflecting boundaries there is zero contribution.

$\underline{X = \nu \; \Sigma_f(n)}$

$$G_i(n) = \frac{V_i}{k} \phi_{i,n} \sum_g \chi(m,g) \; \phi^*_{i,g} \; . \tag{721-12}$$

Calculation of a temperature or power coefficient of reactivity would be done directly from the partial derivatives discussed above using additional data,

$$\frac{\partial k}{\partial P} = \sum_\ell \left[\frac{\partial k}{\partial X_\ell}\right] \frac{dX_\ell}{dP} \; ,$$

where X_ℓ refers to each contributing macroscopic property including cross sections and diffusion constants. To consider the general situation, discrete changes would have to be considered. Thus resonance calculations may be done at two temperatures representing some desired change, and the generated microscopic data used in the form:

$$\frac{1}{k}\frac{\partial k}{\partial P} = \sum_\ell \frac{\partial k}{\partial X_\ell}\left[X_\ell(P_1) - X_\ell(P_2)\right] , \tag{721-13}$$

where $X_\ell(P_1)$ refers to a macroscopic cross section determined from initial nuclide densities and the originally specified microscopic cross sections; $X_\ell(P_2)$ refers to the altered value due to specified changes in nuclide densities and new microscopic data.

Importance maps over space may be obtained. "Importance" is used here to mean the contribution to the multiplication factor per unit volume from some factor, namely

$$I_i(c) = \frac{\sum_\ell X_{\ell,i}\ (c)\ \phi_i\ \phi_i^*}{\frac{1}{k}\sum_i \nu\ \Sigma_{f,i}\ V_i\ \phi_i\ \phi_i^*} , \tag{721-14}$$

for the one-group situation treated above, where i represents a mesh point location and the contribution from component c to the macroscopic cross section X on a unit volume basis is shown to be given the flux times adjoint weighting.

Prompt Neutron Lifetime

For the estimate of the prompt neutron lifetime, the weighting is of reciprocal neutron velocity, Eq. (721-15) applies

$$\ell = \frac{\sum_n \sum_i \frac{V_i}{v(n)}\ \phi_{i,n}^*\ \phi_{i,n}}{\frac{1}{k}\sum_i V_i \sum_g \chi(m,g)\ \phi_{i,g}^* \sum_n \nu\ \Sigma_{f,n}\ \phi_{i,n}} . \tag{721-15}$$

Results Produced

Given forward and adjoint flux solutions, the derivatives of k with respect to each macroscopic (zone) cross section are calculated and edited, Eqs. (721-9) through (721-12) above. No calculations are done which require reaccess of microscopic data or nuclide concentrations. The basic zone integrals, $V_i \phi_i \phi_i^*$, are written on an interface data file for further use. On option, pointwise importance maps are edited of $V\Sigma_f$, Σ_a, and $V\Sigma_f - \Sigma_a$.

To produce additional information at the macroscopic cross section level, the effects of relative changes in the cross sections are calculated. Consider

$$\Delta k = \sum \frac{\partial k}{\partial \Sigma} (f\Sigma) = f \sum \frac{\partial k}{\partial \Sigma} (\Sigma) \tag{721-16}$$

where f represents a fractional change, set to unity for the calculations (100% change). The contributions to Δk are determined for neutron production, absorption, scattering and transport and the total for the common value of f unity. These results are edited by option to reflect energy, zone dependence, summed over zones to yield energy dependence, summed over energy to yield zone dependence, and totals are generated.

Additional information is produced to indicate the effect of uncertainties at the macroscopic cross section level. Consider that in an uncertainty sense,

$$\delta k = \left\{ \sum \left[\frac{\partial k}{\partial \Sigma} (f\Sigma) \right]^2 \right\}^{\frac{1}{2}} = f \left\{ \sum \left[\frac{\partial k}{\partial \Sigma} (\Sigma) \right]^2 \right\}^{\frac{1}{2}} \tag{721-17}$$

and again f is set at unity. The results are obtained for individual contributions, summed over zones, energy, zones and energy, and

individual components added. In this calculation, transfer from group-to-group is treated as an entity (loss and source), correlated rather than independent.

END OF SECTION

CONCLUSION AND GLOSSARY

We expect this code block and its documentation to improve with time. Feedback of information from analysts applying the procedures to general situations and quite special problems allows upgrading the capability; it also permits the documentation to be improved, removal of errors and inconsistencies and expansion of the coverage to further address and clarify troublesome areas. Keep us posted!

The capability contained in the VENTURE code block is a direct reflection of experience in nuclear reactor analysis and the requirements found over a period of years at ORNL. Several analysts have made direct contributions. Methods in use have undergone a continuing improvement which has been in part a trial-and-error process, but also benefitted from the direct contributions of several individuals, and we particularly acknowledge those of M. L. Tobias.

A glossary follows which is intended to convey an intended meaning of certain terms used in this report.

Glossary

Absolute Convergence. The difference between an estimated or iterate value of dependent variable and its value at solution divided by the latter, giving a direct error measure.

Acceleration. The iterate estimate of the flux values are driven in some manner toward an apparent solution.

Adjoint Solution. As opposed to the direct, forward or regular solution of the differential equations expressing a neutron balance, these equations are recast in the true adjoint eigenvalue problem form appropriate to perturbation theory (matrix elements are transposed about the main diagonals), but an arbitrary fixed source adjoint problem may also be solved.

Blunder. That which produced an error, more often having human source than machine (as developers always say, "check the input first!").

Convergence Criterion. The specified maximum relative change between iterations of a dependent variable used to terminate an interative process.

Convergence Level (Relative Convergence Level). The relative change from one iteration to the next of the iterate value of a dependent variable, generally the maximum of a set when several variables are involved such as point flux, is termed the convergence level.

Convergence Rate Plot. A graph of the logarithm of the convergence level as dependent on iteration number, which is asymptotically linear for a wide variety of problems as a solution is approached but

fluctuates about some value when further resolution is not possible due to limited significant figures carried in digital calculations.

Discrete Formulation. A differential and/or integral equation involving continuous functions is recast into a finite-difference representation by discretization of some or all of the independent variables. Thus the neutron population is divided into groups, each associated with an energy range over which there is no energy dependence.

Direct Search. The search eigenvalue problem is iterated directly toward a desired solution without using the conventional approach of solving each of a series of problems for the multiplication factor.

Eigenvalue. Root of the determinate of a matrix, often used as the most positive root. Given a set of N equations for N unknown neutron flux values, there remains one unknown in a multiplying system; this unknown multiplication factor is termed the eigenvalue of the problem and an additional equation must be used to supply a complete set of equations.

Extrapolation. This term is reserved herein to mean that occasionally a complete iterate set of flux values are driven to a new extrapolated set for use in the next iteration; driving is generally in the direction of the individual changes between the last two iterations (or last and two iterations back) and is based on the iterative behavior over three or more previous iterations.

Fission Source Distribution Function. In the discrete, multienergy-group representation, neutrons produced from the fission reactions at one geometric location are summed and the total is then distributed in energy by this distribution function.

Flux. Neutron flux is neutron density times speed. Since flux times cross section gives reaction rate, flux is total track length per unit volume.

Foot-Draggers Disease. This expression is reserved for the situation where either a poor arrangement of the terms in equations or the ordered sweep of the equations causes slow rate of convergence (per Tobias).

Inner-Iteration. Several sweeps are made of only part of the whole problem, generally over geometric space at one energy; the process is continued until a set number of inner-iterations on this partitioned iterative problem is reached, at which time the calculation proceeds to the next partitioned problem for iteration. Only after a complete sweep has been made of all the space-energy mesh points is an outer-iteration completed and a new estimate made of the eigenvalue of the problem for use in the next sweep.

Line Relaxation. The equations for the flux values along a row of points at one energy are solved simultaneously (a forward-backward sweep to solve a tri-diagonal matrix with simple coupling); source terms are held fixed as are flux values along adjacent rows.

Material. A material is considered to be homogeneous and have nuclear properties which are proportional to individual nuclide densities and additive in the usual sense. See Zone.

Outer-Iteration. A complete sweep of the mesh points; that is, the equations for each unknown flux value have been solved, individually, at least once (more than once with inner-iteration).

Overrelaxation. The newly calculated value of each dependent variable is driven in the direction of the change between iterations to

accelerate the iterative process, and these overrelaxed, iterate values of the flux are used at latest values during an inner- or outer-iteration.

Predominant Error Mode. Contributions to the error in iterate flux estimate are dominated by one or two error vectors, usually those having the largest eigenvalues. Contributions from the others have decayed and therefore have but little influence on the changes in point flux values with iteration; they tend to move in a single mode.

Primitive Conversion Ratio. The ratio of volume integrated capture rate in defined fertile nuclides to the volume integrated absorption rate in defined fissile nuclides.

Production Cross Section. This is used to mean the product of the cross section for fission and the number of neutrons produced by the fission reaction, either in a macroscopic or a microscopic sense, e.g., $\nu \Sigma_f = \nu (\Sigma_f)$.

Rate of Convergence. A measure of the rate of approach to a solution: often the reciprocal of the number of iterations (computer mesh sweeps) required to reduce the relative flux change by a factor of e or to reduce the absolute error by a factor of e.

Region. A volume containing mesh points which are located at the geometric centroids of finite-difference volume elements of equal volume.

Removal Cross Section (Σ_t). This is used as the sum of all cross sections for removal of neutrons from the energy of interest including absorption (sink) and out-of-energy scatter.

Residue. The equation used for solution of an unknown (point neutron balance) is rearranged with all terms on one side and the result obtained by use of current iterate estimates of the unknowns is called

here the residue of the equation for the iterate set. Weighting is arbitrarily on true volumetric reactions.

Slab Geometry. This refers to the cartesian coordinate system with orthogonal axes (one-dimensional slab geometry has symmetry in two dimensions as would be the situation if conditions were uniform over all space in these dimensions).

Time, Machine. The machine time reported to resolve a problem by iteration is the total time required for the calculation but generally excludes that for auxiliary operations of reading data, setting up the problems, and processing results. Both the amount of time the central processor is active and the total (clock) time are measured.

Zone. A volume, consisting of one or more Regions, within which macroscopic nuclear properties are constant. A zone may contain material (have nuclide concentrations) and additionally contain one or more subzones of material having specified volumes (each having nuclide concentrations).

END OF SECTION

Appendix A: CROSS-SECTION PROCESSOR CODE BLOCK

Presented herein is primary documentation of a code block designed to process microscopic cross-section data. For example, it will convert a nuclide-ordered ISOTXS file to a group-ordered GRUPXS file as would usually be required before the VENTURE neutronics code could be used. Locally we call this code block CasSandraPiC. The following items are covered:

SUBJECT

SECTION		PAGES
A1.	Code Block Specifications	A1-1,3
A2.	Tasks Performed and Order of Performance	A2-1
A3.	Computer Requirements	A3-1
A4.	Use of Logical Data Storage Units and Interface Files	A4-1,4
A5.	Code Structure and Subroutine Referencing	A5-1,4
A6.	File Specifications, VERSION-III for cross sections excluding an extended blocking of the principal cross sections in GRUPXS, and the special code block dependent interface file CXSPRR	A6-1,5

Code Block Specification

Code Block — Broad Group Microscopic Cross Section Processor

Basic Functions —

1. Convert a microscopic library order by nuclide to a microscopic library ordered by group — going from one standard interface format to another. As an option, a second nuclide-ordered library consistent with the group-ordered file may be generated.
2. Provides selectivity to eliminate extraneous data.
3. Provides flexibility to collect data for isotopes or other mixtures as desired.
4. Provides for adding libraries (files) together, as well as selecting data from two or more nuclide-ordered files.

(not done) 5. Provides for basic integrals (reaction rates) over energy of principal cross sections to test data.

6. Provides for condensation of such data as $\chi\nu\sigma_f(g \rightarrow g')$ for simple treatment.
7. Provides for user input of data to override that in the library in short, select data blocks as well as full data for additional nuclides.
8. Provides at least elementary capability for converting data from old formats.

Energy Groups — 1 to 1,000, but fully variably dimensioned.

Nuclides — 1 to 500, but fully variably dimensioned.

Legendre Order — Provision through order 20.

Library Protection and Recovery

Care and some sacrifice in efficiency is to be taken to protect libraries. Reasonable tests are to be made to insure integrity of data. Full recovery is normally possible when old libraries are preserved and the nature of failure is made known. Even the possibility of misunderstanding of procedures on the part of the production user is to be taken into account.

Edits – Not under user option:

1. Description of what was done by the code block when accessed, and associated data storage use.
2. Integrals over energy (reaction rates) when these calculations are requested.

Under user option:

Full edits of final interface data files.

Special Input Data Requirements – See interface file CONTRL, record XCPINS (Section 204):

1. Control options for selection of procedures and data file handling.
2. Edit control.
3. Input data control.
4. Select data to override that in the library.
5. Nuclide data for adding to the library.
6. A broad-group neutron flux spectrum for integrals and for condensing such data as $\chi\nu\sigma_f(g\rightarrow g')$.

Data Conversion —

Initially only simple CITATION cross-section data, elementary 1DX,[a] and basic LASL S_n[a] forms of data are to be converted to the nuclide-ordered standard interface data file as needed at several installations to support methods development effort.

Programming Note —

It is noted that direct-access techniques must be used to permit efficient data processing.

Interface Data Files —

Used	Generated
ISOTXS	GRUPXS (ISOTXS)

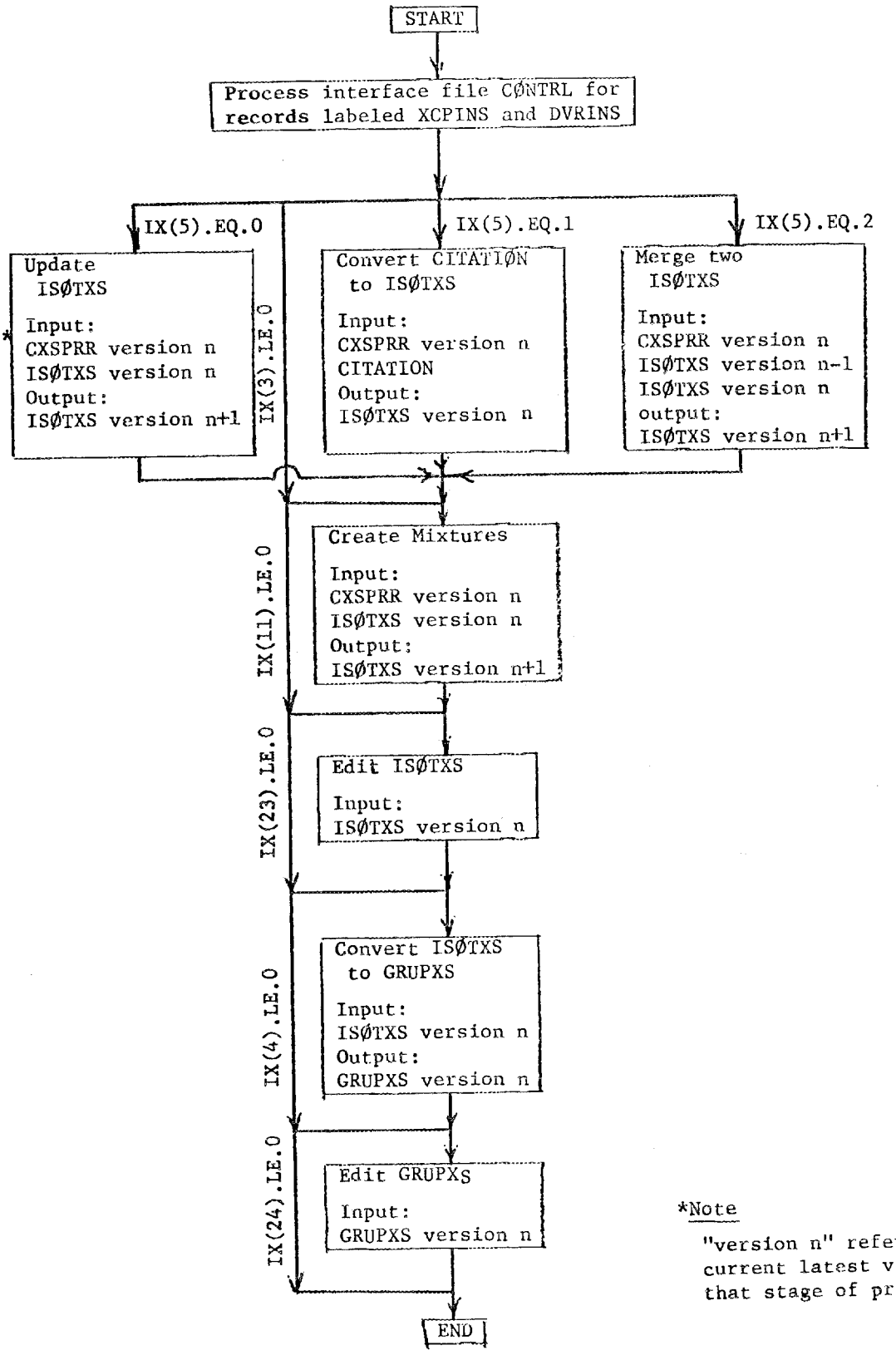
[a]Not done.

Tasks Performed

A primary function of the code is to convert a nuclide-ordered cross-section interface file (ISOTXS) to a group-ordered cross-section interface file (GRUPXS).

Additional functions include creating a nuclide-ordered file from the ORNL CITATION code cross-section format, updating an existing nuclide-ordered file, or merging two existing nuclide-ordered files. Each of these functions may, on option, eliminate selected nuclides or replace certain data (for example, Hollerith names) for a nuclide.

The capability for creating nuclide mixtures is also available. It is possible to generate a complete set of macroscopic data in the nuclide-ordered format. Any nuclide used in a mixture will be excluded from the resulting interface file.



*Note

"version n" refers to the current latest version at that stage of processing.

Computer Requirements

The requirements of this code on an IBM-360/370 machine are given here.

	Core Storage (4-byte words)	
Allocation to	Without Overlay	With Overlay
Program	33K	14K
System Routines	7K	7K
Data	10K	10K
Typical Buffers	9K	9K
Total	59K	40K

Use of Logical Data Storage Units and Interface Files

The use of logical units and interface files for each task is presented here. Unit numbers shown are for default assignment of unit numbers to the interface files at the control module level.

Always Required

ITRL (A)	CØNTRL	10 (stand-alone unit, typical)

ISOTXS to ISOTXS (Update)

IØUT	standard output	6
ICXS (A)	CXSPRR	30
ICIT (A)	input ISØTXS	32
ISØT (B)	output ISØTXS	34[a]
ISCR	scratch	45

CITATIØN to ISØTXS (Create)

IØUT	standard output	6
ICXS (A)	CXSPRR	30
ICIT	CITATIØN	8
ISØT (D)	output ISØTXS	32
ISCR	scratch	45

ISØTXS + ISØTXS to ISØTXS (Merge)

IØUT	standard output	6
ICXS (A)	CXSPRR	30
ICIT (C)	primary input ISØTXS	31

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[a] In general this is the first available unassigned interface data file number in the allowed set.

IØTH (A)	secondary input ISØTXS	32
ISØT (B)	output ISØTXS	34[a]
ISCR	scratch	45

ISØTXS to ISØTXS (Create Mixtures)

IØUT	standard output	6
ICXS (A)	CXSPRR	30
ICIT (A)	input ISØTXS	32 or 34
ISØT (B)	output ISØTXS	34 or 35
ISCR	scratch	45
ISC2	scratch	46
IDA3	scratch (direct access)	40

EDIT ISØTXS

IØUT	standard output	6
ISØT (A)	ISØTXS	32 or 34 or 35

ISØTXS to GRUPXS

IØUT	standard output	6
ISØT (A)	ISØTXS	32 or 34 or 35
IGRU (D)	GRUPXS	11
ISCR	scratch	45
IDA1	scratch (direct access)	27
IDA2	scratch (direct access)	24

[a]In general this is the first available unassigned interface data file number in the allowed set.

EDIT GRUPXS

IØUT	standard output	6
IGRU (A)	GRUPXS	11[a]

Notes:

(A) Asks SEEK for latest version to read.

(B) Asks SEEK for a new version to write.

(C) Asks SEEK for the next to the latest version to read.

(D) Asks SEEK for the latest version to write, if none available, asks SEEK for a new version to write.

---

[a]Or the first available unassigned interface data file unit number in the allowed set if not assigned by the default procedure at the control module level.

CROSS SECTION PROCESSOR MODULE SCRATCH INPUT/OUTPUT

```
C*********************************************************************
C
C          DIRECT ACCESS
C     LOGICAL UNIT 40 (IDA3)
C       NUMBER OF RECORDS     MIXO*(1 + NGROUP*(1 + (MAXORD + 1)*NTYPE))
C       LENGTH OF RECORD      MAXIMUM( 3*IDP + 7 ,
C                                      22 + 2*(MAXORD + 1) ,
C                                      4 + NGROUP )            WORDS
C       ALWAYS REQUIRED IN CREATING MIXTURES
C     LOGICAL UNIT 27 (IDA1)
C       NUMBER OF RECORDS     NISO*(1 + NGROUP)
C       LENGTH OF RECORD      MAXIMUM( 3*IDP + 7 ,
C                                      22 + 2*(MAXORD + 1) )   WORDS
C       ALWAYS REQUIRED IN CONVERTING ISOTXS TO GRUPXS
C     LOGICAL UNIT 24 (IDA2)
C       NUMBER OF RECORDS     NISO*ITYPE*(NEWORD + 1)*NGROUP
C       LENGTH OF RECORD      4 + MUD        WORDS
C       ALWAYS REQUIRED IN CONVERTING ISOTXS TO GRUPXS
C
C          SEQUENTIAL
C     LOGICAL UNIT 45 (ISCR)
C       TOTAL(APPROXIMATE)    (3*IDP + 17)*NISO
C                             + (12 + 2*(MAXORD + 1))*NISO*NGROUP
C                             + NISO*NTYPE*(MAXORD + 1)*NGROUP*MUD  WORDS
C       ALWAYS REQUIRED WHEN WRITING AN ISOTXS
C        AND IN CONVERTING ISOTXS TO GRUPXS IF CHI MATRIX DATA IS
C        PRESENT
C     LOGICAL UNIT 46 (ISC2)
C       TOTAL(APPROXIMATE)    (3*IDP + 17)*MUSO
C                             + (12 + 2*(MAXORD + 1))*MUSO*NGROUP
C                             + MUSO*NTYPE*(MAXORD + 1)*NGROUP*MUD  WORDS
C       ALWAYS REQUIRED IN CREATING MIXTURES
C
C          DEFINITIONS
C     MIXO   = MUSO + MIX
C     MUD    = MINIMUM( MAXUP + MAXDN + 1 , NGROUP)
C     NGROUP  NUMBER OF ENERGY GROUPS
C     NISO    NUMBER OF NUCLIDES IN CROSS SECTIONS
C     MAXUP   MAXIMUM NUMBER OF UPSCATTER GROUPS
C     MAXDN   MAXIMUM NUMBER OF DOWNSCATTER GROUPS
C     MAXORD  MAXIMUM SCATTERING ORDER
C     NSCMAX  MAXIMUM NUMBER OF BLOCKS OF SCATTERING DATA
C     IDP     2 FOR SHORT WORD MACHINE, 1 FOR LONG WORD MACHINE
C     NTYPE   NUMBER OF DIFFERENT SCATTERING TYPES
C     MUSO    NUMBER OF DIFFERENT NUCLIDES IN MIXTURES
C     MIX     NUMBER OF MIXTURES
C     NEWORD  MAXIMUM SCATTERING ORDER TO BE PUT ON GRUPXS
C     ITYPE   1 OR 4 DEPENDING ON THE VALUE OF NSCMAX, AND WHETHER ONLY
C              THE TOTAL SCATTERING IS TO BE PUT ON GRUPXS, AND
C              WHETHER THE TOTAL SCATTERING IS TO BE COMPUTED
C
C*********************************************************************
```

INFORMATION ABOUT SUBROUTINES

```
C*********************************************************************
C
C     CROSS SECTION PROCESSOR MODULE SUBROUTINE DESCRIPTICN
C
C     CHOL    CONVERT HOLLERITH TYPE
C     CTI1    CITATION TO ISOTXS
C     CTI2    CITATION TO ISOTXS
C     CTI3    CITATION TO ISOTXS
C     GXS1    EDIT GRUPXS
C     GXS2    EDIT GRUPXS
C     HCHK    CHECK FOR UNIQUENESS IN NUCLIDE NAMES
C     ITI1    UPDATE ISOTXS
C     ITI2    UPDATE ISOTXS
C     IXS1    EDIT ISOTXS
C     IXS2    EDIT ISOTXS
C     MAIN    INITIALIZE INPUT/OUTPUT UNITS
C     MIXC    CREATE NUCLIDE MIXTURES ON ISOTXS
C     MIX1    CREATE NUCLIDE MIXTURES ON ISOTXS
C     MIX2    CREATE NUCLIDE MIXTURES ON ISOTXS
C     MIX3    CREATE NUCLIDE MIXTURES ON ISOTXS
C     MIX4    CREATE NUCLIDE MIXTURES ON ISOTXS
C     MIX5    CREATE NUCLIDE MIXTURES ON ISOTXS
C     M2I1    MERGE ISOTXS
C     M2I2    MERGE ISOTXS
C     NPCR    CALCULATE NUMBER OF PRINCIPAL CROSS SECTIONS
C     TRLR    CCNTROLS PROCESSING OPTIONS
C     XLEI    DETERMINE SCATTERING TYPE AND ORDER FOR EDIT
C     XORD    DETERMINE SCATTERING TYPE AND ORDER
C     XSCI    OBTAIN CROSS SECTION PROCESSOR CONTROL INFORMATION FROM
C              INTERFACE CONTRL
C     XSCU    SETUP DYNAMIC DATA STORAGE SPACE
C     XSC1    CONVERT ISOTXS TO GRUPXS
C     XSC2    CCNVERT ISOTXS TO GRUPXS
C     XSC3    CONVERT ISOTXS TO GRUPXS
C     XSC4    CONVERT ISOTXS TO GRUPXS
C     XSC5    CCNVERT ISOTXS TO GRUPXS
C
C*********************************************************************
```

(CONT)

```
C*********************************************************************
C
C     CROSS SECTION PROCESSOR SUBROUTINE CROSS-REFERENCING
C
C  SUBROUTINE ***************  CALLED SUBROUTINE  *********************
C
C     CHOL
C     CTI1     CTI2     CTI3     REED     SEEK
C     CTI2     CHOL     HCHK     ISTR     REED     RITE     RSTI
C     CTI3     REED
C     GXS1     GXS2     REED     SEEK
C     GXS2     REED     XLEI
C     HCHK
C     ITI1     ITI2     REED     SEEK
C     ITI2     HCHK     ISTR     NPCR     REED     RITE     RSTI
C     IXS1     IXS2     REED     SEEK
C     IXS2     ISTR     REED     XLEI
C     MAIN     DOPC     XSCI     XSCU
C     MIXC     REED
C     MIX1     MIX2     REED     SEEK
C     MIX2     DOPC     HCHK     ISTR     MIXC     MIX3     MIX4     MIX5
C              NPCR     REED     RITE     XORD
C     MIX3     ISTR     NPCR     REED     RITE     RSTI     XORD
C     MIX4     ISTR     REED     RITE     RSTI
C     MIX5     NPCR     REED     RITE     STOR     XORD
C     M2I1     M2I2     REED     SEEK
C     M2I2     HCHK     ISTR     NPCR     REED     RITE     RSTI
C     NPCR
C     TRLR     CTI1     GXS1     ITI1     IXS1     MIX1     M2I1     XSC1
C     XLEI
C     XORD
C     XSCI     FERR     REED     SEEK     SKER
C     XSCU     DOPC     ROXX     ROXY     TRLR     FRECOR   GETCOR
C     XSC1     DOPC     REED     SEEK     XSC2
C     XSC2     REED     RITE     RSTI     STOR     XORD     XSC3     XSC4
C              XSC5
C     XSC3     ISTR     REED     RITE
C     XSC4     HCHK     REED     RITE     XORD
C     XSC5     ISTR     REED     RITE     RSTI
C
C*********************************************************************

C*********************************************************************
C
C     CROSS SECTION PROCESSOR SUBROUTINE CROSS-REFERENCING
C
C  SUBROUTINE **************  CALLED FROM SUBROUTINE  ****************
C
C     CHOL     CTI2
C     CTI1     TRLR
C     CTI2     CTI1
C     CTI3     CTI1
```

(CONT)

```
C     DOPC     MAIN     MIX2     XSCU     XSC1
C     FERR     XSCI
C     FRECOR   XSCU
C     GETCOR   XSCU
C     GXS1     TRLR
C     GXS2     GXS1
C     HCHK     CTI2     ITI2     MIX2     M2I2     XSC4
C     ISTR     CTI2     ITI2     IXS2     MIX2     MIX3     MIX4     M2I2
C              XSC3     XSC5
C     ITI1     TRLR
C     ITI2     ITI1
C     IXS1     TRLR
C     IXS2     IXS1
C     MAIN
C     MIXC     MIX2
C     MIX1     TRLR
C     MIX2     MIX1
C     MIX3     MIX2
C     MIX4     MIX2
C     MIX5     MIX2
C     M2I1     TRLR
C     M2I2     M2I1
C     NPCR     ITI2     MIX2     MIX3     MIX5     M2I2
C     REED     CTI1     CTI2     CTI3     GXS1     GXS2     ITI1     ITI2
C              IXS1     IXS2     MIXC     MIX1     MIX2     MIX3     MIX4
C              MIX5     M2I1     M2I2     XSCI     XSC1     XSC2     XSC3
C              XSC4     XSC5
C     RITE     CTI2     ITI2     MIX2     MIX3     MIX4     MIX5     M2I2
C              XSC2     XSC3     XSC4     XSC5
C     RCXX     XSCU
C     RCXY     XSCU
C     RSTI     CTI2     ITI2     MIX3     MIX4     M2I2     XSC2     XSC5
C     SEEK     CTI1     GXS1     ITI1     IXS1     MIX1     M2I1     XSCI
C              XSC1
C     SKER     XSCI
C     STOR     MIX5     XSC2
C     TRLR     XSCU
C     XIEI     GXS2     IXS2
C     XORD     MIX2     MIX3     MIX5     XSC2     XSC4
C     XSCI     MAIN
C     XSCU     MAIN
C     XSC1     TRLR
C     XSC2     XSC1
C     XSC3     XSC2
C     XSC4     XSC2
C     XSC5     XSC2
C*****************************************************************************
```

(CONT)

```
C*********************************************************************
C
C     SIMPLE OVERLAY STRUCTURE FOR CROSS SECTION PROCESSOR
C
C                              MAIN
C                              XSCI
C                              XSCU
C                              TRLR
C                              HCHK
C                              NPCR
C                              XORD
C                              XLEI
C                              DOPC(ROXY)        LIBRARY
C                              RITE(REED,ROXX)   LIBRARY
C                              SEEK              LIBRARY
C                              STOR              LIBRARY
C                              ISTR              LIBRARY
C                              RSTI              LIBRARY
C                              SKER              LIBRARY
C                              FERR              LIBRARY
C                              GETCOR            LIBRARY
C                              FRECOR            LIBRARY
C                              DEFILE            LIBRARY
C                              CLOSDA            LIBRARY
C                               *
C                               *
C      ***********************************************
C      *       *       *       *       *       *       *
C     ITI1    CTI1    M2I1    MIX1    IXS1    XSC1    GXS1
C     ITI2    CTI2    M2I2    MIX2    IXS2    XSC2    GXS2
C             CTI3            MIX3            XSC3
C             CHOL            MIXC            XSC4
C                             MIX4            XSC5
C                             MIX5
C*********************************************************************
C*********************************************************************
C     NON-STANDARD SUBROUTINE USAGE IN CROSS SECTION PROCESSOR
C
C     DEFILE        (CALLED FROM DOPC) ASSEMBLER LANGUAGE ROUTINE
C                   USED TO OPEN DIRECT ACCESS FILES - REPLACES THE
C                   IBM DEFINE FILE STATEMENT
C     CLOSDA        (CALLED FROM DOPC) ASSEMBLER LANGUAGE ROUTINE
C                   USED TO CLOSE DIRECT ACCESS FILES OPENED
C                   WITH DEFILE
C     GETCOR/FRECOR (CALLED FROM XSCU) ASSEMBLER LANGUAGE ROUTINES
C                   USED TO DYNAMICALLY ALLOCATE AND RELEASE MAIN
C                   CORE STORAGE
C     CHOL          (CALLED FROM CTI2) NON-STANDARD FORTRAN ROUTINE
C                   USED TO CONVERT FOUR CHARACTER SINGLE PRECISION
C                   HOLLERITH WORDS TO SIX CHARACTER DOUBLE PRECISION
C                   HOLLERITH WORDS. USED ONLY IN CONVERSION OF
C                   CITATION CROSS SECTIONS TO ISOTXS
C
C*********************************************************************
```

INTERFACE DATA FILE SPECIFICATIONS

```
C*********************************************************************
C                        PREPARED 10/18/73                           -
C                                                                    -
CF          CXSPRR                                                   -
CE          DATA FOR CROSS SECTION PROCESSOR                         -
C                                                                    -
CN          SEE INTERFACE FILE CONTRL, RECORD XCPINS, FOR REFERENCES -
CN          TC ARRAY IX                                              -
C                                                                    -
C*********************************************************************

C-------------------------------------------------------------------
CS          FILE STRUCTURE                                           -
CS                                                                   -
CS             RECORD TYPE                          PRESENT IF       -
CS             ==============================     ===============   -
CS             FILE IDENTIFICATION                  ALWAYS           -
CS             FILE CONTROL                         ALWAYS           -
CS             CITATION SET NUMBERS                 NOP(1) GT 0      -
CS             NEUTRON ENERGY SPECTRUM              NOP(3) GT 0      -
CS             TRANSPORT MULTIPLIERS                NOP(4) GT 0      -
CS                                                                   -
CS          ******(REPEAT FROM 1 TO NOP(5))                          -
CS          *  ISOTOPE DATA                         NOP(5) GT 0      -
CS          ******                                                   -
CS                                                                   -
CS          ******(REPEAT FROM 1 TO NOP(6))                          -
CS          *  ISOTOPE NAMES IN MIXTURE             NOP(6) GT 0      -
CS          *  ISOTOPE DENSITIES IN MIXTURE         NOP(6) GT 0      -
CS          ******                                                   -
CS                                                                   -
CS          ******(REPEAT FROM 1 TO NOP(6))                          -
CS          *  MIXTURE DATA                         NOP(6) GT 0      -
CS          ******                                                   -
C                                                                    -
C-------------------------------------------------------------------

C-------------------------------------------------------------------
CR          FILE IDENTIFICATION                                      -
C                                                                    -
CL     HNAME,(HUSE(I),I=1,2),IVERS                                   -
C                                                                    -
CW     3*MULT + 1                                                    -
C                                                                    -
CD     HNAME          HOLLERITH FILE NAME - CXSPRR - (A6)            -
CD     HUSE           HOLLERITH USER IDENTIFICATION (A6)             -
CD     IVERS          FILE VERSION NUMBER                            -
CD     MULT           DOUBLE PRECISION PARAMETER                     -
CD                        1 - A6 WORD IS SINGLE WORD                 -
CD                        2 - A6 WORD IS DOUBLE PRECISION WORD       -
C                                                                    -
C-------------------------------------------------------------------
```

(CONT)

```
C-----------------------------------------------------------------------
CR          FILE CONTROL                                              -
C                                                                     -
CL    (NOP(I),I=1,24)                                                 -
C                                                                     -
CW    24                                                              -
C                                                                     -
CD    NOP(1)          NUMBER OF CITATION CROSS SECTION SETS TO PROCESS -
CD                        (IF NOP(1) EQ 0 AND IX(3) EQ 1 AND IX(5) EQ 1, -
CD                        SET ONE WILL BE PROCESSED)                  -
CD    NOP(2)          SCATTERING BLOCKING FACTOR FOR NUCLIDE-ORDERED  -
CD                        FILE CREATED FROM CITATION CROSS SECTIONS   -
CD                        0 - NSBLOK = 1                              -
CD                        N - NSBLOK = N, IF (NGROUP/N)*N EQ NGROUP,  -
CD                              OTHERWISE NSBLOK = 1                  -
CD    NOP(3)          OPTION TO INPUT A NEUTRON ENERGY SPECTRUM       -
CD                        0 - NO                                      -
CD                        N - YES (N SHOULD BE EQUAL TO THE NUMBER OF -
CD                              ENERGY GROUPS ON THE CROSS SECTION FILE) -
CD    NOP(4)          OPTION TO CREATE PSEUDO DIRECTION DEPENDENT     -
CD                        TRANSPORT DATA                              -
CD                        0 - NO                                      -
CD                        1 - YES                                     -
CD    NOP(5)          OPTION TO INPUT OVERRIDE DATA FOR ISOTOPES      -
CD                        0 - NO                                      -
CD                        N - YES (N IS THE NUMBER OF RECORDS OF DATA) -
CD    NOP(6)          NUMBER OF MIXTURES (REQUIRED IF IX(11) EQ 1)    -
CD    NOP(7)          MAXIMUM NUMBER OF ISOTOPES IN ANY MIXTURE       -
CD                        (REQUIRED IF IX(11) EQ 1)                   -
CD    NOP(8-9)        RESERVED                                        -
CD    NOP(10)         OPTION ON USE OF THE OVERRIDE DATA FOR ISOTOPES -
CD                        WHEN NOP(5) GT 0  (APPLICABLE ONLY WHEN     -
CD                        IX(3) EQ 1 AND IX(5) EQ 0)                  -
CD                        0 - DATA CORRESPONDS WITH THE ORDER OF      -
CD                              ISOTOPES IN THE FILE                  -
CD                        1 - DATA IDENTIFIES ISOTOPES TO BE SELECTED -
CD                              BY UNIQUE ISOTOPE LABEL               -
CD    NOP(11-23)      RESERVED                                        -
CD    NOP(24)         OPTION ON EDIT DURING CITATION CROSS SECTION    -
CD                        PROCESSING                                  -
CD                        0 - NO                                      -
CD                        1 - YES                                     -
C                                                                     -
C-----------------------------------------------------------------------
```

(CONT)

```
C-----------------------------------------------------------------------
CR          CITATION CROSS SECTION SET NUMBERS                         -
C                                                                      -
CC          PRESENT IF NOP(1) GT 0                                     -
C                                                                      -
CL    (ISET(I),I=1,NOP1)                                               -
C                                                                      -
CW    NOP1 = NOP(1)                                                    -
C                                                                      -
CD    ISET          SET NUMBERS IN ASCENDING ORDER OF APPEARANCE       -
CD                      IN LIBRARY                                     -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          NEUTRON ENERGY SPECTRUM                                    -
C                                                                      -
CC          PRESENT IF NOP(3) GT 0                                     -
C                                                                      -
CL    (WGT(I),I=1,NOP3)                                                -
C                                                                      -
CW    NOP3 = NOP(3)                                                    -
C                                                                      -
CD    WGT           SPECTRUM FOR WEIGHTING IN MIXTURE CALCULATION      -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MULTIPLIERS FOR TRANSPORT CROSS SECTION                    -
C                                                                      -
CC          PRESENT IF NOP(4) GT 0                                     -
C                                                                      -
CL    (TRMOD(I),I=1,3)                                                 -
C                                                                      -
CW    3                                                                -
C                                                                      -
CD    TRMOD         MULTIPLIER FOR EACH COORDINATE DIRECTION           -
CD                      STRPD(I) = TRMOD(I)*STRPL(1) FOR EACH ENERGY   -
C                                                                      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE DATA                                               -
C                                                                      -
CC          PRESENT IF NOP(5) GT 0                                     -
CC          THERE MUST BE NOP(5) RECORDS                               -
C                                                                      -
CN          WHEN NOP(10) EQ 0,                                         -
CN          THIS DATA MAY BE USED WHEN IX(3) EQ 1 TO CONTROL THE       -
CN          PROCESSING OF THE INPUT CROSS SECTIONS. THE ORDER          -
CN          OF THESE RECORDS MUST BE ONE-TO-ONE WITH THE ORDER         -
CN          OF THE ISOTOPES IN THE INPUT CROSS SECTIONS. FOR EACH      -
CN          ISOTOPE READ FROM THE INPUT CROSS SECTIONS, ONE RECORD     -
CN          IS READ FROM THIS DATA                                     -
```

(CONT)

```
CN              A) IF HISONM EQ 6HDELETE, THE DATA FOR THIS ISOTOPE      -
CN                 IS NOT WRITTEN ON THE NEW NUCLIDE-ORDERED FILE        -
CN              B) IF HISONM NE 6HDELETE, THE DATA FOR THIS ISOTOPE      -
CN                 WILL BE COPIED TO THE NEW NUCLIDE-ORDERED FILE        -
CN                 (NON-BLANK OR NON-ZERO DATA WILL REPLACE THE          -
CN                 DATA ON THE NEW FILE)                                 -
CN              C) IF AFTER READING NOP(5) RECORDS, THERE ARE ISOTOPES   -
CN                 REMAINING IN THE INPUT CROSS SECTIONS, THOSE          -
CN                 REMAINING WILL BE DELETED FROM THE NEW FILE           -
CN                                                                       -
CN          WHEN NOP(10) EQ 1,                                           -
CN          THIS DATA MAY BE USED WHEN IX(3) EQ 1 AND IX(5) EQ 0 TO      -
CN          CONTROL THE CONTENT OF THE NEW ISOTXS FILE. THE ORDER        -
CN          OF THE RECORDS IS NOT SPECIFIED SINCE THE UNIQUE LABEL       -
CN          (HISONM) IS USED TO IDENTIFY ISOTOPES TO BE COPIED TO        -
CN          THE NEW FILE. NON-BLANK OR NON-ZERO VALUES FOR THE           -
CN          REST OF THE DATA WILL BE PUT ON THE NEW FILE.                -
CN          THE UNIQUE LABEL CAN NOT BE CHANGED WHEN USING THIS OPTION.-
CN                                                                       -
CN          IF THIS DATA IS NOT PRESENT, ALL ISOTOPES ON THE INPUT       -
CN          CROSS SECTIONS WILL BE COPIED TO THE NEW FILE                -
C                                                                        -
CL    HISONM,HABSID,HMAT,AMASS,EFISS,ECAPT,KBR,(IOP(I),I=1,3)            -
C                                                                        -
CW    3*MULT + 7                                                         -
C                                                                        -
CD    HISONM        HOLLERITH ISOTOPE LABEL (UNIQUE)   (A6)              -
CD    HABSID        HOLLERITH ISOTOPE LABEL (ABSOLUTE)   (A6)            -
CD    HMAT          HOLLERITH ISOTOPE LABEL (REFERENCE)   (A6)           -
CD    AMASS         GRAM ATOMIC WEIGHT                                   -
CD    EFISS         TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)      -
CD    ECAPT         TOTAL THERMAL ENERGY YIELD/CAPTURE(N,GAMMA)          -
CD                      (W.SEC/CAPT)                                     -
CD    KBR           ISOTOPE CLASSIFICATION                               -
CD    IOP           RESERVED                                             -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          ISOTOPE NAMES IN MIXTURE                                     -
C                                                                        -
CC          PRESENT IF NOP(6) GT 0                                       -
CC          THIS RECORD AND THE RECORD FOLLOWING APPEAR IN PAIRS         -
CC          THERE MUST BE NOP(6) PAIRS                                   -
C                                                                        -
CL    (HISOMX(I),I=1,NOP7)                                               -
C                                                                        -
CW    MULT*NOP7 = MULT*NOP(7)                                            -
C                                                                        -
CD    HISOMX        UNIQUE NAME OF ISOTOPE TO BE INCLUDED IN MIXTURE     -
CD                      (BLANK NAMES ARE IGNORED)                        -
C                                                                        -
CN          ANY ISOTOPE INCLUDED IN A MIXTURE WILL BE DELETED FROM THE -
CN             NEW FILE                                                  -
C-----------------------------------------------------------------------
```

(CONT)

```
C-----------------------------------------------------------------------
CR          ISOTOPE DENSITIES IN MIXTURE                              -
C                                                                     -
CC          PRESENT IF NOP(6) GT 0                                    -
C                                                                     -
CL    (RDENS(I),I=1,NOP7)                                             -
C                                                                     -
CW    NOP7 = NOP(7)                                                   -
C                                                                     -
CD    RDENS         DENSITY OF ISOTOPE TO BE INCLUDED IN MIXTURE      -
C-----------------------------------------------------------------------

C-----------------------------------------------------------------------
CR          MIXTURE DATA                                              -
C                                                                     -
CC          PRESENT IF NOP(6) GT 0                                    -
CC          THERE MUST BE NOP(6) RECORDS                              -
C                                                                     -
CL    HISONM,HABSID,HMAT,AMASS,EFISS,ECAPT,KBR,(IOP(I),I=1,3)         -
C                                                                     -
CW    3*MULT + 7                                                      -
C                                                                     -
CD    HISONM        HOLLERITH MIXTURE LABEL (UNIQUE)  (A6)            -
CD    HABSID        HOLLERITH MIXTURE LABEL (ABSOLUTE)  (A6)          -
CD    HMAT          HOLLERITH MIXTURE LABEL (REFERENCE)  (A6)         -
CD    AMASS         GRAM ATOMIC WEIGHT                                -
CD    EFISS         TOTAL THERMAL ENERGY YIELD/FISSION (W.SEC/FISS)   -
CD    ECAPT         TOTAL THERMAL ENERGY YIELD/CAPTURE(N,GAMMA)       -
CD                      (W.SEC/CAPT)                                  -
CD    KBR           MIXTURE CLASSIFICATION                            -
CD    IOP           RESERVED                                          -
C                                                                     -
CN          NON-BLANK DATA SHOULD BE SUPPLIED FOR LABELS              -
CN          AND NON-ZERO DATA FOR KBR                                 -
CN          AMASS, EFISS, AND ECAPT ARE CALCULATED FOR MIXTURE BUT    -
CN          MAY BE REPLACED BY NON-ZERO ENTRIES                       -
C                                                                     -
C-----------------------------------------------------------------------

CEOF
```

END OF APPENDIX A

Appendix B: CODE BLOCK TO CALCULATE REACTION RATES, ETC.

This code block reaction rate integrals by nuclide, certain summary tables, and such auxiliary results as the primitive fuel conversion (breeding) ratio. It is compatible with the VENTURE code and operational locally as a separate module in the code system requiring less than 50K words total memory usually. File communication is compatible with VENTURE. Basic control parameters are indicated in the specifications for the CONTRL file in the body of this report.

It is intended that this code block perform a variety of tasks on demand, independent of the neutronics model applied, using cross sections and nuclide concentrations from the fiels used by the neutronics codes and flux data produced by neutronics codes, and perhaps generate a new interface data file. A preliminary list of the tasks follows, but only the first is implemented in the present release version.

1. Calculate by zone (and subzone) average neutron, nuclide reaction rates and integrated summary tables using interface data files with user control over edit levels
    a. Using files NDXSRF, ZNATDN, RZFLUX AND GRUPXS.
    b. Repeat with flux, adjoint weighting on option using file PERTUB.
2. Edit selected maps of individual reaction rates (traverse or on a plane)
3. Basic cross section collapse capability in Energy and space.

The code structure and subroutine referencing start on page B1-1 and information about logical input/output units on B2-1. An overlay structure will not be needed for this release version.

INFORMATION ABOUT SUBROUTINES

```
C*********************************************************************
C
C     REACTION RATE MODULE SUBROUTINE DESCRIPTION
C
C     AUXR     WRITE CONDENSED EDIT
C     MAIN     INITIALIZE INPUT/OUTPUT UNITS
C     RRCI     OBTAIN REACTION RATE CONTROL INFORMATION FRCM CONTRL
C     RRDS     SETUP DYNAMIC DATA STORAGE SPACE
C     RRTA     COMPUTE SPECIFIC REACTION RATES FOR ABSORPTION, FISSION,
C               NU*FISSION, (N,G), (N,A), (N,P), (N,2N), (N,D), AND (N,T)
C     RRTB     COMPUTE REACTION RATES, INVENTORY, AND POWER PER UNIT
C               VOLUME BY ZONE AND SUBZONE
C     RRTC     COMPUTE REACTION RATES, INVENTORY, AND POWER BY ZONE, SUBZ
C     RRTD     EDIT    REACTION RATES, INVENTORY, AND POWER BY ZONE, SUBZ
C     RRTE     WRITE   REACTION RATES, INVENTORY, AND POWER ON SCRATCH
C               CNE RECORD FOR EACH ZONE AND SUBZONE (IF NOT ON DIRECT
C               ACCESS UNIT)
C     RRTF     SETUP INTERNAL CROSS-REFERENCING INFORMATION FOR ABSOLUTE
C               NUCLIDE, NUCLIDE CLASS, AND ZONE CLASS
C     RRTG     COMPUTE REACTION RATES, INVENTORY, AND POWER BY ZONE
C     RRTH     EDIT    REACTION RATES, INVENTORY, AND POWER BY ZONE
C     RRTI     COMPUTE REACTION RATES, INVENTORY, AND POWER BY ZONE CLASS
C     RRTJ     EDIT    REACTION RATES, INVENTORY, AND POWER BY ZONE CLASS
C     RRTK     COMPUTE TOTAL REACTION RATES, INVENTORY, AND POWER BY
C               UNIQUE NUCLIDE
C     RRTL     EDIT    TOTAL REACTION RATES, INVENTORY, AND POWER BY
C               UNIQUE NUCLIDE
C     RRTM     COMPUTE TOTAL REACTION RATES, INVENTORY, AND POWER BY
C               ABSOLUTE NUCLIDE
C     RRTN     EDIT    TOTAL REACTION RATES, INVENTORY, AND POWER BY
C               ABSOLUTE NUCLIDE
C     RRTO     PREPARE AND EDIT FINAL SUMMARY TABLE
C     RRTP     COMPUTE AND EDIT ENERGY PRODUCING UNIQUE NUCLIDES
C     RRTS     DETERMINE STORAGE REQUIRED AND MODE OF SOLUTION AND
C               INITIALIZE DIRECT ACCESS UNITS IF NEEDED
C     RRTT     PRE-WRITE DIRECT ACCESS UNITS IF NEEDED
C     RRT1     CONTROLS INTERFACE FILE PROCESSING AND DATA PREPARATION
C              AND CALCULATION
C     RRT2     COMPUTE ZONE VOLUMES FROM REGION VOLUMES
C     RRT3     PROCESS RZFLUX AND WRITE ZONE AVERAGE FLUX ON SCRATCH
C               ONE GROUP AT A TIME
C     RRT4     CHECK NAMES AND CLASSES ON NDXSRF AND GRUPXS FOR AGREEMENT
C     RRT5     CHECK ZONE VOLUMES
C     RRT6     PUT     REACTION RATES, INVENTORY, AND POWER BY ZONE CLASS
C               ON WHOLE SYSTEM BASIS(DIVIDE BY FRACTION OF CORE TREATED)
C     RRT7     COPY PRINCIPAL CROSS SECTIONS FROM GRUPXS TO SCRATCH
C     RRT8     COMPUTE TOTAL DESTRUCTION RATE BY UNIQUE NUCLIDE
C     RRT9     PROCESS INTERFACE FILE PERTUB AND WRITE ZONE FORWARD-
C               ADJOINT FLUX INTEGRALS ON SCRATCH ONE GROUP AT A TIME
C
C*********************************************************************
```

(CONT)

```
C*********************************************************************
C
C     REACTION RATE MODULE SUBROUTINE CROSS-REFERENCING
C
C  SUBROUTINE ****************  CALLED SUBROUTINE  ********************
C
C     AUXR
C     MAIN     DOPC     RRCI     RRDS
C     RRCI     FERR     REED     SEEK     SKER
C     RRDS     DOPC     ROXX     ROXY     RRT1     FRECOR   GETCOR
C     RRTA     REED     RITE
C     RRTB     REED     RITE
C     RRTC     REED     RITE
C     RRTD     REED
C     RRTE     RITE
C     RRTF
C     RRTG     REED     RITE
C     RRTH     REED
C     RRTI     REED     RITE
C     RRTJ     REED
C     RRTK     REED
C     RRTL
C     RRTM
C     RRTN
C     RRTO     AUXR     REED
C     RRTP
C     RRTS     DOPC     FERR
C     RRTT     RITE
C     RRT1     FERR     REED     RRTA     RRTB     RRTC     RRTD     RRTE
C              RRTF     RRTG     RRTH     RRTI     RRTJ     RRTK     RRTL
C              RRTM     RRTN     RRTO     RRTP     RRTS     RRTT     RRT2
C              RRT3     RRT4     RRT5     RRT6     RRT7     RRT8     RRT9
C              SEEK     SKER     STOR
C     RRT2
C     RRT3     REED     RITE     SEEK     SKER
C     RRT4
C     RRT5
C     RRT6     REED     RITE
C     RRT7     REED     RITE
C     RRT8
C     RRT9     REED     RITE     SEEK     SKER
C
C*********************************************************************
```

(CONT)

```
C*********************************************************************
C
C     REACTION RATE MODULE SUBROUTINE CROSS-REFERENCING
C
C  SUBROUTINE **************  CALLED FROM SUBROUTINE  ******************
C
C     AUXR     RRTO
C     DOPC     MAIN     RRDS     RRTS
C     FERR     RRCI     RRTS     RRT1
C     FRECOR   RRDS
C     GETCOR   RRDS
C     MAIN
C     REED     RRCI     RRTA     RRTB     RRTC     RRTD     RRTG     RRTH
C              RRTI     RRTJ     RRTK     RRTO     RRT1     RRT3     RRT6
C              RRT7     RRT9
C     RITE     RRTA     RRTB     RRTC     RRTE     RRTG     RRTI     RRTT
C              RRT3     RRT6     RRT7     RRT9
C     RCXX     RRDS
C     RCXY     RRDS
C     RRCI     MAIN
C     RRDS     MAIN
C     RRTA     RRT1
C     RRTB     RRT1
C     RRTC     RRT1
C     RRTD     RRT1
C     RRTE     RRT1
C     RRTF     RRT1
C     RRTG     RRT1
C     RRTH     RRT1
C     RRTI     RRT1
C     RRTJ     RRT1
C     RRTK     RRT1
C     RRTL     RRT1
C     RRTM     RRT1
C     RRTN     RRT1
C     RRTO     RRT1
C     RRTP     RRT1
C     RRTS     RRT1
C     RRTT     RRT1
C     RRT1     RRDS
C     RRT2     RRT1
C     RRT3     RRT1
C     RRT4     RRT1
C     RRT5     RRT1
C     RRT6     RRT1
C     RRT7     RRT1
C     RRT8     RRT1
C     RRT9     RRT1
C     SEEK     RRCI     RRT1     RRT3     RRT9
C     SKER     RRCI     RRT1     RRT3     RRT9
C     STOR     RRT1
C
C*********************************************************************
```

(CONT)

```
C*********************************************************************
C
C     SIMPLE OVERLAY STRUCTURE FOR REACTION RATE MODULE
C     MODULE MAY BE USED WITHOUT OVERLAY AT THIS TIME
C
C                              MAIN
C                              RRCI
C                              RRDS
C                              RRT1
C                              DOPC(ROXY)        LIBRARY
C                              RITE(REED,ROXX)   LIBRARY
C                              SEEK              LIBRARY
C                              STOR              LIBRARY
C                              SKER              LIBRARY
C                              FERR              LIBRARY
C                              GETCOR            LIBRARY
C                              FRECOR            LIBRARY
C                              DEFILE            LIBRARY
C                              CLOSDA            LIBRARY
C                               *
C                               *
C      ****************************************
C      *       *       *       *       *       *
C     RRT2    RRT3    RRTA    RRTG    RRTI    RRTO
C     RRT5    RRT9    RRTB    RRTH    RRTJ    RRTP
C     RRT7    RRTT    RRTC            RRT6    AUXR
C     RRT4            RRTD            RRTK
C     RRTF            RRTE            RRTL
C     RRTS                            RRTM
C                                     RRTN
C                                     RRT8
C
C*********************************************************************

C*********************************************************************
C
C     NON-STANDARD SUBROUTINE USAGE IN REACTION RATE MODULE
C
C     DEFILE        (CALLED FROM DOPC) ASSEMBLER LANGUAGE ROUTINE
C                   USED TO OPEN DIRECT ACCESS FILES - REPLACES THE
C                   IBM DEFINE FILE STATEMENT
C     CLOSDA        (CALLED FROM DOPC) ASSEMBLER LANGUAGE ROUTINE
C                   USED TO CLOSE DIRECT ACCESS FILES OPENED
C                   WITH DEFILE
C     GETCOR/FRECOR(CALLED FROM RRDS) ASSEMBLER LANGUAGE ROUTINES
C                   USED TO DYNAMICALLY ALLOCATE AND RELEASE MAIN
C                   CORE STORAGE
C
C*********************************************************************
```

REACTION RATE MODULE SCRATCH INPUT/OUTPUT

```
C*********************************************************************
C
C          DIRECT ACCESS
C
C     LOGICAL UNIT 40 (IDA1)   REACTION RATES BY ZONE
C       NUMBER OF RECORDS     NZONE
C       LENGTH OF RECORD      NACT*NISOU      WORDS
C       OPTIONAL DEPENDING ON MEMORY STORAGE AVAILABLE
C
C     LOGICAL UNIT 24 (IDA2)   REACTION RATES BY ZONE AND SUBZONE
C       NUMBER OF RECORDS     NZONE + NSZ
C       LENGTH OF RECORD      NACT*NNS        WORDS
C       OPTIONAL DEPENDING ON MEMORY STORAGE AVAILABLE
C
C     LOGICAL UNIT 27 (IDA3)   REACTION RATES BY ZONE CLASS
C       NUMBER OF RECORDS     NZCLAS
C       LENGTH OF RECORD      NACT*NISOU      WORDS
C       OPTIONAL DEPENDING ON MEMORY STORAGE AVAILABLE
C
C          SEQUENTIAL
C
C     LOGICAL UNIT 45 (ISR1)   ZONE AVERAGE FLUX
C       NUMBER OF RECORDS     NGROUP
C       LENGTH OF RECORD      NZONE           WORDS
C       ALWAYS USED
C
C     LOGICAL UNIT 46 (ISR2)   REACTION RATES BY ZONE AND SUBZONE
C       NUMBER OF RECORDS     NZONE + NSZ
C       LENGTH OF RECORD      NACT*NNS        WORDS
C       USED WHEN LOGICAL UNIT 24 IS NOT USED
C
C     LOGICAL UNIT 48 (ISR3)   PRINCIPAL CROSS SECTIONS
C       NUMBER OF RECORDS     NGROUP
C       LENGTH OF RECORD      NPSCS           WORDS
C       ALWAYS USED
C
C     LOGICAL UNIT 49 (ISR4)   ZONE AVERAGE FORWARD-ADJOINT FLUX
C       NUMBER OF RECORDS     NGROUP
C       LENGTH OF RECORD      NZONE           WORDS
C       OPTIONAL
C
C          DEFINITIONS
C
C     IRSUM = IALF + INP + IN2N + IND + INT
C     NACT  = 7 + IRSUM
C     NPSCS = (4 + IRSUM + 2*(MAXORD + 1) + NSTRPD)*NISO
C
C     NGROUP  NUMBER OF ENERGY GROUPS
C     NISO    NUMBER OF NUCLIDES IN CROSS SECTION DATA
C     MAXORD  MAXIMUM SCATTERING ORDER
C     NPSCS   LENGTH OF PRINCIPAL CROSS SECTION RECORD
C     NSTRPD  NUMBER OF COORDINATE DIRECTIONS FOR WHICH TRANSPORT
C              CROSS SECTIONS ARE GIVEN
C     IALF    (N,A)  CROSS SECTION FLAG 0,1
C     INP     (N,P)  CROSS SECTION FLAG 0,1
C     IN2N    (N,2N) CROSS SECTION FLAG 0,1
C     IND     (N,D)  CROSS SECTION FLAG 0,1
C     INT     (N,T)  CROSS SECTION FLAG 0,1
C     NZONE   NUMBER OF ZONES
C     NSZ     NUMBER OF SUBZONES
C     NNS     MAXIMUM NUMBER OF NUCLIDES IN ANY SET
C     NISOU   NUMBER OF DIFFERENT UNIQUE NUCLIDES FOUND IN SYSTEM
C     NZCLAS  NUMBER OF DIFFERENT ZONE CLASSES
C
C*********************************************************************
```

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