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THE ARGONNE REACTOR COMPUTATION
(ARC) SYSTEM

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Printed in the United States of America

Available from

Clearinghouse for Federal Scientific and Technical Information
National Bureau of Standards, U. S. Department of Commerce
Springfield, Virginia 22151

Price: Printed Copy \$3.00; Microfiche \$0.65

ANL-7332

Reactor Technology

(TID-4500)

AEC Research and

Development Report

ARGONNE NATIONAL LABORATORY

9700 South Cass Avenue

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THE ARGONNE REACTOR COMPUTATION
(ARC) SYSTEM

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THE ARGONNE REACTOR COMPUTATION (ARC) SYSTEM

by

B. J. Toppel

I. INTRODUCTION

The reactor physicist is primarily concerned with solving the Boltzmann equation for a particular physical configuration. In addition, the reactor designer is involved with numerous adjunct problems to further define the interaction of the reactor with its environment. In this area, for example, the problem will be influenced by the engineering realities of the physical system.

Table I illustrates the scope of the problems confronting the reactor designer. Three broad categories are indicated, and several examples are listed in each of these.

TABLE I. Scope of Reactor Problems

Problem Category	Examples
Cross-section Manipulations	Unresolved resonances, resolved resonances, elastic scattering, inelastic scattering, $n, 2n$ considerations, thermal-region treatment, ...
Solution of the Boltzmann Equation	1D, 2D, 3D diffusion theory, P_n transport theory, S_n transport theory, Monte Carlo treatment, ...
Adjunct Calculations	Fuel cycle, economics, neutron inventory, perturbation analysis, kinetics, thermodynamics, hydrodynamics, engineering considerations, spatial synthesis, ...

Reactor problems have been traditionally attacked with the help of computers by using a number of self-contained and unrelated codes, each having unique input requirements and furnishing results on a variety of output media such as printed page, tape, punched cards, etc. Problems requiring the application of several such codes, with results of one code used as input for another, normally involve several unrelated computer runs with intervening human manipulation of data. Also, because of the

TABLE II. Problems for a Typical
Reactor-physics Computation

-
1. Generate multigroup cross sections
 2. Solve 1-D multigroup diffusion-theory equations
 3. Calculate neutron inventory for the system
 4. Perform perturbation analyses on the system
-

sovereign nature of such traditional programs, the use of several codes involved with similar algorithms has invariably required the preparation of unique input for each, and frequently, human involvement in data reduction in order to compare results.

As an example, Table II lists the problems for a typical reactor-physics computation.

The steps traditionally involved in accomplishing the task outlined in this table can be illustrated by referring to specific codes for the sake of definiteness. The codes referred to are IBM-704 codes, although that fact is irrelevant to the argument.

Table III lists the steps concerned with setting up a cross-section set for a thermal-reactor problem. Note that three separate uses of the computer are involved.

TABLE III. Steps for Cross-section Generation

Manual	Computer
Prepare and punch input for GAM I ¹	Run GAM I code
Manipulate GAM I output	
Prepare and punch input for SOFOCATE ²	Run SOFOCATE code
Manipulate SOFOCATE output	
Prepare and punch input to REX LIB ³	Run REX LIB code and generate cross-section library tape

Table IV involves solution of the diffusion-theory equation followed by the neutron-inventory and perturbation-theory calculations. Here, two separate computer runs are involved. No neutron-inventory code is available for direct use with a REX output so that the neutron inventory would be obtained from a desk calculation.

The situation as exemplified by the above example provides repeated opportunity for human error and involves the expenditure of extensive time for both the hand manipulations and the computer runs.

TABLE IV. Neutronics Calculations

Manual	Computer
Prepare and punch input for REX ⁴	Run REX code and generate real and adjoint flux tape
Compute neutron inventory	
Prepare and punch input for DEL ⁵	Run DEL code

There have been a number of attempts to automate computer usage in regard to such a sequence of interrelated calculations. Table V lists examples of some of these.

TABLE V. Examples of Automated Reactor Computations

1. KAPL KARE System
2. ANL MACH 1 System
3. KAPL NOVA System
4. ANL ARC System

The KARE system⁶ developed at KAPL consists of a collection of machine-language programs. Each program depends on the other programs of the system and will not function alone. KARE is designed to deal with rather specific classes of problems involving neutronics and depletion studies.

The MACH 1⁷ system is based on the AIM⁸ diffusion-theory code and includes a collection of adjunct routines intended to follow the neutronics calculation. These include, for example, neutron inventory, perturbation theory, and a calculation of β_{eff} and the prompt-neutron life-time. MACH 1 is a FORTRAN-programmed code package and so is much more amenable than is KARE for use by other installations.

The KAPL KARE system and the ANL MACH 1 system both suffer from some serious drawbacks. In particular, extending these systems is difficult because of the extreme dependence of each program on other programs in the system. Also, many aspects of reactor theory, such as Monte Carlo methods and higher-order approximations to the transport equation, are not incorporated in these rather specialized code packages. For KARE, particularly, applying this system to a simple problem is often difficult.

The NOVA system currently under development at KAPL⁶ on a CDC-6600 computer is an attempt to eliminate these problems. NOVA is a modular system designed to facilitate elaborate program linkages and automate data storage and retrieval. NOVA uses the KAPL-developed DATATRAN language⁹ for data handling and module linkages.

The remainder of this report describes the Argonne Reactor Computation (ARC) system under development at the Argonne National Laboratory.

II. PURPOSE AND BASIC CONCEPTS OF THE ARC SYSTEM

The ARC system, which is being implemented on an IBM System/360 Model 50-75 computer complex, represents a break with past computer methods in essentially all respects. The ARC system enjoys two major advantages as compared with conventional computer codes. These are:

- (1) The ability to automate the linkage of computational modules in an arbitrarily complex manner, without human intervention for data handling, in order to attack sophisticated reactor problems.
- (2) The ability to simply store away, and, at a later time, retrieve data generated by an ARC run to facilitate the rerunning of previous problems with data changes, or the extension of previous problems into further computational areas.

The ARC system consists of:

- (1) The Datapool--The collection of data and computational algorithms that can be used by ARC.
- (2) Computational Modules--Conventional program subroutines.
- (3) Standard Paths--Control programs similar to the driver or executive portions of large conventional codes containing numerous subroutines or overlays.
- (4) Operating System--Collection of codes which form the interface between ARC and the computer hardware.

The computational modules and standard paths operate under the direction of the operating system in an automated and unified manner.

The route to be taken through ARC may be determined by selecting a previously cataloged FORTRAN IV control program known as a standard path, or by programming the required path at run time. In the latter case, the full capability of the FORTRAN compiler is brought to bear on setting up the current ARC run. The only limit to the complexity of the route to be taken through ARC is that imposed by the ingenuity of the user.

The individual computational modules are highly restricted in scope so that, for example, neutronics-calculations modules such as 1D-Diffusion, 2D-Transport etc., are concerned only with the algorithms involved in computing fluxes, k_{eff} , etc. They are specifically not involved in manipulating input or output.

The computational modules are also highly standardized with regard to their interface quantities. In particular, the adjunct calculations modules, which depend to a large extent on data generated by the neutronics-calculations modules, will be compatible with any of these modules. Thus, for example, only one Neutron Inventory module is required for the ARC system, rather than one for each different type of neutronics module.

Once the interfaces are defined for any of the computation modules in ARC, these modules can be programmed without knowledge of other modules of the system. This aspect of the system is extremely important in that it permits programming and assembling a limited ARC system which can be put into use while further subsequent modules are being developed. It also encourages module exchanges with other laboratories since the generally tedious input-output efforts are handled separately. The modules are being programmed using FORTRAN IV to facilitate their use by other installations.

The independence of the various computational modules is actually made possible by use of the datapool concept.

The ARC system uses a datapool with all external inputs, the computational modules, the standard paths, the utility programs, and the results generated by all the computational modules being stored in the datapool under the direction of the operating system. Similarly all the data needed by a module are retrieved from the datapool by the operating system.

In its most elementary form, the datapool might consist of files on a magnetic tape or tapes. However, since the disk and data cell storage capacity of modern computers is measured in the tens of millions, such modern random-access memory devices are more appropriate and are utilized for the datapool of ARC, supplemented by tape storage for low-activity files.

The datapool is organized into data sets consistent with the implementation of ARC on the IBM System/360. The data sets in general correspond to particular categories of data such as 1D-diffusion theory real flux, geometry data, cross-section data, etc. The user can designate which data are to be cataloged away into the datapool from the current ARC run and which previously generated data sets are to be retrieved for use during the current run. This capability facilitates the rerunning of previous problems with slight parameter changes, the restarts of problems not yet completed, or the running of new problems requiring the results of previous computations, and is one of the most powerful aspects of the ARC concept.

The datapool can also be loaded at run time using the operating system. Thus, the user may supply some of the data that normally would be generated by a computation module.

Figure 1 is a schematic representation of the ARC system. The configuration represented corresponds to the situation in which the operating system has transferred control to a standard path which has in turn called a particular computational module into the fast core from the datapool.

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Fig. 1. Schematic Representation of the ARC System

The ARC system is open-ended and can be extended indefinitely. In particular, use of the general FORTRAN compiler is available so that the user may generate at run time a module or path not yet available in the system. In the latter case, the program generated is designated as a nonstandard path. Clearly, all standard paths are initially nonstandard paths.

From the user's point of view, the ARC system facilitates reactor-physics calculations that involve many independent computations. These computations may be processed serially and may incorporate logical decisions.

A standard path may be used to link ARC program modules in such a manner as to effectively generate the equivalent of a present-day self-standing code. On the other hand, because of the flexibility of the system, we may easily use standard paths to perform comparative calculations, either with regard to variations in input data, or with regard to computational algorithmic methods. Indeed, since logical decisions can be made during execution of a path, the particular algorithms to be invoked need not be predetermined. Such paths involving branches based upon logical decisions use the full capability of the ARC system.

III. COMPUTATIONAL SCOPE OF THE SYSTEM

Table VI reflects the current thinking in regard to modules for the ARC system. The module names describe the function of the modules. The box marked ARC MODULE in Fig. 1 may correspond to any of the Table VI modules. The module FORTRAN names are also given in the table.

TABLE VI. ARC System Modules

I. Cross-section Preparation Modules

A. Input Modules

1. Epithermal Cross-section Specifications CSI001
2. Thermal Cross-section Specifications CSI002
- 3.

B. Computational Modules

1. Resonance Cross Sections CSC001
2. Nonresonant Cross Sections and Fundamental-mode Spectrum CSC002
3. Thermal Cross Sections CSC003
4. Broad-group Cross Sections and Fundamental-mode Spectrum CSC004
- 5.

C. Output Edit Modules

1. Thermal Cross-section Edit CSE001
- 2.

II. Neutronics Calculations Modules

A. Input Modules

1. Cross-section Homogenization Specifications NUI001
2. Geometry Specifications NUI002
3. Neutronics Specifications NUI003
4. 1D-Transport Specifications NUI004
5. 2D-Transport Specifications NUI005
6. Diffusion-mesh Refinement Specifications NUI006
7. Transport-mesh Refinement Specifications NUI007
8. Neutronics Output Manipulation Specifications NUI008
- 9.

B. Computational Modules

1. Cross-section Homogenization NUC001
2. 1D-Diffusion NUC002
3. 1D-Transport NUC003
4. 2D-Diffusion NUC004

TABLE VI (Contd.)

-
5. 2D-Transport NUC005
 6. Diffusion-mesh Refinement NUC006
 7. Transport-mesh Refinement NUC007
 8. Criticality Search NUC008
 - 9.

C. Output Edit Modules

1. Neutronics Output Manipulation NUE001
- 2.

III. Adjunct Calculations Modules

A. Input Modules

1. Neutron Inventory Specifications AJI001
2. Diffusion Perturbation Specifications AJI002
3. Transport Perturbation Specifications AJI003
4. Spatial Synthesis Specifications AJI004
5. Group Collapse Specifications AJI005
6. Bivariate Cross-section Interpolation Specifications AJI006
- 7.

B. Computational Modules

1. Neutron Inventory AJC001
2. Diffusion Perturbation AJC002
3. Transport Perturbation AJC003
4. Spatial Synthesis AJC004
5. Group Collapse AJC005
6. Bivariate Cross-section Interpolation AJC006
- 7.

C. Output Edit Modules

1. Neutron Inventory Edit AJE001
2. Diffusion Perturbation Edit AJE002
3. Transport Perturbation Edit AJE003
4. Spatial Synthesis Edit AJE004
5. Group Collapse Edit AJE005
6. Bivariate Cross-section Interpolation Edit AJE006
- 7.

IV. Fuel-cycle and Depletion Calculation Modules

A. Input Modules

1. Fuel-cycle Specifications FCI001
2. Economics Specifications FCI002
- 3.

TABLE VI (Contd.)

B. Computational Modules

1. Fuel Cycle FCC001
2. Economics FCC002
- 3.

C. Output Edit Modules

1. Fuel-cycle Edit FCE001
2. Economics Edit FCE002
- 3.

V. Safety and Accident Calculations Modules

A. Input Modules

1. Point Kinetics Specifications SAI001
2. Spatial Kinetics Specifications SAI002
3. Heat Transfer Specifications SAI003
4. Two-phase Coolant Flow Specifications SAI004
5. Core Compaction Specifications SAI005
6. Compressible Fluid Hydrodynamics Specifications SAI006
7. Fuel-element Deformations Specifications SAI007
8. Initiating Mechanisms Specifications SAI008
9. Fuel-Coolant Interaction Specifications SAI009
- 10.

B. Computational Modules

1. Point Kinetics SAC001
2. Spatial Kinetics SAC002
3. Heat Transfer SAC003
4. Two-phase Coolant Flow SAC004
5. Core Compaction SAC005
6. Compressible-fluid Hydrodynamics SAC006
7. Fuel-element Deformations SAC007
8. Initiating Mechanisms SAC008
9. Fuel-Coolant Interaction SAC009
- 10.

C. Output Edit Modules

1. Point-kinetics Edit SAE001
 2. Spatial-kinetics Edit SAE002
 3. Heat-transfer Edit SAE003
 4. Two-phase Coolant Flow Edit SAE004
 5. Core Compaction Edit SAE005
 6. Compressible Fluid Hydrodynamics Edit SAE006
 7. Fuel-element Deformations Edit SAE007
 8. Initiating Mechanisms Edit SAE008
 9. Fuel-Coolant Interaction Edit SAE009
 - 10.
-

The listing has been grouped into five main categories. Within each category, the modules are further organized into Input, Computational, and Output Edit modules. In each category, a blank entry has been included to imply the open-ended nature of the ARC module library.

The input modules have BCD card-image upper-interface data sets, while the computational modules generally deal with binary data sets. The edit modules have both BCD and binary upper-interface data sets. Eventually, selective edits will be possible depending upon user choice. For the initial implementation, most edit modules will be similar to the output routines of classical codes in that little or no selectivity is provided in the output complexity.

The various modules, together with their pertinent interface quantities, are further described in Appendix B.

The Phase I version of ARC, currently under development, will include the following capability:

1. Cross-section generation modules based on the MC² code.¹⁰ In addition, the Argonne-revised version of the thermal-energy code, THERMOS,¹¹ will be incorporated into the system. These comprise modules in categories IA, B, and C in Table VI.
2. One- and two-dimensional diffusion- and transport-theory neutronics modules related to the present CANDID1D,³ CANDID2D,³ SNARG1D,¹² and SNARG2D³ codes, but with some extension of the present capability of these codes such as improvements in convergence, inclusion of internal logarithmic boundary conditions, volume and surface sources, improved scaling of boundary fluxes (SNARG), and an improved negative-flux fix-up routine. The associated modules fall into categories IIA, B, and C of Table VI.
3. Fuel-burnup modules, including isotopic change and fuel management algorithms.¹³ A general isotopic change capability will be included, specifically including radioactive decays and various neutron-heavy-particle reactions. The fuel-management capability will permit study of the equilibrium fuel cycle directly, as well as displaying the approach to equilibrium in detail. These modules are listed in categories IVA, B, and C in Table VI.
4. Various of the adjunct modules concerned with neutron inventory and perturbation theory listed in categories IIA, B, and C of Table VI.

Increasing the utility of the system beyond Phase I requires implementation of other of the modules listed in Table VI, particularly in the areas of Safety and Accident Calculations.

Additions to the system in the areas of Monte Carlo and three-dimensional neutronics capabilities are also obvious and desirable extensions which will be made to the ARC system computational algorithms.

Finally, we may mention some of the future system-capability objectives for ARC.

Rapid retrieval of stored data sets to verify that they are the particular sets one wants to use for other problems is clearly desirable. In general, however, having this information in permanent form will not be necessary. Thus, it would be appropriate to have these data sets displayed on remote cathode-ray screens.

In addition to the contents of the data sets, it would be useful to the casual user to have at hand a brief description of the data-set contents. This might most easily be accomplished via automated report-writing features. Again it will be profitable to generate these reports on a transitory medium such as an image on a remote cathode-ray screen, at the user's option.

We may also foresee in the future the use of a remote console with light pen and extended keyboard to monitor long problems by printing out on request the current status of certain data sets or of particular elements of these data sets. Such a facility would provide the capability of data revision during execution in order to expedite long calculations.

The ultimate objective of the ARC system is to provide a flexible computation system of high utility to facilitate solution of any of the problems of interest to the reactor designer. The ARC system will clearly never be completed.

APPENDIX A

System Structure

Program linkages and data management in the ARC system are accomplished through the facilities provided by the IBM System/360 Operating System and the ARC system-modules.[†] Some of the ARC system-modules occupy core for the entire ARC run, and others are called in as required.

The ARC system-modules provide the following functions:

- (1) Dynamic loading of programs.
- (2) Location of data sets.
- (3) Dynamic data-storage allocation.
- (4) Production of BCD data sets from card input.
- (5) Maintenance of tables required during an ARC run.

The executable programs in the ARC system are stored in a partitioned data set (library) called ARC.MODLIB whose members may be:

- (1) Computational modules.
- (2) ARC system-modules.
- (3) Path drivers or executive modules.
- (4) Overlay structures containing (1), (2), and (3).

Figure 2 is a picture of core-storage allocation, with time increasing from left to right. A description of events in each time interval follows.

<u>Interval</u>	<u>Events</u>
1	PATH1 is to be executed so it is in core. ARC system-module SYSTEM is part of this initial load module.
2	PATH1 called SYSTEM causing INITIAL, SNIFF, and BCDDS to be loaded.
3	INITIAL, SNIFF, and BCDDS are executed for the first time, causing tables to be initialized and flags to be set so that a subsequent call to any of these modules will not reinitialize the tables. The first call to BCDDS loads SCAN to process all of the input data into one data set. This data set will be processed piecemeal by STUFF.

[†]Complete details are contained in AMD Technical Memorandum No. 157 by L. C. Just and S. Sparck.

Interval	Events
4	PATH1 needs BCD data, so a call to BCDDS results in the loading of STUFF to process the input data for the first call from PATH1.
5	CALL LINK ('MODULEA') causes loading and execution of MODULEA (see Table VII).
6	CALL LINK ('MODULEB') causes loading and execution of MODULEB.
7	PATH1 executed CALL LINK ('PATH2'). PATH2 is loaded and given control. PATH2 tries to initialize the system but cannot, so PATH1 is still in control of tables.
8	PATH2 needs BCD data, so a call to BCDDS causes STUFF to be loaded and executed.
9	PATH2 executes CALL LINK ('MODULEC').
10	PATH2 executes CALL LINK ('MODULEA').
11	Control has passed back to PATH1, which has executed CALL LINK ('MODULED').

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Fig. 2. Core Storage Allocation during an ARC Run. Modules marked with * are ARC system-modules.

Table VII lists the system-modules with a brief description of the functions performed. With the exception of LOAD and LINK, all system-modules are written in FORTRAN IV.

TABLE VII. ARC System-module Descriptions

Module	Language	Function
LOAD	Assembly	This module locates a module in a library and loads it into core, generally for the duration of the run.
LINK	Assembly	Causes execution of modules already loaded into core, and loading and execution of those that are not in core.
SYSTEM	FORTRAN IV	The first executable statement in a path driver must be CALL SYSTEM. This causes the system to be initialized. This module also contains LINK and LOAD. SYSTEM must be part of every nonsystem-module in the library.
SNIFF	FORTRAN IV	Given a data set name, SNIFF returns the data-set reference number and also maintains tables of data-set usage.
BCDDS	FORTRAN IV	With modules SCAN and STUFF, BCDDS creates BCD data sets from card input.
SCAN	FORTRAN IV	This module is only called once to create a data set containing all of the card input.
STUFF	FORTRAN IV	This module provides BCD data sets as they need to be created.
INITIAL	FORTRAN IV	This module works with SYSTEM to initialize the system.

A path uses a number of data sets. Each data set that can be referenced by a path has a number assigned to it; this is done by the path driver. When a module calls SNIFF, with the data-set name as a parameter, the number (N) associated with that data set is returned so that READ (N) LIST, will read the data set. For example, if the data set GEOM is to be referenced in a module, a data set of the form ARC.GEOM.RII must be available at run time. The operating system requires that an identifier of the type FTNNF001 be assigned to this data set if a FORTRAN program is to reference it as NN. SNIFF returns NN when called with GEOM as a parameter.

As the system exists today, path execution is a nonautomated procedure. Many IBM Job Control Language (JCL) cards must be used to interface properly with the operating system. This problem could be eliminated with a simplified user-oriented language, ARC Control Language (ACL), which would serve as input to a program (ARCOMP) that would produce the JCL needed to run the job.

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Fig. 3. Relationship between ARC Control Language and Job Control Language

Figure 3 shows the relationships between these elements.

Note that the user can appear in two places; he could write in ACL or JCL and provide identical functions. While ACL was being developed, functions not yet implemented in ACL could be had through JCL. All of the capability afforded by the JCL could ultimately be available through the simplified user-oriented ACL.

The specifications for such an automated user-oriented system will be published in a forthcoming technical memorandum. Implementation of the system is not expected to begin until experience is gained through the first nonautomated use of the ARC system.

APPENDIX B

ARC Module Descriptions

The obvious complexity of the ARC system makes it imperative that rigorous discipline be maintained in regard to organization, book-keeping, FORTRAN symbol standardization, etc. Since the various modules of the system will be programmed by different individuals, standardizing the documentation package for the modules is also clearly important so as to ultimately produce a unified description of the system and to facilitate module exchanges with other laboratories.

A dossier will eventually exist for each module in the system comprising the ARC module standard-documentation package. The format of this dossier is outlined in Fig. 4.

TITLE: Module name.

PROGRAMMER: Programmer's name.

DESCRIPTION OF THE PROBLEM: A detailed statement of the purpose of the program. May include analytical equations which clearly define the algorithms to be used.

REFERENCES: All references to memoranda, reports, etc., pertinent to the physical problem as well as the machine program.

INTERFACE QUANTITIES REQUIRED: A description and definition of the interface data sets used by the module. Glossary names will be used, and subscript order will be noted.

INTERFACE QUANTITIES OUTPUT: A listing of the output interface data sets generated by the module, with definitions and subscript order noted.

APPENDIX A. MATHEMATICAL METHOD AND NUMERICAL ANALYSIS: All analytical equations to be solved and the methods to be used, such as quadrature formulas, necessary approximations, etc.

APPENDIX B. DETAILED SCHEMATIC FLOW DIAGRAMS: Flow diagrams of module and subroutines, when pertinent. The flow should be described with meaningful prose and/or equations that are easily related to Appendixes A and C.

APPENDIX C. FORTRAN LISTING: Heavily annotated listing using comment cards that are closely related to the detailed schematic flow diagram.

APPENDIX D. TEST PROBLEMS

SPECIFICATIONS: A prose description of the problems being solved and the problem input interface quantities.

RESULTS: The interface quantities generated by the module.

VERIFICATION: Comparisons with hand calculations, results of other proven codes, etc.

Fig. 4. ARC Module Dossier Format

For the purposes of this report, since ARC is still in its initial developmental stages, the module descriptions that follow are much less complete than the ultimate dossier. They convey the current thinking in regard to scope and algorithmic methods. Whenever possible, data-set correspondences have been included.

Not all the modules listed in Table VI are represented in this appendix as, indeed, not all the modules in the ARC system are even listed in Table VI. Each module description given below will conform more or less to the following format depending upon the degree to which the module has been finalized.

1. Person responsible for description
2. Module name
3. Nature of physical problem solved
4. Method of solution
5. Related programs
6. References
7. Machine requirements
8. Upper and lower interface quantities

Output edit modules have no lower interface data sets since current plans call for edit modules to output directly to peripheral printers.

1. Epithermal Cross-section Specifications CSI001

Prepared by: A. L. Rago

a. Nature of Physical Problem Solved

This module reads the BCD card image data set for epithermal cross-section generation modules.

b. Method of Solution

This module reads input data, checks input requests of the evaluated nuclear-data library, and makes a consistency check of all input data.

c. Related Programs

This routine is analogous to the subroutine INPUT of the CDC-3600 automated multigroup cross-section generation program, MC².

d. Reference

B. J. Toppel, A. L. Rago, and D. M. O'Shea, MC²--A Code to Calculate Multigroup Cross Sections, ANL-7318 (June 1967).

e. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

Quantities Used

A.XSSPC

Problem identification. Maximum and minimum energy boundaries. Fine-group lethargy width. Convergence criteria. Isotope temperatures. Buckling iteration data. Isotope identification. Option parameters. Heterogeneous geometry factors. Fuel-pin concentration. Homogenized clad-coolant concentration. Atom densities for fundamental-mode calculation. Thermal cross section (optional). Fundamental-mode spectrum (optional). Broad-group energy boundaries.

XS.ENDF

Isotope names of basic nuclear data library.

Lower-interface Data Modules

Quantities Produced

B.XSSPC

Problem identification. Maximum and minimum energy boundaries. Fine-group lethargy width. Broad-group lethargy

Lower-interface Data ModulesQuantities Produced

B.XSSPC (Contd.)

boundaries. Convergence criteria.
Buckling iteration data. Option parameters. Heterogeneous geometry factors. Fuel-pin concentrations. Homogenized clad-coolant concentration. Atom densities for fundamental-mode calculation. Isotope temperatures. Isotope identification. Broad-group energy boundaries.

XS.THERM

Thermal-group cross sections.

FR.FM

Fundamental-mode spectrum.

2. Thermal Cross-section Specifications CSI002

Prepared by: D. A. Sargis

a. Nature of Physical Problem Solved

The module reads BCD card images. Consistency checks are made on the input data.

b. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

Quantities Used

A.THIN

General descriptive data, such as mixture specifications. Mesh structure. Region-mesh correspondence. Mixture-mesh correspondence. Source, transfer cross section, geometry. User-supplied cross-section data.

Lower-interface Data Module

Quantities Produced

B.THIN

General descriptive data, such as mixture specifications. Mesh structure. Region-mesh correspondence. Mixture-mesh correspondence. Source, transfer cross sections, geometry, cross-section flags. User-supplied cross-section data.

3. Resonance Cross Sections CSC001

Prepared by: A. L. Rago

a. Nature of Physical Problem Solved

Cross sections in the resolved resonance region are calculated using Doppler-broadened line shapes with an equivalence relation to account for heterogeneities. The interference between resonance and potential scattering, and the interference with overlapping resonances in other isotopes are included.

Cross sections in the unresolved resonance region are computed by taking averages over suitable Porter-Thomas distributions of the neutron and fission widths. The program does the calculation for both s and p wave neutrons, and includes a summation over spin states in each case. The program also permits energy variation of the fission and neutron widths over the unresolved region. A flux-correction factor is used consistent with the treatment used in the resolved-resonance region.

b. Method of Solution

Calculations in the resonance region may be either for homogeneous mixtures, or for heterogeneous systems.

For heterogeneous calculations, cross sections for materials present in the pin region are obtained using the equivalence relation in which the total potential scattering cross section is augmented by an "escape" cross section. Outer region materials have cross sections obtained using a homogeneous treatment in which the total cross section used in the calculation results from the volume-weighted mixture of pin and outer-region contributions. If a material appears in both pin and outer region, the code obtains its resonance cross sections as an outer-region material. Thus, for example, for a sodium-logged oxide fuel with an outer sodium coolant region, the resonant sodium capture cross section is obtained with a total cross-section weighting corresponding to the volume-weighted pin and outer-region mixture.

The single-level Breit-Wigner formalism is used for calculation of resonance cross sections.

For the unresolved resonance calculations, cross sections are evaluated at discrete energy points E^* in the unresolved energy region.

To calculate the effective unresolved capture and fission cross sections, respectively, at energy E^* for isotope m , the module uses

$$\overline{\sigma_c^m(E^*)} = \sum_s^m \frac{\frac{\sigma_p \Gamma_\gamma^s}{\langle D^s \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(u) \int_0^\infty \frac{\psi^s}{\psi^s + \beta^s} dx dr du}{1 - \frac{1}{\langle D^s \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(u) \Gamma^s \int_0^\infty \frac{\psi^s}{\psi^s + \beta^s} dx dr du}, \quad (1)$$

and

$$\overline{\sigma_f^m(E^*)} = \sum_s^m \frac{\frac{\sigma_p}{\langle D^s \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(u) \overline{\Gamma_f(E^*)} \int_0^\infty \frac{\psi^s}{\psi^s + \beta^s} dx dr du}{1 - \frac{1}{\langle D^s \rangle} \int_0^\infty P_n(r) \int_0^\infty P_k(u) \Gamma^s \int_0^\infty \frac{\psi^s}{\psi^s + \beta^s} dx dr du}. \quad (2)$$

Here s represents a particular sequence of resonances (particular angular momentum and channel spin), $\langle D^s \rangle$ is the average spacing of resonances of sequence s , $P_n(r)$ is a chi-squared distribution with n degrees of freedom, and r and u are, respectively, the ratio of neutron width at E to mean neutron width at E^* , and fission width at E to mean fission width at E^* . The module allows values of k from 1 to 5 and n of 1 or 2. The library tabulation specifies the number of degrees of freedom to be used in the two width distributions.

Also,

$$\beta^s = \frac{\sigma_p}{\sigma_0^s},$$

$$\sigma_0^s = 4\pi g \lambda^2 \frac{\Gamma_n^s}{\Gamma^s},$$

$\psi^s = \psi(\xi^s, x^s)$, the usual Doppler-broadened line-shape function,

$$\xi^s = \left(\frac{A \Gamma^s{}^2}{4 E_0 k T} \right)^{1/2} = \frac{\Gamma^s}{\Delta},$$

$$x^s = \frac{2(E - E_0^s)}{\Gamma^s},$$

and all widths are measured at the resonance energy E_0^s .

For fertile isotopes, the integral over the chi-squared distribution $P_k(u)$ for the fission widths would drop out of Eq. 1 and Eq. 2 would drop out entirely.

In these equations the total cross section has been broken into a resonant part and a remainder, the remainder being denoted as σ_p . The resonances contributing to the resonant portion are assumed to be narrow so σ_p includes the resolved resonant total cross sections for all nonnarrow resonances in the mixture, and the total background potential scattering cross section for all materials present. The module includes resonant contributions to σ_p for all materials in the mixture of mass less than 100; σ_p is evaluated at E^* , and for heterogeneous calculation of pin materials, according to the equivalence relation, the escape cross section per absorber atom is also included. In deriving Eqs. 1 and 2 (see Reference), we have neglected overlap effects between different resonances of the same sequence, overlap between more than two sequences, and interference effects.

The module also allows the unresolved region to overlap the resolved resonance region. This is convenient, for example, at higher energies, where a large number of weak p-wave resonances may be unresolved, whereas members of the s-wave population are resolved.

The calculation of the effective ultrafine (or fine) group cross sections in the resolved resonant region involves a flux weighting assuming $\phi(E) \sim 1/\Sigma_t(E)$, so that for group i and isotope m ,

$$\langle \sigma_c^m \rangle_i = \frac{\sum_j \int_{E_i}^{E_{i+1}} \frac{\sigma_c^m(E)_j}{\Sigma_t(E)} dE}{\int_{E_i}^{E_{i+1}} \frac{dE}{\Sigma_t(E)}} \quad (3)$$

The E_i and E_{i+1} are, respectively, the lower and upper energy boundaries of group i . The sum is over all resonances j belonging to isotope m which contribute to the group i cross section. $\Sigma_t(E)$ includes contributions from all resonances of all isotopes, including interference effects.

The $\langle \sigma_f^m \rangle_{ij}$ is obtained by multiplying Eq. 3 by Γ_f/Γ_γ , the ratio of fission to radiative capture widths.

c. Related Programs

This module is analogous to the RESRES and UNRES subroutines of the CDC 3600 cross-section generation program MC². It performs a calculation similar to the GA codes TUZ and ZUT.

d. Reference

B. J. Toppel, A. L. Rago, and D. M. O'Shea, MC²--A Code to Calculate Multigroup Cross Sections, ANL-7318 (June 1967).

e. Upper- and Lower-interface Data ModulesUpper-interface Data ModulesQuantities Used

B.XSSPC

Group structure. Convergence criteria. Option parameters. Resonance calculation densities. Fine-group energy boundaries. Fine group-ultrafine group relation. Convergence criteria. Option parameters. Heterogeneous geometry factors. Fuel-pin concentration. Homogenized clad-coolant concentration. Isotope temperatures. Isotope identification.

XS.ENDF

Re, W, Im W, real and imaginary parts of complex probability integral used to evaluate ψ and χ functions. Flags for unresolved resonance calculation. Abundances for isotopes in unresolved resonance calculation. Number of angular momentum states. P-wave penetration factor. Number of channel spin states. E^* , energies at which unresolved cross sections are calculated for each angular-momentum state. $\langle \Gamma_n^0 \rangle$, $\langle \Gamma_\gamma \rangle$, $\langle D \rangle$, $\langle \Gamma_f \rangle$. Degrees of freedom in neutron and fission width distribution. Abundances for resolved-resonance calculation. σ_p , E_0 , Γ , Γ_f , Γ_γ , Γ_n .

$$4\pi\kappa_{0g}^2 \frac{\Gamma_n}{\Gamma E_0}, \left(\frac{A\Gamma^2}{4kE_0} \right)^{1/2}, \left(\sigma_p \sigma_{0g} \frac{\Gamma_n}{\Gamma} \right)^{1/2}$$

Masses. Coefficients for ν expression.

Lower-interface Data ModulesQuantities Produced

XS.I.RES

σ_c^i , σ_f^i isotope-dependent resolved-resonant group (ultrafine or fine) capture and fission cross section. Weighting spectrum for resolved-resonance cross sections.

<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
XS.UNRES	E^* , $\sigma_c(E^*)$, $\sigma_f(E^*)$, unresolved energy point capture and fission cross sections.
XS.C.RES	σ_c , σ_f , $\nu\sigma_f$, composition resolved-resonant (ultrafine or fine) capture, fission, and ν times fission cross section.

4. Nonresonant Cross Sections and Fundamental-mode Spectrum CSC002

Prepared by: A. L. Rago

a. Nature of Physical Problem Solved

Nonresonant quantities are represented in the library by the coordinates of end points of linear segments taken from $\ln E$ versus $\ln \sigma$, $\ln E$ versus σ , or E versus σ graphs, where σ may be a cross section or other quantity of interest which varies with energy E . Since the quantities tabulated are then linear functions of the energy, they may be easily integrated analytically using an assumed flux shape, to obtain a suitable average over a fine group of arbitrary width.

Inelastic scattering and $n, 2n$ matrices are computed from excitation functions for individual levels and by using a nuclear evaporation model above the region of resolved levels.

Elastic scattering and transport cross sections computed from Legendre coefficients for the expansions of the scattering angular distribution data are utilized in calculating the fundamental-mode weighting spectrum.

The fundamental-mode weighting spectrum may be calculated in either the ordinary Pl approximation or the consistent Pl or Bl approximations. Iteration on buckling to criticality may be done if desired.

b. Method of Solution

Fine-group effective cross sections for various nonresonant quantities are obtained. These quantities, represented as continuous curves by means of linear segments, include σ_s , $\bar{\mu}$, $\sigma_{\text{inelastic}}$, σ_f , σ_c , $\sigma_{n,2n}$, $\sigma_{n,p}$, and $\sigma_{n,\alpha}$. The σ_c and σ_f are intended to supply any deficiency between the observed capture and fission cross sections, and the quantities calculated using the resonance parameters. For an ultrafine-group problem, $\sigma_{\text{inelastic}}$ and $\sigma_{n,2n}$ are obtained for the ultrafine groups.

The cross sections and corresponding discrete energy points are given as pairs of numbers (σ_n, E_n) , and each type of quantity is associated with one of three types of interpolation laws. These are: $\ln E$ versus $\ln \sigma$, $\ln E$ versus σ , and E versus σ .

In obtaining effective quantities for the fine groups, the module assumes a flux weighting spectrum $\phi(E)$ which is user-designated as either $1/E$, constant, or E , so that for fine group i and material m ,

$$\langle \sigma_x^m \rangle_i = \frac{\int_{E_i}^{E_{i+1}} \sigma_x^m(E) \phi(E) dE}{\int_{E_i}^{E_{i+1}} \phi(E) dE}. \quad (4)$$

In addition to the various cross-section types listed above, such as inelastic, capture, etc., the x also corresponds to the unresolved resonant contribution to the capture and fission cross section utilizing the E^* , $\sigma(E^*)$ pairs calculated by the resonance module.

The integral in Eq. 4 is evaluated by piecewise integration over the linear segments. The term $\sigma_x^m(E)$ may also correspond to $\nu^m(E)$, the number of fission neutrons produced per fission. This is expressed as a cubic polynomial for isotope m . For isotopes not using elastic scattering angular-distribution data, elastic removal to the next lower fine group only is allowed and elastic transport evaluated as $\sigma_s(1 - \bar{\mu})$. Utilization of elastic scattering angular-distribution data involves use of elastic scattering and transport group cross sections calculated by the method of the ELMOE program. An analytical expression is used for scattering and capture for hydrogen in a direct numerical integration of Eq. 4.

Inelastic and $n,2n$ cross sections are calculated. The inelastic calculation uses both discrete-level excitation cross sections, and a statistical nuclear evaporation model where discrete data are lacking.

The discrete-level data are stored as above, using linear segments to describe the excitation of the various levels for each material. With each level excitation is associated a discrete energy loss, E_γ , corresponding to the energy of the gamma ray emitted when the particular level is excited. The material inelastic cross sections are obtained from the summation over the levels involved and are based on the energetics of the events. For example, the average fine group i to fine group j inelastic cross section for material n is given by

$$\langle \sigma_{\text{inel}}^m \rangle_{i \rightarrow j} = \frac{\int_{E_j + E_\gamma}^{E_{j+1} + E_\gamma} \sigma_{\text{inel}}^m(E \rightarrow E - E_\gamma) \phi(E) dE}{\int_{E_i}^{E_{i+1}} \phi(E) dE}, \quad (5)$$

where, as before, $\phi(E)$ may be $1/E$, constant, or E .

In the statistical region, a nuclear evaporation model is used with an energy distribution for the emitted neutrons given by

$$N(E) = E e^{-E/T}. \quad (6)$$

In Eq. 6, T is the appropriate nuclear temperature. The library stores nuclear temperature as a function of energy again as linear segments. The module calculates $\langle T^m \rangle_j$, the material m average temperature appropriate for fine group j , and then evaluates the normalized secondary neutron scattering probability,

$$P_{j \rightarrow k}^m = \frac{\int_{E_k}^{E_{k+1}} E e^{-E/\langle T^m \rangle_j} dE}{\sum_{k=j}^n \int_{E_k}^{E_{k+1}} E e^{-E/\langle T^m \rangle_j} dE} \quad (7)$$

In Eq. 7, the sum in the denominator is over all groups of energy less than or equal to that of group j .

The library contains linear segment data for σ_{inelst}^m , the difference between the total inelastic, and that due to the contribution of all the discrete levels. Averaging σ_{inelst}^m over group j as before using Eq. 4, we finally have, for the statistical contribution to the inelastic cross section

$$\langle \sigma_{inelst}^m \rangle_{j \rightarrow k} = \langle \sigma_{inelst}^m \rangle_j P_{j \rightarrow k} \quad (8)$$

The use of σ_{inelst}^m for the unresolved region allows a smooth transition in the inelastic distributions when going from the discrete to the statistical region. The

$$\langle \sigma_{inel}^m \rangle_{j \rightarrow k} \text{ and } \langle \sigma_{inelst}^m \rangle_{j \rightarrow k}$$

are combined to get the complete inelastic scattering cross section.

The $n, 2n$ cross sections are evaluated following the methods used in the statistical inelastic treatment using appropriate nuclear temperatures and values for the total $n, 2n$ cross sections.

The group fission spectrum is evaluated by a direct numerical integration of the generalized fission spectrum,

$$\chi(E) = \alpha \frac{E}{T^2} e^{-E/T} + (1 - \alpha) \sqrt{\frac{4E}{\pi \beta^3}} e^{-E/\beta}, \quad (9)$$

to yield the normalized group values,

$$\chi_i = \frac{\int_{E_i}^{E_{i+1}} \chi(E) dE}{\sum_{j=1}^n \int_{E_j}^{E_{j+1}} \chi(E) dE} \quad (10)$$

The sum in the denominator is over all groups in the problem.

The library has various sets of α , β , and τ appropriate to the various isotopes, and the user specifies the desired spectrum as part of the problem input.

The P1 fundamental-mode spectrum is calculated using the buckling B^2 and the homogenized macroscopic effective group cross sections, which are obtained using

$$\langle \Sigma_x \rangle_j = \sum_m N^m \langle \sigma_x^m \rangle_j. \quad (11)$$

The x refers to capture, fission, elastic removal, etc., and N^m is the specified atom density for material m . The sum is over all materials in the composition.

For an all-fine-group problem, or for an ultrafine-group problem above the top of the Legendre-coefficient data, the code calculates the fine-group fluxes for the case of the ordinary P1 option using

$$\phi_K^{fg} = \frac{\chi_K + \sum_{J \neq K} \langle \Sigma_{inel} \rangle_{J \rightarrow K} \phi_J^{fg} + \langle \Sigma_{el} \rangle_{K-1 \rightarrow K} \phi_{K-1}^{fg} + 2 \sum_{J \neq K} \langle \Sigma_{n,zn} \rangle_{J \rightarrow K} \phi_J^{fg}}{\text{DENOM}}, \quad (12)$$

where

$$\begin{aligned} \text{DENOM} = & \frac{B^2}{3 \langle \Sigma_{tr} \rangle_K} + \langle \Sigma_c \rangle_K + \langle \Sigma_{np} \rangle_K + \langle \Sigma_{na} \rangle_K + \langle \Sigma_f \rangle_K + \langle \Sigma_{el} \rangle_{K \rightarrow K+1} \\ & + \langle \Sigma_{inel} \rangle_K + \langle \Sigma_{n,zn} \rangle_K - \langle \Sigma_{inel} \rangle_{K \rightarrow K} - 2 \langle \Sigma_{n,zn} \rangle \end{aligned}$$

and

$$\begin{aligned} \langle \Sigma_{tr} \rangle_K &= \langle \Sigma_{eltr} \rangle_K + \langle \Sigma_{inel} \rangle_K + \langle \Sigma_c \rangle_K + \langle \Sigma_f \rangle_K + \langle \Sigma_{n,zn} \rangle_K + \langle \Sigma_{np} \rangle_K + \langle \Sigma_{na} \rangle_K \\ &= \langle \Sigma_{eltr} \rangle_K + \langle \Sigma_a \rangle_K. \end{aligned} \quad (13)$$

In Eqs. 12 and 13, all cross sections are fine-group values obtained from the nonresonant calculation described above, except that in the resolved resonance region, Σ_{cK} and Σ_{fK} include contributions from the resonance module, although in this case, these too are fine-group values.

For an ultrafine-group problem below the top of the Legendre-coefficient library, the module evaluates ultrafine-group fluxes. Let the source into fine group K be written as

$$S_K^{fg} = \sum_{J \neq K} \left[\sum_{j \text{ in } J} \Sigma_{inel,j}^{ufg} \phi_j^{ufg} \frac{\langle \Sigma_{inel} \rangle_{J \rightarrow K}}{\langle \Sigma_{inel} \rangle_J} + \sum_{j \text{ in } J} \Sigma_{n,2n,j}^{ufg} \phi_j^{ufg} \frac{2 \langle \Sigma_{n,2n} \rangle_{J \rightarrow K}}{\langle \Sigma_{n,2n} \rangle_J} \right] + \langle \Sigma_{el} \rangle_{K-1 \rightarrow K} \phi_{K-1}^{fg} \quad (14)$$

In Eq. 14, $\Sigma_{inel,j}^{ufg}$ and $\Sigma_{n,2n,j}^{ufg}$ are evaluated using Eq. 4 with the integration extending over an ultrafine group. The quantities in the angular brackets are fine-group quantities.

The module then defines the source into ultrafine group k, contained within fine group K, as

$$S_k^{ufg} = S_K^{fg} \frac{\Delta e_k^{ufg}}{\Delta e_K^{fg}} + \sum_{j \neq k} \Sigma_{el,j \rightarrow k}^{ufg} \phi_j^{ufg} + \chi_k^{ufg} \quad (15)$$

In Eq. 15, the Δe_k^{ufg} and Δe_K^{fg} are respectively the energy widths of ultrafine group k and fine group K. The ultrafine-group contribution in Eq. 15 is due to the contribution of Legendre coefficient materials. The $\Sigma_{el,j \rightarrow k}^{ufg}$ is written with the superscript to emphasize that it is an ultrafine-group value. For the first ultrafine group at the top of the Legendre-coefficient data, since there is no ultrafine scattering-in source available, the Legendre materials are treated as they are above the Legendre region and contribute to the elastic term as in Eq. 14. This situation does not arise if the maximum problem energy corresponds to 10 MeV or less.

The ultrafine-group flux for ultrafine-group k may be written as

$$\phi_k^{ufg} = \frac{S_k^{ufg}}{L_k} \quad (16)$$

where

$$L_k = \frac{B^2}{3 \Sigma_{tr,k}} + \langle \Sigma_c \rangle_K + \Sigma_{c,k}^{ufg} + \langle \Sigma_f \rangle_K + \Sigma_{f,k}^{ufg} + \langle \Sigma_{el} \rangle_{K \rightarrow K+1} + \Sigma_{el,k}^{ufg} + \Sigma_{inel,k}^{ufg} \left[1 - \frac{\langle \Sigma_{inel} \rangle_{K \rightarrow K}}{\langle \Sigma_{inel} \rangle_K} \right] + \Sigma_{n,2n,k}^{ufg} \left[1 - \frac{2 \langle \Sigma_{n,2n} \rangle_{K \rightarrow K}}{\langle \Sigma_{n,2n} \rangle_K} \right] + \langle \Sigma_{np} \rangle_K + \langle \Sigma_{na} \rangle_K \quad (17)$$

and

$$\begin{aligned} \Sigma_{tr_k} = & \langle \Sigma_{eltr} \rangle_K + \Sigma_{eltr_k}^{ufg} + \Sigma_{inel_k}^{ufg} + \Sigma_{n,2n_k}^{ufg} + \langle \Sigma_c \rangle_K \\ & + \Sigma_{c_k}^{ufg} + \langle \Sigma_f \rangle_K \Sigma_{f_k}^{ufg} + \langle \Sigma_{np} \rangle_K + \langle \Sigma_{n\alpha} \rangle_K. \end{aligned} \quad (18)$$

In Eqs. 15-18, the ultrafine-group quantities use a lower-case subscript and in addition are pointed out by using the ufg superscript. Fine-group quantities, denoted by the upper-case subscript, are treated as being constant for all ultrafine groups contained within the fine group. The $\Sigma_{c_k}^{ufg}$ and $\Sigma_{f_k}^{ufg}$ are obtained in the resonant module. For the region above the resolved resonant region, $\Sigma_{c_k}^{ufg}$ and $\Sigma_{f_k}^{ufg}$ do not appear in the above equations.

The code calculates the total fission source after determining all of the fine- and ultrafine-group fluxes. This is given by

$$S_f = \sum_K \langle \nu \rangle_K \langle \Sigma_f \rangle_K \phi_K^{fg} + \sum_k \langle \nu \rangle_k^{ufg} \langle \Sigma_f \rangle_k^{ufg} \phi_k^{ufg} + \nu_{th} \Sigma_{fth} \phi_{th}. \quad (19)$$

If the user wishes to iterate on B^2 , S_f is compared with one, and if

$$|S_f - 1| > \epsilon, \quad (20)$$

the module computes a new value of B^2 and recalculates the spectrum as above. The procedure is continued until S_f deviates from one by less than or equal to the input convergence criterion ϵ .

If the user inputs thermal-group cross section Σ_{cth} , Σ_{fth} , Σ_{npth} , $\Sigma_{n\alpha th}$, and Σ_{trth} , the module calculates the thermal flux from

$$\phi_{th} = \frac{\langle \Sigma_{el} \rangle_{N \rightarrow N+1} \phi_N^{fg} + \sum_{j>th} \sum_{k>th} \Sigma_{el,j \rightarrow k}^{ufg} \phi_j^{ufg}}{\frac{B^2}{3\Sigma_{trth}} + \Sigma_{cth} + \Sigma_{fth} + \Sigma_{npth} + \Sigma_{n\alpha th}}. \quad (21)$$

In Eq. 21, it is explicitly assumed that there is no fission, inelastic, or $n,2n$ source into the thermal group. The first term in the numerator of Eq. 21 is the fine-group elastic source from the last epithermal fine group, N . The ultrafine-group elastic-source term results from j ranging

over all possible ultrafine groups above the thermal group, and k over all pseudo ultrafine groups in the thermal group. If the user does not input thermal cross sections, ϕ_{th} is set equal to zero.

For consistent Pl and consistent Bl options, the single equation for flux such as Eq. 16 is replaced with a pair of coupled equations for the current and the flux.

The consistent equations, for the current and flux at a buckling of B^2 , may then be written as

$$J_k^{ufg} = \frac{B\phi_k^{ufg}}{3\gamma_k \Sigma_{totk}} + \frac{1}{\gamma_k \Sigma_{totk}} \sum_{j \neq k} \Sigma_{elj \rightarrow k}^{1ufg} J_j^{ufg} \quad (22)$$

and

$$\phi_k^{ufg} = \frac{S_k^{ufg} - \frac{B}{\gamma_k \Sigma_{totk}} \sum_{j \neq k} \Sigma_{j \rightarrow k}^{1ufg} J_j^{ufg}}{L_k^1} \quad (23)$$

In Eq. 23, L_k^1 is obtained from Eq. 17 by replacing Σ_{trk} by $\gamma_k \Sigma_{totk}$, where γ_k and Σ_{totk} are defined.

The module makes the usual transport approximation in regard to the within-group scattering so that there is no $\Sigma_{elj \rightarrow j}^{1ufg}$ term involved, and in Eqs. 22 and 23

$$\Sigma_{totk} = \Sigma_{trk} - \Sigma_{eltrk}^{ufg} + \Sigma_{elrk}^{ufg} \quad (24)$$

with Σ_{trk} given by Eq. 18. The Σ_{eltrk}^{ufg} and Σ_{elrk}^{kufg} are obtained by use of detailed angular-distribution data. Only Legendre-coefficient materials (or hydrogen if present) contribute to the Σ_{eltrk}^{ufg} and Σ_{elrk}^{ufg} .

The consistent Pl equations are obtained by setting γ_k equal to one in Eqs. 22 and 23. For the consistent Bl equations, if B^2 is greater than zero,

$$\gamma_k = \frac{\alpha_k \tan^{-1} \alpha_k}{3 \left(1 - \frac{\tan^{-1} \alpha_k}{\alpha_k} \right)} \quad (25)$$

and

$$\alpha_k = \frac{B}{\Sigma_{\text{tot}_k}} \quad (26)$$

For negative buckling, Eq. 25 is replaced by

$$\gamma_k = \frac{-\alpha_k \tanh^{-1} \alpha_k}{3 \left(1 - \frac{\tanh^{-1} \alpha_k}{\alpha_k} \right)} \quad (27)$$

In this case, only values of α_k less than one are permissible. In the abnormal case, for which $B \geq \Sigma_{\text{tot}_k}$, the code sets α_k equal to one and $\tanh^{-1} \alpha_k$ equal to 10^{70} , and an error message is returned. In the limiting case of zero buckling Eq. 22 yields one for γ_k so that the consistent B1 and consistent P1 equations are identical in this case. Facility is available in all specified above to handle hydrogen.

c. Related Programs

This module is analogous to overlays 3 and 4 of the ANL cross-section generation code MC². The fundamental-mode calculation is also analogous to the ELMOE code.

d. References

A. L. Rago and H. H. Hummel, ELMOE: An IBM-704 Program Treating Elastic Scattering Resonances in Fast Reactors, ANL-6805 (Jan 1964).

B. J. Toppel, A. L. Rago, and D. M. O'Shea, MC²--A Code to Calculate Multigroup Cross Sections, ANL-7318 (June 1967).

e. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

B.XSSPC

Quantities Used

Fine-group energy boundaries. Fine-group lethargy width. Maximum-energy boundary. Minimum-energy boundary. Buckling iteration data. Option parameters. Atom densities for fundamental-mode calculation. Thermal cross sections (optional). Fundamental-mode spectrum (optional). Isotope identification. Fine group-ultrafine group relation.

Upper-interface Data ModulesQuantities Used

XS.UNRES

E^* , $\sigma_c(E^*)$, $\sigma_f(E^*)$, unresolved energy point capture and fission cross sections.

XS.C.RES

σ_c , σ_f , $\nu\sigma_f$, composition-resolved resonant (ultrafine or fine) capture, fission, and ν times fission cross section.

XS.ENDF3

Isotope identification. Masses. Interpolation law flags. $\sigma_x(E_i)$, E_i pairs, where σ_x may be any of σ_s , $\bar{\mu}$, $\sigma_{\text{inelastic}}$, σ_f , σ_c , $\sigma_{n,2n}$, $\sigma_{n,p}$, and $\sigma_{n,\alpha}$. σ_c and σ_f are the nonresonant contribution to the capture and fission cross section. Coefficients for evaluation of $\nu(E)$. Inelastic data parameters E_γ ; $\sigma_{\text{inelastic}}(E_i \rightarrow E_i - E_\gamma)$, E_i pairs for the discrete levels. Nuclear-temperature parameters $T(E_i)$, E_i pairs for statistical contribution to inelastic scattering. Statistical inelastic parameters $\sigma_{\text{inelst}}(E_i)$, E_i pairs, where σ_{inelst} is the difference between the total inelastic and the discrete contribution. $n,2n$ parameters. $\sigma_{n,2n}(E_i)$, E_i pairs for $n,2n$ process. Constants for fission-source spectrum. Elastic scattering angular distribution data.

XS.THERM

Thermal-group cross sections.

Lower-interface Data ModulesQuantities Produced

XS.C.SMT

Microscopic nonresonant σ_c , σ_f , σ_s , $\bar{\mu}$, $\sigma_{\text{inelastic}}$, $\sigma_{n,2n}$, $\sigma_{n,p}$, $\sigma_{n,\alpha}$ group cross sections, discrete-level inelastic group cross sections, statistical inelastic group cross sections, $n,2n$ scattering group cross sections, and unresolved resonant capture and fission group cross sections all for each isotope specified.

XS.C.UFG

Macroscopic $\sigma_{el}^0(j \rightarrow k)$, $\sigma_{el}^1(j \rightarrow k)$, σ_{eltr} , $\bar{\mu}\sigma_{elr}$, σ_{elr} .

FR.FM

Fine-group and ultrafine-group real fluxes and currents. k_{eff} . B^2 , the critical buckling.

Lower-interface Data ModulesQuantities Produced

XS.I.UFG

Microscopic $\sigma_{el}^0(j \rightarrow k)$, $\sigma_{el}^1(j \rightarrow k)$, σ_{eltr} ,
 $\bar{\mu}\sigma_{elr}$, σ_{elr} .

XS.SORS

Fission-source group data.

5. Thermal Cross Sections CSC003

Prepared by: D. A. Sargis

a. Nature of Physical Problem Solved

This module computes the scalar thermal-neutron flux as a function of energy and position in a lattice by solving the integral transport equation with isotropic scattering. One-dimensional slab or cylindrical geometry may be used along with vacuum and reflecting-cell boundary conditions. Arbitrary scattering kernels may be employed, but the Brown-St. John free-gas kernel is built into the module.

The slowing-down sources are computed within the module by assuming the epithermal flux varies as $1/E$ and the down-scattering cross sections are isotropic in the center-of-mass system.

Space- and energy-dependent absorption and total cross sections are calculated for the cell mixtures. Energy-dependent cross sections are also generated for each individual cell isotope. The isotropic-scattering kernels for all isotopes and the space-dependent isotropic-scattering kernels for the mixtures are calculated.

A transfer cross-section option is also available to generate transfer cross sections from each coarse-energy group to all other coarse groups for each space point, and flux- and volume-averaged transfer cross sections for the regional mixtures, as well as for individual cell and edit isotopes.

b. Method of Solution

The integral transport equation is written as

$$vN(\vec{r}, v) = \int d\vec{r}' T(\vec{r}, \vec{r}', v) \left\{ S(\vec{r}', v) + \int_0^{v^*} dv' P(\vec{r}', v, v') N(\vec{r}', v') \right\}, \quad (28)$$

where $N(\vec{r}, v)$ is the space- and speed-dependent neutron density, and $P(\vec{r}', v, v')$ is the differential scattering cross section from speed v' to speed v at $\vec{r}'$. The slowing-down source $S(\vec{r}', v)$ is given by

$$S(\vec{r}', v) = \int_{v^*}^{\infty} dv' P(\vec{r}', v, v') N(\vec{r}', v'), \quad (29)$$

where v^* is the speed corresponding to the cutoff energy between the thermal and epithermal groups. $T(\vec{r}, \vec{r}', v)$ is the transport kernel representing the flux at $\vec{r}$ due to a unit isotropic point source at $\vec{r}'$,

$$T(\vec{r}, \vec{r}', v) = \frac{1}{4\pi |\vec{r} - \vec{r}'|^2} \exp \left\{ - \left| \int_{\vec{r}'}^{\vec{r}} dx \Sigma_t(x, v) \right| \right\}. \quad (30)$$

The scattering kernels $P(\vec{r}', v, v')$ may be supplied by the user or may be calculated within the module using the Brown-St. John free-gas formulation. The slowing-down sources $S(\vec{r}, v)$ are calculated within the module using an age-theory asymptotic flux, or are supplied by epithermal cross-section generating modules.

Cross sections for the isotopes of interest are either input by the user or are read in from a permanent library data set. Mixture cross sections as a function of position and energy group are then computed.

The Thermal Cross-section Module solves Eq. 28 by a power-iteration method to obtain the neutron density $N(\vec{r}, v)$ and neutron flux $\phi(\vec{r}, v)$. Renormalization, extrapolation, and over relaxation schemes are employed to accelerate convergence of the iteration technique.

c. Related Programs and References

H. C. Honeck, A Thermalization Transport Theory Code for Reactor Lattice Calculations, BNL-5826 (Sept 1961).

B. J. Toppel and I. Baksys, The Argonne-revised THERMOS Code, ANL-7023 (March 1965).

d. Machine Requirements

64 K Memory and 8 Tape Units.

e. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
B.THIN	General descriptive data, such as mixture specifications. Mesh structure. Region-mesh correspondence. Mixture-mesh correspondence. Source, transfer cross section, geometry, cross-section flags. User-supplied cross-section data.
XS.TH	Isotope thermal cross sections, $\sigma_a(v)$, $\sigma_f(v)$, $\sigma_s(v)$, $\nu(v)$, $\bar{\mu}(v)$.
XS.KER.I	Isotope scattering kernels.
EN	Energy group structure parameters, such as number of groups and group boundaries.

<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
LPR	The first flight nonleakage probability at $\vec{r}$ and v , $Q(\vec{r}, v)$.
FR.D1	The neutron flux at $\vec{r}$ and v , $\Phi(\vec{r}, v)$.
XS.MIX	The space-dependent mixture cross sections, $\Sigma_a(\vec{r}, v)$, $\Sigma_T(\vec{r}, v)$.
XS.KER.M	Scattering kernels for mixtures.
XS.TH.U	Isotope thermal cross sections for user-supplied data, $\sigma_a(v)$, $\sigma_f(v)$, $\sigma_s(v)$, $\nu(v)$, $\bar{\mu}(v)$.
XS.KER.U	Scattering kernels for user-supplied isotopes.
SDS	Space- and speed-dependent slowing-down source, $S(\vec{r}, v)$.
INTEG	Spatial and energy integration limits.

6. Broad-group Cross Sections and Fundamental-mode Spectrum CSC004

Prepared by A. L. Rago

a. Nature of Physical Problem Solved

This module prepares microscopic multigroup cross sections by a flux-weighted group contraction of quantities calculated by various cross-section generation modules and uses these cross sections to calculate the fundamental-mode real and adjoint spectrum iterating on buckling until criticality is reached.

b. Method of Solution

The algorithms used to obtain the various cross sections are described below according to type. The superscripts bg, fg, and ufg denote broad-group, fine-group, and ultrafine-group quantities, respectively.

(1) Inelastic Scattering Matrix

$$\overline{\sigma_{\text{inel}}^m}^{\text{bg}}_{J \rightarrow K} = \frac{\sum_{k \text{ in } K} \sum_{j \text{ in } J} \langle \sigma_{\text{inel}}^m \rangle_{j \rightarrow k}^{\text{fg}} \phi_j^{\text{fg}}}{\sum_{j \text{ in } J} \phi_j^{\text{fg}}} \quad (31)$$

(2) n,2n Matrix

$$\overline{\sigma_{n,2n}^m}^{\text{bg}}_{J \rightarrow K} = \frac{\sum_{k \text{ in } K} \sum_{j \text{ in } J} \langle \sigma_{n,2n}^m \rangle_{j \rightarrow k}^{\text{fg}} \phi_j^{\text{fg}}}{\sum_{j \text{ in } J} \phi_j^{\text{fg}}} \quad (32)$$

(3) Capture Cross Section. The unresolved-resonant, the resolved-resonant, and the total broad-group cross sections are calculated separately:

$$\left(\overline{\sigma_c^m}^{\text{bg}} \right)_{\text{unresolved}} = \frac{\sum_{j \text{ in } J} \left(\langle \sigma_c^m \rangle_j^{\text{fg}} \right)_{\text{unresolved}} \phi_j^{\text{fg}}}{\phi_J^{\text{bg}}} \quad (33)$$

and

$$\left(\overline{\sigma_{cJ}^{bg}} \right)_{\text{resolved}} = \frac{\sum_{j \text{ in } J} \left(\left\langle \sigma_c^m \right\rangle_j \right)_{\text{resolved}}^{\text{ufg}} \int_{E_j}^{E_{j+1}} \frac{dE}{\Sigma_t(E)} S_j^{\text{ufg}}}{\sum_{j \text{ in } J} \int_{E_j}^{E_{j+1}} \frac{dE}{\Sigma_t(E)} S_j^{\text{ufg}}}, \quad (34)$$

where the integral is the weighting function used in calculating

$$\left(\left\langle \sigma_c^m \right\rangle_j \right)_{\text{resolved}}^{\text{ufg}},$$

and S_j^{ufg} is the source into the ultrafine group j obtained from the fundamental-mode calculation.

In an all-fine-group problem, Eq. 34 involves only fine-group quantities.

The total capture is given by the sum of Eqs. 33 and 34 plus any nonresonant contribution.

(4) Fission Cross Section. As above, the resolved resonant is displayed separately from the unresolved resonant cross section:

$$\left(\overline{\sigma_{fJ}^{bg}} \right)_{\text{unresolved}} = \frac{\sum_{j \text{ in } J} \left(\left\langle \sigma_f^m \right\rangle_j \right)_{\text{unresolved}}^{\text{fg}} \phi_j^{\text{fg}}}{\phi_J^{\text{bg}}} \quad (35)$$

and

$$\left(\overline{\sigma_{fJ}^{bg}} \right)_{\text{resolved}} = \frac{\sum_{j \text{ in } J} \left(\left\langle \sigma_f^m \right\rangle_j \right)_{\text{resolved}}^{\text{ufg}} \int_{E_j}^{E_{j+1}} \frac{dE}{\Sigma_t(E)} S_j^{\text{ufg}}}{\sum_{j \text{ in } J} \int_{E_j}^{E_{j+1}} \frac{dE}{\Sigma_t(E)} S_j^{\text{ufg}}}, \quad (36)$$

and the total fission is the sum of Eqs. 35 and 36 plus any nonresonant contribution.

(5) Average Number of Neutrons per Fission

$$\overline{\nu}_j^{bg} = \frac{\sum_{j \text{ in } J} \langle \nu^m \rangle_j^{fg} \langle \sigma_f^m \rangle_j^{fg} \phi_j^{fg} + \sum_{j \text{ in } J} \langle \nu^m \rangle_j^{ufg} \langle \sigma_f^m \rangle_j^{ufg} \phi_j^{ufg}}{\phi_J^{bg} \overline{\sigma}_{fJ}^{bg}} \quad (37)$$

The $\overline{\sigma}_{fJ}^{bg}$ is the total broad-group J fission cross section given by Eq. 35 and 36.

(6) Inelastic Cross Section

$$\overline{\sigma}_{inelJ}^{bg} = \frac{\sum_{j \text{ in } J} \langle \sigma_{inel}^m \rangle_j^{fg} \phi_j^{fg}}{\phi_J^{bg}} \quad (38)$$

(7) n,2n Cross Section

$$\overline{\sigma}_{n,2nJ}^{bg} = \frac{\sum_{j \text{ in } J} \langle \sigma_{n,2n}^m \rangle_j^{fg} \phi_j^{fg}}{\phi_J^{bg}} \quad (39)$$

(8) n,p Cross Section

$$\overline{\sigma}_{n,pJ}^{bg} = \frac{\sum_{j \text{ in } J} \langle \sigma_{n,p}^m \rangle_j^{fg} \phi_j^{fg}}{\phi_J^{bg}} \quad (40)$$

(9) n,α Cross Section

$$\overline{\sigma}_{n,\alpha J}^{bg} = \frac{\sum_{j \text{ in } J} \langle \sigma_{n,\alpha}^m \rangle_j^{fg} \phi_j^{fg}}{\phi_J^{bg}} \quad (41)$$

(10) Transport Cross Section. The definition of the transport cross section depends upon the option chosen. For the ordinary Pl option,

$$\overline{\sigma}_{trJ}^{bg} = \frac{\sum_{j \text{ in } J} \frac{\langle \sigma_{tr}^m \rangle_j^{fg} \phi_j^{fg}}{\langle \Sigma_{tr} \rangle_j^{fg}} + \sum_{j \text{ in } J} \frac{\sigma_{trJ}^{m,ufg} \phi_j^{ufg}}{\Sigma_{trJ}^{ufg}}}{\sum_{j \text{ in } J} \frac{\phi_j^{fg}}{\langle \Sigma_{tr} \rangle_j^{fg}} + \sum_{j \text{ in } J} \frac{\phi_j^{ufg}}{\Sigma_{trJ}^{ufg}}} \quad (42)$$

where

$$\left\langle \Sigma_{tr} \right\rangle_j^{fg} \text{ and } \Sigma_{trj}^{ufg}$$

are macroscopic quantities for the mixture. The

$$\left\langle \sigma_{tr}^m \right\rangle_j^{fg} \text{ and } \sigma_{trj}^{m,ufg}$$

are evaluated in the Nonresonant Cross Section and Fundamental-mode Spectrum Module.

For an all-fine-group problem, only the fine-group quantities appear in Eq. 42. For an ultrafine-group problem and for Legendre materials, below 10 MeV only the ultrafine-group contributions appear in Eq. 42. In this range, the non-Legendre material transport cross section is given by

$$\overline{\sigma_{trJ}^{m,bg}} = \frac{\sum_{j \text{ in } J} \frac{\left\langle \sigma_{tr}^m \right\rangle_j^{fg} \phi_j^{ufg}}{\Sigma_{trj}^{ufg}}}{\sum_{j \text{ in } J} \frac{\phi_j^{ufg}}{\Sigma_{trj}^{ufg}}}, \quad (43)$$

where the $\left\langle \sigma_{tr}^m \right\rangle_j^{fg}$ is assumed to be constant for all ultrafine groups contained in the fine group over which the average was obtained.

If a consistent option is chosen, Legendre materials and hydrogen have

$$\overline{\sigma_{trJ}^{m,bg}} = \frac{\sum_{j \text{ in } J} \gamma_j \sigma_{totj}^m J_j^{ufg} - \sum_{j \text{ in } J} \sum_{k \neq j} \sigma_{e\ell_{k \rightarrow j}}^{m,ufg} J_k^{ufg}}{J_J^{bg}}, \quad (44)$$

where $\sigma_{e\ell_{k \rightarrow j}}^{m,ufg}$ and σ_{totj}^m are given in the Nonresonant Cross Section and Fundamental-mode Spectrum Module. The γ_j are defined in the same module and are equal to one for the consistent Pl option.

For the non-Legendre materials,

$$\overline{\sigma_{tr}^m}^{bg}_J = \frac{\sum_{j \text{ in } J} \langle \sigma_{tr}^m \rangle_j^{fg} \phi_j^{ufg}}{J_J^{bg}}, \quad (45)$$

and $\langle \sigma_{tr}^m \rangle_j^{fg}$ is assumed to be constant for all ultrafine groups in the corresponding fine groups.

(11) Elastic Scattering Matrix. For non-Legendre materials,

$$\overline{\sigma_{el}^m}^{bg}_{K \rightarrow K+1} = \frac{\phi_j^{fg}}{\phi_K^{bg}} \langle \sigma_{el}^m \rangle_{j \rightarrow j+1}^{fg} \quad (46)$$

Similarly, if m is hydrogen,

$$\overline{\sigma_{el}^H}^{bg}_{J \rightarrow K} = \frac{\Delta E_K}{\phi_J^{bg}} \sum_{j \text{ in } J} \frac{\phi_j^{fg} \langle \sigma_{elr}^H \rangle_j^{fg}}{E_{j+1}}, \quad (47)$$

where ΔE_K is the energy width of broad group K , $\langle \sigma_{elr}^H \rangle_j^{fg}$ is the fine group j average elastic removal cross section due to hydrogen, and E_{j+1} is the lower energy of fine group j .

For Legendre materials in an ultrafine-group problem,

$$\overline{\sigma_{el}^m}^{bg}_{J \rightarrow K} = \frac{\sum_{k \text{ in } K} \sum_{j \text{ in } J} \sigma_{el,j \rightarrow k}^{m,ufg} \phi_j^{ufg}}{\phi_J^{bg}} \quad (48)$$

The module also generates the Pl scattering matrix

$$\overline{\sigma_{el}^m}^{bg}_{J \rightarrow K} = \frac{\sum_{k \text{ in } K} \sum_{j \text{ in } J} \sigma_{el,j \rightarrow k}^{m,ufg} \phi_j^{ufg}}{J_J^{bg}} \quad (49)$$

If hydrogen is present, Eq. 48 includes the contribution

$$\overline{\sigma_{elJ \rightarrow K}^{Hbg}} = \frac{\Delta E_K}{\phi_J^{bg}} \sum_{j \text{ in } J} \frac{1}{2} \left[\sigma_S^H(E_j) \frac{E_{j+1}}{E_j} + \sigma_S^H(E_{j+1}) \right] \frac{\phi_j^{ufg}}{E_{j+1}}, \quad (50)$$

where E_j and E_{j+1} are the upper and lower energies of ultrafine group j in broad group J and the σ_S^H are evaluated in the Nonresonant Cross-section Fundamental-mode Spectrum Module.

The hydrogen contributes to Eq. 49 the amount

$$\overline{\sigma_{elJ \rightarrow K}^{Hbg}} = \frac{\sum_{k \text{ in } K} \Delta e_k^{ufg} E_k^{1/2} \sum_{j \text{ in } J} \frac{1}{2} \left[\sigma_S^H(E_j) \frac{E_{j+1}}{E_j} + \sigma_S^H(E_{j+1}) \right] \frac{J_j^{ufg}}{E_{j+1}^{3/2}}}{J_J^{bg}}, \quad (51)$$

where Δe_k^{ufg} is the energy width of ultrafine group k . The J_j^{ufg} and J_J^{bg} are, respectively, the currents for ultrafine group j and broad group J . No Pl scattering component is calculated for hydrogen for scattering into the thermal group.

The self-scattering in the broad group is obtained by subtracting the sum of all events that remove a neutron from the group from the broad-group transport cross section. Therefore

$$\begin{aligned} \overline{\sigma_{elJ \rightarrow J}^{mbg}} &= \overline{\sigma_{trJ}^{mbg}} - \sum_{k \neq J} \overline{\sigma_{elJ \rightarrow K}^{mbg}} - \overline{\sigma_{n,pJ}^{mbg}} - \overline{\sigma_{n,\alpha J}^{mbg}} - \overline{\sigma_{inelJ}^{mbg}} \\ &\quad - \overline{\sigma_{n,2nJ}^{mbg}} - \overline{\sigma_{cJ}^{mbg}} - \overline{\sigma_{fJ}^{mbg}}. \end{aligned} \quad (52)$$

The module also generates an "anisotropic" self-scattering in the broad group, $\Sigma_{elJ \rightarrow J}^{anisbg}$. This number, when added to the sum of all events that remove a neutron from the group, yields the broad-group total cross section:

$$\begin{aligned} \overline{\sigma_{elJ \rightarrow J}^{anismbg}} &= \overline{\sigma_{totJ}^{mbg}} - \sum_{K \neq J} \overline{\sigma_{elJ \rightarrow K}^{mbg}} - \overline{\sigma_{n,pJ}^{mbg}} - \overline{\sigma_{n,\alpha J}^{mbg}} \\ &\quad - \overline{\sigma_{inelJ}^{mbg}} - \overline{\sigma_{n,2nJ}^{mbg}} - \overline{\sigma_{cJ}^{mbg}} - \overline{\sigma_{fJ}^{mbg}}. \end{aligned} \quad (53)$$

The real flux is evaluated as

$$\phi_k^i = \frac{\chi_k + \psi_k}{DB_i^2 + \Sigma_{rem}^k}, \quad (54)$$

where

ϕ_k^i = i th iterate of the real flux for group k ;

χ_k = fraction of fission source in group k ;

$$\psi_k = \sum_{j=1}^{k-1} \left(\Sigma_{el}^{j \rightarrow k} + \Sigma_{inelastic}^{j \rightarrow k} + 2\Sigma_{n,2n}^{j \rightarrow k} \right) \phi_j^i$$

= scattering source from higher energies;

$\Sigma_{el}^{j \rightarrow k}$ = elastic scattering cross section, group j to group k ;

$\Sigma_{inelastic}^{j \rightarrow k}$ = inelastic scattering cross section, group j to group k ;

$\Sigma_{n,2n}^{j \rightarrow k}$ = $n, 2n$ scattering cross section, group j to group k ;

$D = \frac{1}{3} \Sigma_{tr}^k$, where Σ_{tr}^k = transport cross section for group k ;

B_i^2 = i th iteration of the buckling;

and

Σ_{rem}^k = total removal cross section from group k .

This equation is successively evaluated, iterating on the buckling, B^2 , until

$$|k_{eff} - 1| \leq \epsilon, \quad (55)$$

where

$$k_{eff} = \sum_{j=1}^J \nu \Sigma_j^f \phi_j$$

and

$\nu \Sigma_j^f$ = neutrons per fission times fission cross section for group k,

ϵ = convergence criterion for k_{eff} .

The adjoint flux is evaluated as

$$\phi_k^{+i} = \frac{\nu \sigma_k + \psi_k^+}{DB_i^2 + \Sigma_{\text{rem}}^k}, \quad (56)$$

where

$$\psi_k^+ = \sum_{j=k+1}^K \left(\sigma_{\text{inelastic}}^{k \rightarrow j} + \sigma_{\text{el}}^{k \rightarrow j} + \sigma_{\text{n,2n}}^{k \rightarrow j} \right) \phi_j^+ \quad (57)$$

and all other terms are as previously defined. Here successive evaluation takes place until

$$\left| \sum_{j=1}^J \chi_j \phi_j^+ - 1 \right| \leq \epsilon. \quad (58)$$

c. Related Programs

This routine is analogous to the subroutines AVER, AVERI, and BGPONE of the ANL automated multigroup cross-section generation program, MC².

d. Reference

B. J. Toppel, A. L. Rago, and D. M. O'Shea, MC²--A Code to Calculate Multigroup Cross Sections, ANL-7318 (June 1967).

e. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

XS.I.INP

Quantities Used

Fine-group energy boundaries. Fine-group lethargy width. Thermal cross sections. Isotope identification. Fundamental-mode spectrum. Fine group-ultrafine group relation. Option parameters. Broad-group energy boundaries. Maximum and minimum energy boundaries.

Upper-interface Data ModulesQuantities Used

XS.I.UFG

Group structure parameters $\sigma_{el}^0(j \rightarrow k)$,
 $\sigma_{el}^1(j \rightarrow k)$, $\sigma_{el \text{ tr}}$, $\bar{\mu} \sigma_{el \text{ r}}$, $\sigma_{el \text{ r}}$

XS.THERM

Thermal cross sections.

XS.C.SMT

Microscopic nonresonant σ_c , σ_f , σ_s , $\bar{\mu}$,
 $\sigma_{\text{inelastic}}$, $\sigma_{n,2n}$, $\sigma_{n,p}$, $\sigma_{n,\alpha}$ group cross
sections, discrete-level inelastic group
cross sections, n,2n scattering group
cross sections, and unresolved resonant
capture and fission-group cross sections,
all for each isotope specified.

XS.C.UFG

Macroscopic $\sigma_{el}^0(j \rightarrow k)$, $\sigma_{el}^1(j \rightarrow k)$, $\sigma_{el \text{ tr}}$,
 $\bar{\mu} \sigma_{el \text{ r}}$, $\sigma_{el \text{ r}}$.

FR.FM

Fine-group and ultrafine-group real fluxes
and currents. $k_{\text{eff}} \cdot B^2$, the critical
buckling.

XS.I.RES

Resolved Resonant microscopic capture
and fission cross sections σ_c and σ_f .

Lower-interface Data ModulesQuantities Produced

XS.ISO

Cross-section set name, number of groups,
number of isotopes, energy boundaries,
lethargy boundaries, velocities, fission
spectrum, cross-section flags and
parameters, σ_{tr} , $\sigma_{n,\gamma}$, $\sigma_{n,\alpha}$, $\sigma_{n,p}$,
 $\sigma_{j \rightarrow j}^{\text{aniso}}$, σ_f , $\nu \sigma_f$, $\sigma_{el}^i(j \rightarrow k)$, $\sigma_{\text{inelastic}}^i(j \rightarrow k)$,
 $\sigma_{n,2n}^i(j \rightarrow k)$.

FR.BGFM

Real and adjoint fluxes, k_{eff} , B^2 .

7. Thermal Cross-section Edit CSE001

Prepared by: D. A. Sargis

a. Nature of Physical Problem Solved

This module uses previously calculated space- and speed-dependent fluxes and cross sections to generate thermal-group cross sections and fluxes. The module computes flux- and volume-averaged values for Σ_a , Σ_f , $\nu\Sigma_f$, Σ_s , and $D = (3\Sigma_{tr})^{-1}$ for the cell composition, and Σ_a , Σ_f , $\nu\Sigma_f$, Σ_s , and Σ_{tr} for all the isotopic constituents.

A "pseudo material" generating option is included in which one problem generates a correct energy-dependent, spatially averaged set of cross sections for use in the next problem. This feature facilitates solution of geometrically complex systems.

A transfer cross-section option is available to generate transfer cross sections from each coarse group to all other coarse groups, for each space point, and flux- and volume-averaged cross sections for each region.

In addition, a consistent P1 or B1 option is available which utilizes the first two Legendre components of the spatially averaged slowing-down source to generate thermal-group cross sections.

b. Method of Solution

This module generates cross sections of interest at each point j , and over a sequence of points, SUM, as well as volume- and flux-averaged quantities given by V AVE and F AVE, respectively. In addition, the transfer cross-section option may be employed to give transfer cross sections from coarse group I to coarse group K. The cross sections and transfer cross sections are given below for the cell composition and for individual cell and edit materials:

(1) For the Cell Composition

<u>Point</u>	<u>Volume</u>	<u>Cross Section</u>	<u>SIGMA I to K</u>
j	V_j	$V_j \int_{v_L}^{v_U} dv \Sigma_x(\vec{r}, v) \phi(\vec{r}, v)$	$V_j \int_{v_{KL}}^{v_{KU}} dv' \int_{v_{IL}}^{v_{IU}} dv \Sigma_S(\vec{r}, v \rightarrow v') \phi(\vec{r}, v)$
SUM	V_J	$\int_J d\vec{r} \int_{v_L}^{v_U} dv \Sigma_x(\vec{r}, v) \phi(\vec{r}, v)$	$\int_J d\vec{r} \int_{v_{KL}}^{v_{KU}} dv' \int_{v_{IL}}^{v_{IU}} dv \Sigma_S(\vec{r}, v \rightarrow v') \phi(\vec{r}, v)$

	<u>Point</u>	<u>Volume</u>	<u>Cross Section</u>	<u>SIGMA I to K</u>
V AVE	V_j	$\frac{1}{V_j} \int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\frac{1}{V_j} \int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$
F AVE	V_j	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$

(2) For Each Cell Material

	<u>Point</u>	<u>Volume</u>	<u>Cross Section</u>	<u>SIGMA I to K</u>
EVENTS	V_j	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$	$\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)$
AVE	V_j	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$

(3) For Each Edit Material

	<u>Point</u>	<u>Volume</u>	<u>Cross Section</u>	<u>SIGMA I to K</u>
j	V_j	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$	$\frac{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}{\int_V d\tau \int_U d\nu \Sigma^x(\vec{r}, \nu) \phi(\vec{r}, \nu)}$

<u>Point</u>	<u>Volume</u>	<u>Cross Section</u>	<u>SIGMA I to K</u>
AVE	V_j	$\frac{\int_J d\vec{r} \int_{v_L}^{v_U} dv \Sigma_x(\vec{r}, v) \phi(\vec{r}, v)}{\int_J d\vec{r} \int_{v_L}^{v_U} dv \phi(\vec{r}, v)}$	$\frac{\int_J d\vec{r} \int_{v_{KL}}^{v_{KU}} dv' \int_{v_{IL}}^{v_{IU}} dv \Sigma_S(\vec{r}, v \rightarrow v') \phi(\vec{r}, v)}{\int_J d\vec{r} \int_{v_{IL}}^{v_{IU}} dv \phi(\vec{r}, v)}$

Here j refers to a spatial point and J refers to a spatial region consisting of a sequence of points j . $\Sigma_x(\vec{r}, v)$ refers to any of the space- and speed-dependent cross sections of interest, and $\Sigma_S(\vec{r}, v \rightarrow v')$ is the transfer cross section from v to v' at $\vec{r}$. v_{KU} and v_{KL} refer to the upper and lower speed boundaries for the K th coarse group in the transfer cross-section calculation. v_U and v_L are the speed boundaries for the usual cross-section calculation for any specified energy group.

In addition to the cross sections generated, the number density and flux are also averaged over energy and space for the cell composition:

A consistent P1 or B1 calculation may also be performed to obtain the fluxes $\phi_0(v)$ and currents $\phi_1(v)$. Cross sections, $\Sigma_x(\vec{r}, v)$, and slowing-down sources, $S(\vec{r}, v)$, are first spatially averaged in this option according to

$$\langle \Sigma_x(v) \rangle = \frac{\int_{\text{cell}} \Sigma_x(\vec{r}, v) \phi(\vec{r}, v) d\vec{r}}{\int_{\text{cell}} \phi(\vec{r}, v) d\vec{r}} \quad (59)$$

and

$$\bar{S}(v) = \int_{\text{cell}} S(\vec{r}, v) d\vec{r}. \quad (60)$$

The slowing-down source $S(r, v)$ may include both the first and second Legendre moments of the scattering cross section, and can be read in from an epithermal cross-section generating module.

Once the P1 or B1 equations are solved for $\phi_0(v)$ and $\phi_1(v)$, thermal group averaging of the cross sections is easily performed:

$$\left. \begin{aligned} \phi &= \int_0^{v^*} \phi_0(v) dv \\ \Sigma_x &= \int_0^{v^*} \frac{\langle \Sigma_x(v) \rangle \phi_0(v) dv}{\phi} \\ D &= - \int_0^{v^*} \frac{\phi_1(v) dv}{\phi} \end{aligned} \right\} \quad (61)$$

where v^* is the speed corresponding to the thermal cutoff energy.

c. Related Programs and References

H. C. Honeck, A Thermalization Transport Theory Code for Reactor Lattice Calculations, BNL-5826 (1961).

B. J. Toppel and I. Baksys, The Argonne-Revised THERMOS Code, ANL-7023 (March 1965).

d. Machine Requirements

64 K Memory and 8 Tape Units.

e. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
B.THIN	Source. Transfer cross section. Geometry. Cross section. Consistent P1-B1 flags.
LPR	First flight Nonleakage probability, $Q(\vec{r}, v)$.
FR.D1	Neutron flux, $\phi(\vec{r}, v)$.
XS.MIX	Space-dependent mixture cross sections, $\Sigma_a(\vec{r}, v)$, $\Sigma_t(\vec{r}, v)$.
XS.TH	Isotope thermal cross sections, $\sigma_a(v)$, $\sigma_s(v)$, $\sigma_f(v)$, $\nu(v)$, $\bar{\mu}(v)$.
XS.KER.M	Scattering kernels for mixtures.

Upper-interface Data ModulesQuantities Used

SS

Space- and speed-dependent slowing down-source, $S(\vec{r}, v)$.

EN

Energy group structure parameters, such as number of groups, group boundaries, transfer cross-section groups, etc.

XS.KER.I

Isotope scattering kernels.

XS.TH.U

Isotope thermal cross sections for user-supplied data, $\sigma_a(v)$, $\sigma_f(v)$, $\sigma_s(v)$, $\nu(v)$, $\bar{\mu}(v)$.

XS.KER.U

Scattering kernels for user-supplied isotopes.

INTEG

Spatial and energy integration limits.

Lower-interface Data ModulesQuantities Produced

XS.THERM

Thermal-group cross sections.

Printer output

User output.

8. Cross-section Homogenization Specifications NUI001

Prepared by: J. V. Zapatka

a. Nature of Physical Problem Solved

The input to the module is information that defines "materials" as a combination of one or more isotopes and (or) compositions as a combination of one or more "materials" ("isotopes") and information (if any) pertaining to delayed-neutron yield, delayed-neutron spectrum, decay constant, and fractions of delayed-neutron yield that go into a delayed family.

The input can be accepted in the form of a BCD data set containing card images and/or one or more binary data sets.

b. Method of Solution

If the input consists only of the BCD data set A.HOMOG, the card images are processed and the processed information is stored in the binary data sets B.HOMOG and XS.DELAY (if delay data is present).

If the input consists only of the binary data sets B.HOMOG and/or XS.DELAY, no processing is done.

If the input consists of the BCD data set A.HOMOG and either or both of the binary data sets B.HOMOG and XS.DELAY, then the BCD card images that are designated as new information are processed and the processed information is stored in either or both of the binary data sets. Any old information of this kind that may already exist on the binary data sets will be replaced by the new information.

Any errors will be flagged, and execution will be terminated if necessary.

c. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

A.NIP

Quantities Used

Material specifications giving the names of the isotopes that comprise each material. Atom densities of the isotopes that comprise each material. Composition specifications giving the names of the materials (isotopes) that comprise each composition. Volume fractions (atom densities) of materials (isotopes) that comprise each composition.

Upper-interface Data ModulesQuantities Used

XS.DELAY

Delayed-neutron yield for each isotope and each energy group. Fractions of the delayed-neutron yield that go into each delayed family. Delayed-neutron spectrum that depends on the energy group and the delayed family. Decay constant for each isotope and each delayed family.

B.HOMOG

Same quantities as A.NIP except in binary.

XS.ISO

Number of energy groups.

Lower-interface Data ModulesQuantities Produced

B.HOMOG

Same quantities as above.

XS.DELAY

Same quantities as above.

9. Geometry Specifications NUI002

Prepared by: G. C. Jensen

a. Nature of Physical Problem Solved

This module reads and analyzes BCD card images defining reactor geometry and composition assignment. Insufficient or inconsistent input data is noted with an error reference number and processing continues as far as is possible.

b. Upper- and Lower-interface Data Modules

Upper-interface Data Module

A.NIP

Quantities Used

Geometry specifications; Reactor size and shape, regional structure, mesh arrangement; area and/or zone specification. Composition-to-region assignments. Buckling data.

Lower-interface Data Module

GEOM

Quantities Produced

General reactor geometry specifications for location of points, regions, and compositions and, optionally, for areas and/or zones. Buckling data.

10. Neutronics Specifications NUI003

Prepared by: G. C. Jensen

a. Nature of Physical Problem Solved

This module reads and analyzes BCD card images defining boundary conditions, problem type (including criticality specifications), source and flux initial data and external source data. Output data sets contain all input data which is explicit or implied. Consistency and completeness checks are performed where appropriate; in general, processing continues after noting apparent inconsistencies until an obvious fatal error occurs.

b. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
GEOM	General descriptive geometry data and region-mesh correspondence.
A.NIP	Specifications for internal and external boundary conditions, problem type, criticality search. Initial source and flux data. Distributed external source values.
XS.C.MIN	Number of energy groups.
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
BC	External and internal boundary conditions.
ES.D1D (or ES.D2D) [†]	Distributed external source.
ES.D1SH (or ES.D2SH) [†]	External shell source.
FA.D1 (or FA.D2) [†]	Initial adjoint flux.
FA.D1A (or FA.D2A) [†]	Initial adjoint angular flux.
FR.D1 (or FR.D2) [†]	Initial real flux.
FR.D1A (or FR.D2A) [†]	Initial real angular flux.
FSA.D1 (or FSA.D2) [†]	Initial adjoint fission source.
FSR.D1 (or FSR.D2) [†]	Initial real fission source.

[†]For two-dimensional geometries.

Lower-interface Data ModulesQuantities Produced

SP.CRIT

Critical search specifications.

SP.CICN

Problem type and other neutronics
calculation specifications.

11. 1D-Transport Specifications NUI004

Prepared by: G. J. Duffy

a. Nature of Problem Solved

Module-dependent input is accepted in the form of a BCD data set containing card images and/or a binary data set. The input is collected and translated into a form usable by the 1D Transport Theory module.

b. Method of Solution

If only the BCD data set, A.INPTR1, is given as input, the card images are processed and translated into the form of the binary data set, SP.NEUT1. If only the SP.NEUT1 data set is given, no processing takes place. If both data sets are input, A.INPTR1 is scanned to determine what modifications are to be made in SP.NEUT1, and these are processed. If errors occur during the processing, they are flagged, and termination is recommended when the condition is serious and not correctable.

c. Upper - and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Produced</u>
A.INPTR1	Maximum number of inner iterations, outer iterations. S_N order, S_N weights and direction cosines. Groups to be skipped or for which consistent P1 is to be used. Density factors for each region or for each mesh interval. Normalization factor. Parameter oscillation damper for criticality search. L number for each composition.
SP.NEUT1	Same quantities as in A.INPTR1, but in binary..
GEOM	General reactor geometry specifications.
SP.CICN	Code-independent data.
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
SP.NEUT1	Same quantities as in SP.NEUT1 above, in the form of a binary data set.

12. 2D-Transport Specifications NUI005

Prepared by: G. J. Duffy

a. Nature of Problem Solved

Module-dependent input is accepted in the form of a BCD data set containing card images and/or a binary data set. The input is collected and translated into a form usable by a 2D Transport Theory module.

b. Method of Solution

If only the BCD data set, A.INPTR2 is given as input, the card images will be processed and translated into the form of the binary data set, SP.NEUT2. If only the SP.NEUT2 data set is given, no processing takes place. If both data sets are input, A.INPTR2 is scanned to determine what modifications are to be made in SP.NEUT2 and these are processed. If errors occur during the processing, they will be flagged, and termination will be recommended when the condition is serious and not correctable.

c. Upper - and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
A.INPTR2	Maximum number of inner iterations, outer iterations. S_N order, S_N weights, and direction cosines. Density factors for each region or for each mesh interval. Normalization factor. Parameter oscillation damper for criticality search. L number for each composition.
SP.NEUT2	Same quantities as in A.INPTR2 but in binary.
GEOM	General reactor geometry specifications.
SP.CICN	Code-independent data.
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
SP.NEUT2	Same quantities as in SP.NEUT2 above, in the form of a binary data set.

13. Transport-mesh Refinement Specifications NUI007

Prepared by: G. J. Duffy

a. Nature of Problem Solved

Module-dependent input consists of a BCD data set containing card images.

The input is collected and translated into a form usable by the module-handling mesh refinement for one- and two-dimensional transport theory.

b. Method of Solution

This module accepts BCD data set, A.NUI009, and produces binary data set MR.TN by direct translation of A.NUI009.

c. Upper- and Lower-interface Data Modules

Upper-interface Data Module

A.NUI009

Quantities Used

Specified changes in the mesh structure.
Number of dimensions. Type and order of interpolation and extrapolation to be performed on fluxes.

Lower-interface Data Module

MR.TN

Quantities Produced

Binary version of A.NUI009.

14. Neutronics Output Manipulation Specifications NUI008

Prepared by: J. L. Zeman

a. Nature of Physical Problem Solved

Reads the BCD card image data set, A.OUTMAN containing quantities required for output manipulation and writes them in the first binary record of data set OUT.NM.

b. Upper- and Lower-interface Data ModulesUpper-interface Data Module Quantities Used

A.OUTMAN

Normalization option. Output calculation options. Power values.

Lower-interface Data Module Quantities Produced

OUT.NM

Same as above.

15. Cross-section Homogenization NUC001

Prepared by: J. V. Zapatka

a. Nature of the Physical Problem Solved

Given isotopic cross-section data, isotopic fission-spectrum fractions, isotopic delayed-neutron data, material specifications, and composition specifications, the module computes the desired material cross-section data, material fission-spectrum fractions, composition cross-section data, composition fission-spectrum fractions, material delayed-neutron data, and composition delayed-neutron data.

b. Method of Solution

(1) Material Cross Sections. In general, material cross sections are formed by homogenizing isotopic cross sections as follows:

$$\Sigma_x(g,m) = \sum_{i \in m} N(i \in m) \cdot \sigma(g,i),$$

where x is the cross-section type;

$\Sigma_x(g,m)$ is the macroscopic material cross section of type x , group g and material m ;

$\sigma_x(g,i)$ is the microscopic isotopic cross section of type x , group g and isotopic i ;

and $N(i \in m)$ is the atom density of isotope i in material m .

x , $\Sigma_x(g,m)$ and $\sigma_x(g,i)$ can be any of the following:

<u>X = TYPE</u>	<u>SYMBOL (Σ_x)</u>	<u>SYMBOL (σ_x)</u>
1. Inelastic Scattering (Order ℓ)	$\Sigma_{in}^{(\ell)}(g \rightarrow k, m)$	$\sigma_{in}^{(\ell)}(g \rightarrow k, i)$
2. Elastic Scattering (Order ℓ)	$\Sigma_{el}^{(\ell)}(g \rightarrow k, m)$	$\sigma_{el}^{(\ell)}(g \rightarrow k, i)$
3. N2N Scattering (Order ℓ)	$\Sigma_{n,2n}^{(\ell)}(g \rightarrow k, m)$	$\sigma_{n,2n}^{(\ell)}(g \rightarrow k, i)$
4. Capture (m, γ)	$\Sigma_{(n,\gamma)}(g, m)$	$\sigma_{(n,\gamma)}(g, i)$
5. Capture (n, α)	$\Sigma_{(n,\alpha)}(g, m)$	$\sigma_{(n,\alpha)}(g, i)$

<u>X = TYPE</u>	<u>SYMBOL (Σ_x)</u>	<u>SYMBOL (σ_x)</u>
6. Capture (n,p)	$\Sigma_{(n,p)}(g,m)$	$\sigma_{(n,p)}(g,i)$
7. Fission	$\Sigma_f(g,m)$	$\sigma_f(g,i)$
8. Nu times Fission	$\nu\Sigma_f(g,m)$	$\nu\sigma_f(g,i)$
9. Transport	$\Sigma_{tr}(g,m)$	$\sigma_{tr}(g,i)$
10. Anisotropic Self-scattering	$\Sigma_{aniso}(g \rightarrow g,m)$	$\sigma_{aniso}(g \rightarrow g,i)$

Other material cross sections and their formulation are as follows:

<u>TYPE</u>	<u>SYMBOL</u>
1. Inelastic Removal	$\Sigma_{in}^{rem}(g,m)$
$\Sigma_{in}^{rem}(g,m) = \sum_{\substack{k \\ k \neq g}} \Sigma_{in}^{(0)}(g \rightarrow k,m)$	
2. Elastic Removal	$\Sigma_{el}^{rem}(g,m)$
$\Sigma_{el}^{rem}(g,m) = \sum_{\substack{k \\ k \neq g}} \Sigma_{el}^{(0)}(g \rightarrow k,m)$	
3. N2N Removal	$\Sigma_{n2n}^{rem}(g,m)$
$\Sigma_{n2n}^{rem}(g,m) = \sum_{\substack{k \\ k \neq g}} \Sigma_{n2n}^{(0)}(g \rightarrow k,m)$	
4. Total Isotropic Scattering	$\Sigma_{scat}^{(0)}(g \rightarrow k,m)$
$\Sigma_{scat}^{(0)}(g \rightarrow k,m) = \Sigma_{in}^{(0)}(g \rightarrow k,m) + \Sigma_{el}^{(0)}(g \rightarrow k,m) + \Sigma_{n2n}^{(0)}(g \rightarrow k,m)$	

<u>TYPE</u>	<u>SYMBOL</u>
5. Total Anisotropic Scattering	$\Sigma_{\text{scat}}^{(\ell>0)}(g \rightarrow k, m)$
	$\Sigma_{\text{scat}}^{(\ell>0)}(g \rightarrow k, m) = \Sigma_{\text{in}}^{(\ell>0)}(g \rightarrow k, m) + \Sigma_{e\ell}^{(\ell>0)}(g \rightarrow k, m) + \Sigma_{n2n}^{(\ell>0)}(g \rightarrow k, m)$
6. Absorption	$\Sigma_a(g, m)$
	$\Sigma_a(g, m) = \Sigma_{(n,\gamma)}(g, m) + \Sigma_{(n,\alpha)}(g, m) + \Sigma_{(n,p)}(g, m) + \Sigma_f(g, m)$
7. Total Removal	$\Sigma_{\text{total}}^{\text{rem}}(g, m)$
	$\Sigma_{\text{total}}^{\text{rem}}(g, m) = \Sigma_a(g, m) + \Sigma_{\text{in}}^{\text{rem}}(g, m) + \Sigma_{e\ell}^{\text{rem}}(g, m) + \Sigma_{n2n}^{\text{rem}}(g, n)$
8. Total	$\Sigma_t(g, m)$
	$\Sigma_t(g, m) = \Sigma_{\text{tr}}(g, m) + \Sigma_{\text{aniso}}(g \rightarrow g, m) - \Sigma_{e\ell}^{(0)}(g \rightarrow g, m)$

(2) Material Fission-spectrum Fractions

There are two cases:

(a) All fissionable isotopes present have the same parent group-independent vector.

(b) All fissionable isotopes present do not have the same parent group-independent vector.

For Case (a), no homogenization is done and the material fission spectrum fraction is taken to be the same as the isotope fission spectrum fraction.

$$\bar{\chi}(g) = \chi(g)$$

For Case (b), any vector present is expanded to a matrix, each column of which is identical to the vector. Homogenization is performed as follows:

$$\bar{\chi}(k \rightarrow g, m) = \frac{\sum_{i \in m} \chi(k \rightarrow g, i) \cdot N(i \in m) \cdot \nu \sigma_f(k, i)}{\nu \Sigma_f(k, m)},$$

where

$\bar{\chi}(k \rightarrow g, m)$ is the material fission-spectrum fraction for material m from parent group k to daughter group g , and $\chi(k \rightarrow g, i)$ is the isotope fission-spectrum fraction for isotope i .

(3) Material Delayed-neutron Data

(a) Prompt Nu times Fission Material Cross Section

$$\nu_p \Sigma_f(g, m) = \sum_{i \in m} [\nu(g, i) - Y(g, i)] \cdot N(i \in m) \cdot \sigma_f(g, i),$$

where

$\nu_p \Sigma_f(g, m)$ is the prompt nu times fission cross section for material m and group g ,

$\nu(g, i)$ is the nu for isotope i , group g ,

and

$Y(g, i)$ is the delayed neutron yield for isotope i , group g .

(b) Material Delayed Chi

$$\tilde{\chi}(g, F, m) = \sum_{i \in m} A(F, i) \cdot Y(g, i) \cdot N(i \in m) \cdot \sigma_f(g, i) / \nu_p \Sigma_f(g, m)$$

where

$\tilde{\chi}(g, F, m)$ is the delayed chi for material m , family F and group g ;

and

$A(F, i)$ is the fraction of $Y(g, i)$ that goes into family F , $\sum_F A(F, i) = 1$.

(4) Composition Cross Sections

Composition cross sections are formed by homogenizing material cross sections as follows:

$$\bar{\Sigma}_x(g, c) = \sum_{m \in c} V F(m \in c) \cdot \Sigma_x(g, m),$$

where

$\bar{\Sigma}_x(g,c)$ is the macroscopic composition cross section of type x, group g and composition c;

and

$VF(m\epsilon c)$ is the volume fraction of material m in composition c.

x can be any of the cross-section types listed under material cross sections.

(5) Composition Fission-spectrum Fractions

For the two cases mentioned under Material Fission-spectrum Fractions:

$$(a) \bar{\bar{\chi}}(g) = \bar{\chi}(g)$$

$$(b) \bar{\bar{\chi}}(k \rightarrow g, c) = \frac{\sum_{m \in c} \bar{\chi}(k \rightarrow g, m) \cdot VF(m\epsilon c) \cdot \nu \Sigma_f(k, m)}{\bar{\nu} \bar{\Sigma}_f(k, c)}$$

(6) Composition Delayed-neutron Data

(a) Prompt Nu times Fission Composition Cross Section

$$\bar{\nu}_p \bar{\Sigma}_f(g, c) = \sum_{m \in c} VF(m\epsilon c) \cdot \nu_p \Sigma_f(g, m)$$

(b) Composition Delayed Chi

$$\bar{\bar{\chi}}(g, F, c) = \frac{\sum_{m \in c} VF(m\epsilon c) \cdot \chi(g, F, c) \cdot \nu_p \Sigma_f(g, m)}{\bar{\nu}_p \bar{\Sigma}_f(g, c)}$$

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
B.HOMOG	Material definitions. Composition definitions.
XS.ISO or XS.ISO2	Isotope cross section data.
XS.M.ANI	Material cross sections $\Sigma_{\text{scat}}^{(\ell > 0)}$.

Upper-interface Data ModulesQuantities Used

XS.M.AUX

Material cross sections

$$\Sigma_{\text{in}}^{(\ell)}, \Sigma_{\text{e}\ell}^{(\ell)}, \Sigma_{\text{nzn}}^{(\ell)}, \Sigma_{\text{in}}^{\text{rem}}, \Sigma_{\text{e}\ell}^{\text{rem}}, \Sigma_{\text{nzn}}^{\text{rem}},$$

$$\Sigma_{(\text{n},\gamma)}, \Sigma_{(\text{n},\alpha)}, \Sigma_{(\text{n},\text{p})}, \nu_{\text{p}}, \Sigma_{\text{f}}, \tilde{\chi}$$

XS.M.MIN

Material cross sections

$$\Sigma_{\text{a}}, \Sigma_{\text{t}}, \Sigma_{\text{rem}}, \Sigma_{\text{tr}}, \Sigma_{\text{f}}, \nu\Sigma_{\text{f}}, \chi$$

Lower-interface Data ModulesQuantities Produced

XS.ISO2

(XS.ISO2 is a subset of XS.ISO)

XS.M.ANI

(Same as above)

XS.M.AUX

(Same as above)

XS.M.MIN

(Same as above)

XS.C.ANI

Composition cross sections $\bar{\Sigma}_{\text{scat}}^{(\ell>0)}$

XS.C.AUX

$$\bar{\Sigma}_{\text{in}}^{(\ell)}, \bar{\Sigma}_{\text{e}\ell}^{(\ell)}, \bar{\Sigma}_{\text{nzn}}^{(\ell)}, \bar{\Sigma}_{\text{in}}^{\text{rem}}, \bar{\Sigma}_{\text{e}\ell}^{\text{rem}}, \bar{\Sigma}_{\text{nzn}}^{\text{rem}},$$

$$\bar{\Sigma}_{(\text{n},\gamma)}, \bar{\Sigma}_{(\text{n},\alpha)}, \bar{\Sigma}_{(\text{n},\text{p})},$$

XS.C.MIN

Composition cross sections $\bar{\Sigma}_{\text{a}}, \bar{\Sigma}_{\text{t}}, \bar{\Sigma}_{\text{rem}},$
 $\bar{\Sigma}_{\text{tr}}, \bar{\Sigma}_{\text{f}}, \nu\bar{\Sigma}_{\text{f}}, \bar{\chi}, \nu_{\text{p}}\bar{\Sigma}_{\text{f}}, \tilde{\chi}$

16. 1D-Diffusion NUC002

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a. Nature of Physical Problem Solved

The one-dimensional, multigroup, diffusion approximation to the transport equation for the cases of real, adjoint, and external source problems.

b. Method of Solution(1) Introduction

This module is concerned with the solution of the finite-difference approximation to the multigroup diffusion equation. Three basic types of calculations can be made: real k_{eff} , adjoint k_{eff} , and, in the presence of external sources or inhomogeneous boundary conditions, a source calculation. These calculations can be made in any of the three geometries--slab, cylindrical and spherical. The permissible form of the external boundary conditions is linear and homogeneous for k_{eff} calculations, and linear and inhomogeneous for source calculations. Interface conditions across regional boundaries can be specified by the logarithmic derivative condition for black regions or the usual continuity of flux and current in all other cases. Scattering between energy groups is unrestricted in form, so that full up and down scattering can be present.

(2) Derivation of the Finite-difference Equations for the Multigroup One-dimensional Diffusion Equation

The multigroup diffusion equation can be written in the form

$$-\text{div} (D_g \nabla \phi_g) + \sigma_R^g \phi_g = S_g \text{ for } g = 1, 2, \dots, G, \quad (62)$$

where S_g represents the fission and scattering source terms. The finite-difference equations associated with Eq. 62 is derived for the following three geometries:

- (a) Spherical,
- (b) Cylindrical,
- (c) Slab.

In the spherical case, we assume that the reactor configuration is spherically symmetric, so that the flux $\phi(\rho, \theta, \phi) = \phi(\rho)$. Then

$$\text{div} (D \nabla \phi) = \frac{1}{\rho^2} \frac{d}{d\rho} \left(\rho^2 D \frac{d\phi}{d\rho} \right),$$

and $dV = 4\pi\rho^2 d\rho$. Now divide the sphere into intervals $[R_{i-1}, R_i]$, $i = 1, 2, \dots, I$, where $0 = R_0 < R_1 < R_2 \dots < R_I = R$. Then integrate the diffusion equation over each interval, and assume that all cross sections are constant over each interval. Then we obtain

$$-4\pi \left[R_i^2 D_i \phi'(R_i^-) - R_{i-1}^2 D_i \phi'(R_{i-1}^+) \right] + \sigma_{R_i} V_i \phi_i = S_i V_i, \quad (63)$$

where

$$V_i = \frac{4\pi}{3} (R_i^3 - R_{i-1}^3)$$

and

$$\phi_i = \phi(r_i), \quad r_i = \frac{R_i + R_{i-1}}{2}.$$

Here we have made the approximation,

$$4\pi \int_{R_{i-1}}^{R_i} \phi(\rho) \rho^2 d\rho \approx \phi(r_i) V_i.$$

Alternatively apply the mean-value theorem, and identify the mean value ϕ with the value of the flux at the center.

Applying the condition of continuity of flux and current across interfaces leads to[†]

$$-(a_i \phi_{i+1} + c_i \phi_{i-1}) + e_i \phi_i = V_i S_i, \quad (64)$$

where

$$a_i = \frac{3R_i^2 D_i D_{i+1}}{\frac{1}{2}\Delta R_i D_{i+1} + \frac{1}{2}\Delta R_{i+1} D_i}, \quad (65)$$

$$\Delta R_i = R_i - R_{i-1}, \quad (66)$$

$$c_i = \frac{3R_{i-1}^2 D_i D_{i-1}}{\frac{1}{2}\Delta R_i D_{i-1} + \frac{1}{2}\Delta R_{i-1} D_i}, \quad (67)$$

and

$$e_i = a_i + c_i + \bar{V}_i \phi_{R_i}. \quad (68)$$

[†] For this and other references in this portion of Appendix B, see references listed on page 93.

Here we have multiplied by the factor 3 and divided by 4π , so that

$$\bar{V}_i = R_i^3 - R_{i-1}^3.$$

On the other hand, if the interval $[R_i, R_{i+1}]$ is the innermost interval of the region that is black to neutrons in some energy group, then the boundary condition

$$D_i \phi'(R_i) + \Lambda_{m,\ell} \phi(R_i) = 0 \quad (69)$$

is applied. Here m is the region number to which the interval $[R_i, R_{i+1}]$ belongs and ℓ indicates that it is on the left. In this case,²

$$\left. \begin{aligned} \text{i)} \quad a_i &= 0; \\ \text{ii)} \quad e_i &= c_i + \sigma_{R_i} \bar{V}_i + \frac{3D_i \Lambda_{m,\ell} R_i^2}{D_i + \frac{1}{2} \Delta R_i \Lambda_{m,\ell}} \end{aligned} \right\} \quad (70)$$

In the black region, $D = 0$ so that, in this case, $c_{i+1} = 0 = a_{i+1}$, and $e_{i+1} = (\sigma_R)_{i+1} \bar{V}_{i+1}$. If, on the other hand, the interval $[R_{i-1}, R_i]$ was the outermost cell of a region black to neutrons in this group, then $c_i = 0$ and

$$e_i = a_i + \sigma_{R_i} \bar{V}_i + \frac{3D_i \Lambda_{m',r} R_{i-1}^2}{D_i + \frac{1}{2} \Delta R_i \Lambda_{m',r}}.$$

Note that in all cases $c_{i+1} = a_i$. Note also that we have omitted the group indices. In spherical coordinates, the left boundary conditions are always $\phi'(0^+) = 0$; thus $c_1 = 0$. The right boundary conditions are of the form

$$A\phi'(R) + B\phi(R) = C, \quad (71)$$

where A , B , and C are group-dependent. Applying this condition in the last interval leads to

$$\left. \begin{aligned} \text{i)} \quad a_I &= 0; \\ \text{ii)} \quad e_I &= c_I + (\sigma_R)_I \bar{V}_I + \frac{3D_I R^2 B}{A + \frac{1}{2} \Delta R_I B} \end{aligned} \right\} \quad (72)$$

In addition, if $C \neq 0$, an external source term having the following form is created:

$$S_{\text{ext}} = \frac{3D_I R^2 C}{A + \frac{1}{2} \Delta R_I B}. \quad (73)$$

Thus, if $C \neq 0$, the problem takes the form of a source calculation rather than a k -calculation.

In cylindrical geometry, we have

$$\left. \begin{aligned} \text{i) } \operatorname{div} (D \nabla \phi) &= \frac{1}{r} \frac{d}{dr} \left(r D(r) \frac{d\phi}{dr} \right); \\ \text{ii) } dV &= 2\pi H r dr, \end{aligned} \right\} (74)$$

where $\phi(r, \phi, z) = \phi(r) \cos \frac{\pi z}{2H}$, and H is the half height of the reactor.

Thus the finite-difference coefficients are defined by

$$\left. \begin{aligned} a_i &= \frac{2R_i D_i D_{i+1}}{\frac{1}{2}\Delta R_i D_{i+1} + \frac{1}{2}\Delta R_{i+1} D_i}, \\ c_i &= \frac{2R_{i-1} D_i D_{i-1}}{\frac{1}{2}\Delta R_i D_{i-1} + \frac{1}{2}\Delta R_{i-1} D_i}, \\ e_i &= a_i + c_i + \bar{V}_i \sigma_{R_i} + D_i B^2 V_i, \end{aligned} \right\} (75)$$

where

$$\bar{V}_i = R_i^2 - R_{i-1}^2 \text{ and } B^2 = \left(\frac{\pi}{2H} \right)^2.$$

If the i th interval is adjacent to a black region, then

$$\left. \begin{aligned} a_i &= 0 \text{ or } c_i = 0, \\ e_i &= c_i \text{ (or } a_i) + \bar{\sigma}_{R_i} \bar{V}_i + \frac{2D_i \Lambda_{m,(\cdot)} R_i}{D_i + \frac{1}{2}\Delta R_i \Lambda_{m,(\cdot)}}, \end{aligned} \right\} (76)$$

where $\bar{\sigma}_{R_i} = \sigma_{R_i} + D_i B^2$. The left-hand boundary condition is $\phi'(0) = 0$, which leads to

$$c_1 = 0. \quad (77)$$

At the right-hand boundary, a condition of the form $A\phi'(R) + B\phi(R) = C$ can be applied which leads to

$$\left. \begin{aligned}
 a_I &= 0, \\
 e_I &= c_I + \bar{\sigma}_{RI} \bar{V}_I + \frac{2D_I R B}{A + \frac{1}{2}\Delta R_I B}, \\
 \text{and} \\
 S_{\text{ext}} &= \frac{2D_I R C}{A + \frac{1}{2}\Delta R B}.
 \end{aligned} \right\} \quad (78)$$

In slab geometry, we have

$$\left. \begin{aligned}
 \text{div}(D \nabla \phi) &= \frac{d}{dr} \left(D(r) \frac{d\phi}{dr} \right), \\
 dV &= dr, \\
 \text{and} \\
 \phi(x, y, z) &= \phi(x) \cos \frac{y}{2\beta} \cos \frac{z}{2\gamma}
 \end{aligned} \right\} \quad (79)$$

where β, γ are the half-thickness in the y and z direction.

$$\left. \begin{aligned}
 a_i &= \frac{D_i D_{i+1}}{\frac{1}{2}\Delta R_i D_{i+1} + \frac{1}{2}\Delta R_{i+1} D_i} \\
 c_i &= \frac{D_i D_{i-1}}{\frac{1}{2}\Delta R_i D_{i-1} + \frac{1}{2}\Delta R_{i-1} D_i} \\
 e_i &= a_i + c_i + V_i \bar{\sigma}_{Ri}
 \end{aligned} \right\} \quad (80)$$

where $V_i = R_i - R_{i-1}$ and $\bar{\sigma}_{Ri} = \sigma_{Ri} + \left(\frac{\pi}{2\beta}\right)^2 + \left(\frac{\pi}{2\gamma}\right)^2$.

The black-boundary conditions take the form

$$\left. \begin{aligned}
 a_i &= 0 \text{ or } c_i = 0, \\
 e_i &= c_i \text{ (or } a_i) + \bar{\sigma}_{Ri} V_i + \frac{D_i \Lambda_{m,()}}{D_i + \frac{1}{2}\Delta R_i \Lambda_{m,()}}
 \end{aligned} \right\} \quad (81)$$

The left and right boundaries can have the general linear boundary conditions. Thus

$$\left. \begin{aligned}
 c_1 &= 0, \\
 e_1 &= a_1 + \bar{\sigma}_{R1} V_1 + \frac{D_1 B'}{A' + \frac{1}{2} \Delta R_1 B'}, \\
 a_I &= 0, \\
 e_I &= c_I + \bar{\sigma}_{RI} V_I + \frac{D_I B}{A + \frac{1}{2} \Delta R_I B},
 \end{aligned} \right\} \quad (82)$$

with

$$S_{\text{ext},1} = \frac{D_1 C'}{A' + \frac{1}{2} \Delta R_1 B'},$$

and

$$S_{\text{ext},I} = \frac{D_I C}{A + \frac{1}{2} \Delta R_I B}.$$

(3) Solution of the Finite-difference Equations

In Section (2) above, we derived the finite-difference equations associated with the multigroup diffusion equation. Thus, starting with the system

$$-\text{div}(D_g \nabla \phi_g) + \sigma_R^g \phi_g = \sum_{g' \neq g} \sigma^{g'g} \phi_{g'} + \frac{1}{k} \sum_{g'=1}^G X^{g'g} (\nu \sigma_f)_{g'} \phi_{g'}$$

$$\text{for } g = 1, 2, \dots, G,$$

with external boundary conditions of the form

$$A_g \frac{\partial \phi_g}{\partial n} + B_g \phi_g = 0,$$

we obtained the homogeneous finite-difference system

$$-a_{ig} \phi_{i+1,g} + e_{ig} \phi_{ig} - c_{ig} \phi_{i-1,g} = \sum_{g' \neq g} \bar{V}_i \sigma_i^{g'g} \phi_{g'} + \frac{1}{k} \sum_{g'=1}^G \bar{V}_i X_i^{g'g} (\nu \sigma_f)_{ig'} \phi_{g'}$$

$$\text{for } g = 1, 2, \dots, G.$$

Here we seek the largest positive value of k for which the above system has a positive solution $\{\phi_{ig}\}$. If the external boundary conditions were inhomogeneous, or if an external source were present, the finite-difference equations would take the form

$$-a_{ig}\phi_{i+1,g} + e_{ig}\phi_{ig} - c_{ig}\phi_{i-1,g} = \sum_{g' \neq g} \bar{v}_i \sigma_i^{g'g} \phi_{g'} + \sum_{g'=1}^G \chi_i^{g'g} (\nu \sigma_f)_{ig'} \phi_{g'} + S_{ig}$$

for $g = 1, 2, \dots, G$.

Here S_{ig} represents the source term arising from either the boundary conditions or the external source. The basic problem is to solve the above linear system of equations for the flux $\{\phi_{ig}\}$. Three types of calculations are performed: real k_{eff} , adjoint k_{eff} , and source calculations. We shall consider the real k_{eff} calculations first. We first define the following matrices:

$$A_g = \begin{bmatrix} e_{1g} & -a_{1g} & & & \\ -c_{2g} & e_{2g} & -a_{2g} & & \\ & \cdot & \cdot & \cdot & \\ & & \cdot & \cdot & -a_{I-1,g} \\ & & & \cdot & -c_{Ig} & e_{Ig} \end{bmatrix} \quad \text{for } g = 1, 2, \dots, G. \quad (83)$$

$$B^{g'g} = \text{diag}[\bar{v}_i \sigma_i^{g'g}] \quad (84)$$

$$F^{g'g} = \begin{cases} \text{diag}[\chi_i^{g'g} (\nu \sigma_f)_{g'i} \bar{v}_i] & \text{Chi-matrix case} \\ \text{diag}[\chi_i^g (\nu \sigma_f)_{g'i} \bar{v}_i] & \text{Chi-vector case.} \end{cases} \quad (85)$$

With these matrices defined, the basic finite-difference system given by

$$-a_{ig}\phi_{i+1,g} + e_{ig}\phi_{ig} - c_{ig}\phi_{i-1,g} = \sum_{g' \neq g} \bar{v}_i \sigma_i^{g'g} \phi_{g'} + \frac{1}{k} \sum_{g'=1}^G \bar{v}_i \chi_i^{g'g} (\nu \sigma_f)_{ig'} \phi_{g'} \quad (86)$$

can be written in the form

$$A_g \phi_g = \sum_{g' \neq g} B^{g'g} \phi_{g'} + \frac{1}{k} \sum_{g'=1}^G F^{g'g} \phi_{g'}, \quad g = 1, 2, \dots, G, \quad (87)$$

where

$$\phi_g = (\phi_{1g}, \phi_{2g}, \dots, \phi_{IG})'.$$

With the logarithmic condition applied at some interfaces, the matrices A_g are symmetric and tridiagonal. Some of the off-diagonal elements are zero; i.e., $a_{i,g} = c_{i+1,g} = 0$ for some i and g . However, we shall assume that all the elements e_{ig} are positive. Thus each matrix A_g is nonsingular with a nonnegative inverse. We next define the following matrices

$$E = \begin{bmatrix} A_1 & -B^{21} & \dots & -B^{G1} \\ -B^{12} & A_2 & & -B^{G2} \\ \vdots & \vdots & \ddots & \vdots \\ -B^{1G} & \dots & \dots & A_G \end{bmatrix}, \quad (88)$$

and

$$F = \begin{bmatrix} F^{11} & F^{21} & \dots & F^{G1} \\ F^{12} & F^{22} & \dots & F^{G2} \\ \vdots & \vdots & \ddots & \vdots \\ F^{1G} & \dots & \dots & F^{GG} \end{bmatrix}. \quad (88a)$$

Then the system defined by Eq. 87 takes the form

$$E\phi = \frac{1}{k} F\phi, \quad (89)$$

where $\phi = (\phi_1, \phi_2, \dots, \phi_G)'$. Since

$$\sigma_R^g = \sigma_C^g + \sigma_f^g + \sum \sigma^{gg'},$$

we have

$$e_{ig} > \sum_{g' \neq g} \sigma_i^{gg'} \bar{V}_i.$$

Thus E^{-1} exists and is nonnegative. The basic problem then is to find the largest value of k and the corresponding positive flux ϕ that satisfy Eq. 89. The basic method of solution used in this problem is that of power iteration on the matrix $E^{-1}F$. Thus starting with an arbitrary positive flux $\phi^{(0)}$ and a positive scalar $k^{(0)}$, we form iteratively

$$E\phi^{(n+1)} = \frac{1}{k^{(n)}} F\phi^{(n)}, \quad k^{(n+1)} = k^{(n)} \frac{(\phi^{(n+1)}, \phi^{(n+1)})}{(\phi^{(n+1)}, \phi^{(n)})}, \quad n = 0, 1, 2, \dots \quad (90)$$

To find $\phi^{(n+1)}$, we must solve a matrix equation. The solution can be effected directly if there is no up-scattering present since E is block lower triangular in this case. If up-scattering is present, the solution is effected iteratively by means of block Gauss-Seidel applied to the blocks exhibited in Eq. 88. The iterations by which we find $\phi^{(n+1)}$ are called inner iterations.

Thus, if we have $\phi^{(n)}$ and $k^{(n)}$, and we also have the vectors $x_1^{(\ell)}, x_2^{(\ell)}, \dots, x_{g-1}^{(\ell)}$, then we find $x_g^{(\ell)}$ by solving

$$A_g x_g^{(\ell)} = \sum_{g' < g} B^{g'g} x_{g'}^{(\ell)} + \sum_{g' > g} B^{g'g} x_{g'}^{(\ell-1)} + \frac{1}{k^{(n)}} \sum_{g'=1}^G F^{g'g} \phi_{g'}^{(n)}, \quad (91)$$

where we take $x_g^{(0)} \equiv \phi_g^{(n)}$ for all g . Since each matrix A_g^{-1} exists and is nonnegative and each matrix $B^{g'g}$ is also nonnegative, the sequence of vectors $x_g^{(\ell)}$ will converge to the solution $\phi_g^{(n+1)}$ of Eq. 90 for each $g = 1, 2, \dots, G$.² As noted before, if there is no up-scattering, i.e., $B^{g'g} = 0$ for $g' > g$, then no iteration is necessary. The above inner iteration is continued until

$$\sum_{g=1}^G \sum_{i=1}^I \left| x_{ig}^{(\ell)} - x_{ig}^{(\ell-1)} \right| < \epsilon_I \text{ or } \ell \geq \ell_{\max}, \quad (92)$$

at which point we set $\phi_{ig}^{(n+1)} = x_{ig}^{(\ell)}$.

In practice, the iteration scheme defined by Eq. 91 is slightly modified to reduce unnecessary steps. We define $\bar{g}$ to be the smallest value of g into which there is any up-scattering, taking into account all compositions. Then we set

$$\phi_g^{(n+1)} = x_g^{(1)}$$

for $1 \leq g < \bar{g}$. Then, for $\bar{g} \leq g \leq G$, we have the iteration procedure

$$\begin{aligned}
 A_{g'g}^{(\ell)} = & \sum_{\bar{g} \leq g' < g} B^{g'g} x_{g'}^{(\ell)} + \sum_{G > g' > g} B^{g'g} x_{g'}^{(\ell-1)} + \sum_{g'=1}^{\bar{g}-1} B^{g'g} \phi_{g'}^{(n+1)} \\
 & + \frac{1}{k^{(n)}} \sum_{g'=1}^G F^{g'g} \phi_{g'}^{(n)}, \quad \text{for } g = \bar{g}, \dots, G.
 \end{aligned} \tag{93}$$

Each matrix A_g is an $I \times I$ tridiagonal matrix to which we apply a slightly modified Choleski algorithm³ to solve each matrix equation defined by Eq. 91 or 93. In discussing this algorithm, we shall drop the group index g . Thus our problem is to find the solution x to the linear system

$$Ax = f, \tag{94}$$

where A has the form

$$A = \begin{bmatrix} e_1 & -a_1 & & \circ \\ -c_2 & e_2 & -a_2 & \\ & \cdot & \cdot & \cdot \\ \circ & & \cdot & -c_I \cdot e_I \end{bmatrix}$$

with $e_i > 0$, $a_i \geq 0$, and $c_i \geq 0$. The matrix A is factored into the product of a lower and an upper triangular matrix $A = LU$. Letting $\omega = Ux$, we can write the system $Ax = f$ as

$$L\omega = f,$$

$$Ux = \omega.$$

The matrix U has the form

$$U = \begin{bmatrix} 1 & -\gamma_1 & \circ \\ 0 & 1 & -\gamma_2 \\ & & -\gamma_{I-1} \\ \circ & & & 1 \end{bmatrix},$$

and the elements $\{\gamma_i\}_{i=1}^{I-1}$ are stored. The sequence $\{\omega_i\}_{i=1}^I$ is found each time a new f is given. The sequences γ_i and ω_i can be generated in the following way:

$$\gamma_1 = a_1/e_1, \gamma_i = \frac{a_i}{e_i - c_i \gamma_{i-1}}, \quad \text{for } i = 2, \dots, I-1. \tag{95}$$

The sequence $\{\omega_i\}$ can then be found from

$$\omega_1 = f_1/e_1, \omega_i = \frac{f_i + c_i \omega_{i-1}}{e_i - c_i \gamma_{i-1}}, \quad i = 2, 3, \dots, I. \quad (96)$$

Since the sequence γ_i is stored rather than e_i we would rather generate ω_i from

$$\omega_1 = \frac{\gamma_1}{a_1} f_1, \omega_i = \frac{\gamma_i}{a_i} [f_i + c_i \omega_{i-1}], \quad i = 2, 3, \dots, I. \quad (97)$$

with $a_I = 1$ and

$$\gamma_I = \frac{1}{e_I - c_I \gamma_{I-1}}.$$

However, if i_0 is a black cell, then $a_{i_0-1} = 0 = c_{i_0} = a_{i_0}$. Thus $\gamma_{i_0-1} = \gamma_{i_0} = 0$ and Eq. 97 will yield an indeterminate form. Moreover, the solution of $Ux = \omega$ that is the backward sweep is given by

$$x_I = \omega_I, x_i = \omega_i + \gamma_i x_{i+1}, \quad \text{for } i = I-1, I-2, \dots, 1. \quad (98)$$

This algorithm is valid for block cells, i.e., for $\gamma_{i_0-1} = \gamma_{i_0} = 0$. Thus we shall use Eq. 97 if $a_i \neq 0$, and Eq. 96 if $a_i = 0$. This means we have to store $\{e_i: a_i = 0\}$.

The outer iterations are terminated when the following criteria are satisfied:

$$\sum_{g=1}^G \sum_{i=1}^I \left| \phi_{ig}^{(n+1)} - \phi_{ig}^{(n)} \right| < \epsilon_\phi, \quad (99)$$

$$\left| k^{(n+1)} - k^{(n)} \right| < \epsilon_k, \quad (100)$$

and

$$\bar{k}^{(n+1)} - \underline{k}^{(n+1)} < \epsilon_k, \quad (101)$$

where

$$\bar{k}^{(n+1)} = \text{Max}_{i,g} \frac{\phi_{ig}^{(n+1)}}{\phi_{ig}^{(n)}}, \quad \underline{k}^{(n+1)} = \text{Min}_{i,g} \frac{\phi_{ig}^{(n+1)}}{\phi_{ig}^{(n)}}, \quad (102)$$

and the extrema are taken over those elements $\phi_{ig}^{(n)}$ such that $\phi_{ig}^{(n)} > \epsilon_{\phi \min}$.

The inner iterations are not accelerated because the gain would not warrant the additional coding complexity and storage requirements. On the other hand, the outer iterations are accelerated by means of three-term Chebyshev extrapolation.² As we have seen, the outer iterations consist of the power iterates $\phi^{(n+1)}$ defined by

$$\phi^{(n+1)} = \frac{1}{k^{(n)}} T\phi^{(n)}, \quad (103)$$

where $T = E^{-1}F$. (This is true if no up-scattering is present; the matrix E^{-1} must be modified if up-scattering is present.) If we make the standard assumption that the eigenvalues of T are real, we can apply the usual three-term extrapolation procedure. Let the eigenvalues of T be denoted by $\lambda_1 > \lambda_2 \geq \dots \geq \lambda_n$. Let $\sigma = \lambda_2/\lambda_1$, and suppose the ratios λ_j/λ_1 lie in the interval $[a, \sigma]$. The iterates then have the form

$$\phi^{(n)} = \alpha_1 \frac{\lambda_1^n}{\prod_{j=0}^{n-1} k^{(j)}} u_1 + \alpha_2 \frac{\lambda_2^n}{\prod_{j=0}^{n-1} k^{(j)}} u_2 + \dots, \quad (104)$$

where u_j is the eigenvector associated with λ_j . For the sake of simplicity, all eigenvalues are assumed simple. If we assume that the estimates $k^{(n)}$ have converged, then Eq. 104 takes the form

$$\phi^{(n)} = \alpha_1 u_1 + \alpha_2 \sigma^n u_2 + \dots \quad (105)$$

If we apply a polynomial Q_p in T/λ_1 to this iterate, we obtain

$$Q_p(T/\lambda_1) \phi^{(n)} = \alpha_1 Q_p(1) u_1 + \alpha_2 Q_p(\sigma) u_2 + \dots \quad (106)$$

To preserve convergence, we would choose $Q_p(1) = \text{constant}$, taken to be one, and to accelerate convergence, choose $Q_p(x)$ to be minimal in modulus over $[a, \sigma]$ among all polynomials of degree p . As shown in Ref. 2, Q_p then has the form

$$Q_p(x; \sigma; a) = \frac{C_p \left[\frac{2x - \sigma - a}{\sigma - a} \right]}{C_p \left[\frac{2 - \sigma - a}{\sigma - a} \right]}, \quad (107)$$

where $C_p(y)$ is the Chebyshev polynomial of degree p defined by

$$C_p(y) = \cosh p \cosh^{-1} y \text{ for } y > 1. \quad (108)$$

Since the polynomials C_p satisfy a three-term recursive relation, the polynomials Q_p satisfy the following relation:

$$Q_p(x) = Q_{p-1}(x) + \alpha_p(x-1) Q_{p-1} + \beta_p(Q_{p-1} - Q_{p-2}), \quad (109)$$

where α_p and β_p are defined by

$$\left. \begin{aligned} \alpha_1 &= \frac{2}{2 - \sigma - a}, \\ \beta_1 &= 0, \\ \alpha_p &= \frac{4}{\sigma - a} \frac{\cosh(p-1)\gamma}{\cosh p\gamma}, \\ 1 + \beta_p &= \left[1 - \frac{1}{2}(\sigma + a)\right] \alpha_p, \\ \text{for } p &\geq 2, \end{aligned} \right\} \quad (110)$$

$$\text{where } \cosh \gamma = \frac{2 - \sigma - a}{\sigma - a}.$$

Thus to apply an extrapolation of order p starting with the iterate $\phi^{(n)}$, we proceed as follows.

We wish to find $\hat{\phi}^{(n+p)} = Q_p(T/\lambda_1; \sigma; a) \phi^{(n)}$. Suppose we have found $\hat{\phi}^{(n+q-1)}$ for $1 \leq q \leq p$ then we define

$$\left. \begin{aligned} \text{a) } \phi^{(n+q)} &= \frac{T}{k^{(n+q-1)}} \hat{\phi}^{(n+q-1)}, \\ \text{b) } k^{(n+q)} &= k^{(n+q-1)} \cdot \frac{(\phi^{(n+q)}, \phi^{(n+q)})}{(\phi^{(n+q)}, \hat{\phi}^{(n+q-1)})}; \\ \text{c) } \bar{k}^{(n+q)} &= \text{Max} \frac{\phi_{ig}^{(n+q)}}{\hat{\phi}_{ig}^{(n+q-1)}}; \underline{k}^{(n+q)} = \text{Min} \frac{\phi_{ig}^{(n+q)}}{\hat{\phi}_{ig}^{(n+q-1)}}; \\ \text{d) } \epsilon_{\phi}^{(n+q)} &= \sum_{g=1}^G \sum_{i=1}^I \left| \phi_{ig}^{(n+q)} - \hat{\phi}_{ig}^{(n+q-1)} \right|. \end{aligned} \right\} \quad (111)$$

Then,

$$\hat{\phi}^{(n+q)} = \hat{\phi}^{(n+q-1)} + \alpha_q(\phi^{(n+q)} - \hat{\phi}^{(n+q-1)}) + \beta_q(\hat{\phi}^{(n+q-1)} - \hat{\phi}^{(n+q-2)}) \quad (112)$$

With $\hat{\phi}^{(n)} \equiv \phi^{(n)}$, the above relations hold for $q \geq 1$. Since, in practice, $k^{(n)} \neq \lambda_1$, we are not performing the stationary process described by Eq. 106. In addition to the above quantities, we form

$$E_{n,q} = \frac{\epsilon_{\phi}^{(n+q+1)}}{\epsilon_{\phi}^{(n+1)}} \quad \text{for } q \geq 2. \quad (113)$$

For a successful application of the extrapolation procedure, two conditions must be met:

- i) $k^{(n)} = \lambda_1$.
- ii) An accurate estimate of σ must be known.

Neither condition is met until the problem has converged; however, the sequence $k^{(n)}$ converges at a faster rate than the fluxes $\phi^{(n)}$. Thus condition (i) is met quite early in the iteration procedure. An accurate estimate $\sigma = \lambda_2/\lambda_1$ is also impossible until the later stages of convergence. Rather than continually trying to estimate σ by some direct means, we have adopted the method, used in the PDQ programs, of estimating σ from the results of previous extrapolations; i.e., we use the updating method.⁴ First an initial estimate of σ is computed under the assumption that $k^{(n)} \cong \lambda_1$. From Eq. 104,

$$\frac{\epsilon_{\phi}^{(n+1)}}{\epsilon_{\phi}^{(n)}} \cong \sigma. \quad (114)$$

Equation 114 provides an initial estimate; later in the iteration procedure, it provides estimates, when circumstances dictate its use. Now suppose that we have an estimate $\bar{\sigma}$ for σ and that we have performed an extrapolation cycle of order p on the flux $\phi^{(n)}$. In addition, suppose that this cycle was followed by one unextrapolated iteration so that we have the flux $\phi^{(n+p+1)}$ at our disposal. From Eq. 106, we see that the quantity $E_{n,p}$ defined by Eq. 113 has the following approximate value:

$$E_{n,p} = \frac{\epsilon_{\phi}^{(n+p+1)}}{\epsilon_{\phi}^{(n+1)}} \cong Q_p(\sigma; \bar{\sigma}; a). \quad (115)$$

Now if our estimate $\bar{\sigma}$ is equal to the theoretical value σ then our acceleration is optimal for this method and the error reductions ratio is given by

$$Q_p(\bar{\sigma}; \bar{\sigma}; a) = \frac{1}{C_p \left(\frac{2 - \bar{\sigma} - a}{\bar{\sigma} - a} \right)}.$$

Thus the first thing we do is to compare the actual error-reduction ratio, $E_{n,p}$, with the optimal one; i.e., we make the following test

$$E_{n,p} \leq \frac{1}{C_p \left(\frac{2 - \bar{\sigma} - a}{\bar{\sigma} - a} \right)} \quad (116)$$

If this test is satisfied, we keep $\bar{\sigma}$. If this test is not satisfied and $E_{n,p} < 1$, then we estimate $\bar{\sigma}$, for σ is too low. This conclusion rests heavily on the assumption that $k^{(n)} \cong \lambda_1$. Thus, if this assumption is satisfied, we obtain a new estimate for σ by solving the following equation for σ' :

$$E_{n,p} = Q_p(\sigma'; \bar{\sigma}; a). \quad (117)$$

The new estimate σ' is then given by

$$\sigma' = \frac{1}{2} \left\{ (\bar{\sigma} + a) + (\bar{\sigma} - a) \cosh \frac{1}{p} \Omega \right\}, \quad (118)$$

where $\Omega = \cosh^{-1} [E_{n,p} \cosh p\gamma]$, and γ is defined by

$$\gamma = \cosh^{-1} \left(\frac{2 - \bar{\sigma} - a}{\bar{\sigma} - a} \right).$$

It has been shown in Ref. 4 that $1 > \sigma' > \bar{\sigma}$. The monitoring for the effectiveness of the extrapolation begins with $p = 3$ to a maximum of $p = 8$. If during this period the test defined by Inequality 116 is not satisfied, a new estimate is found, and the extrapolation starts over with $p = 1$. When p reaches 8, or three consecutive estimates for σ have not been effective, the code performs three unextrapolated iterations and then begins extrapolation again.

(4) Adjoint Calculation

In the adjoint calculation, we wish to find solution ϕ^* and the corresponding k for the equation adjoint to Eq. 89.

$$E^* \phi^* = \frac{1}{k} F^* \phi^*, \quad (119)$$

where E^* and F^* denote the adjoint or transposed matrices of E and F , respectively. They are defined by

$$E^* = \begin{bmatrix} A_1^* & -B^{12} & \dots & -B^1 G \\ -B^{21} & A_2^* & & -B^2 G \\ \vdots & & \ddots & \\ -B^G 1 & -B^G 2 & \dots & A_G^* \end{bmatrix}. \quad (120)$$

If only black regions are permitted, $a_{ig} = c_{i+1,g}$ so that the matrices A_g are symmetric in this case. The matrix F^* is defined by

$$F^* = \begin{bmatrix} F^{11} & F^{12} & \dots & \dots & F^{1G} \\ F^{21} & F^{22} & & F^{23} & \dots & F^{2G} \\ \vdots & & & & & \\ F^{G1} & F^{G2} & \dots & \dots & \dots & F^{GG} \end{bmatrix} \quad (121)$$

Since the matrix E^* is heavily upper triangular and the iteration algorithms are designed for a lower triangular matrix, we reorder the adjoint flux during the calculation by defining

$$\psi_g = \phi_{G-g+1}^* \quad (122)$$

Having performed this reordering of the indices of the matrix elements, the calculation then proceeds exactly as in the real case. At the end of the calculation the resulting vector is reordered to obtain the adjoint flux in its standard ordering.

(5) Source Calculation

In a source calculation, we are given a fixed external source distributed over the reactor. For this source, we wish to find the corresponding flux; thus, in the notation of Eqs. 88 and 89, we must solve the equation

$$(E - \mu F) \phi = S, \quad (123)$$

where μ is a specified constant that ensures that the reactor in the absence of any source is subcritical. It suffices to consider the case $\mu = 1$. Since, by assumption, the largest eigenvalue of $E^{-1}F$ is less than one, $(E - F)^{-1} \cdot (1 - E^{-1}F)^{-1}E^{-1}$ exists. Moreover it is nonnegative, since both E^{-1} and $E^{-1}F$ are nonnegative. In addition, the off-diagonal elements are nonpositive; thus we can employ any iterative method derived from a regular splitting² of $E - F$. We shall choose a block Gauss-Seidel splitting $E - F = (D - L) - U$, where

$$D - L = \begin{bmatrix} \bar{A}_1 & \circ & & \circ \\ -(B^{12} + F^{12}) & \bar{A}_2 & \circ & \\ \vdots & & & \\ -(B^{1G} + F^{1G}) & \dots & \dots & \bar{A}_G \end{bmatrix} \quad (124)$$

and

$$\bar{A}_g = A_g - Fg g.$$

The matrix U is then the remaining upper triangular portion, and

$D = \text{diag} [\bar{A}_1, \bar{A}_2, \dots, \bar{A}_G]$. Hence the basic iteration scheme is defined by

$$\bar{A}_g \phi_g^{(n+1)} = \sum_{g' < g} (B g' g + F g' g) \phi_{g'}^{(n+1)} + \sum_{g' > g} (B g' g + F g' g) \phi_{g'}^{(n)} + S_g. \quad (125)$$

The tridiagonal matrix $\bar{A}_g$ is inverted by the standard Choleski method used in the k -effective calculation.

Since the block Jacobi matrix $D^{-1}(L + U)$ associated with $E - F$ is nonnegative with zero diagonal blocks, convergent, and weakly cyclic, successive overrelaxation can be used to accelerate the iteration.² Since the block Jacobi matrix is generally inconsistently ordered, an optimal relaxation factor cannot be found by simple means. Instead of attempting to find this optimal factor, we shall find the optimal factor based on the assumption that the block Jacobi matrix is consistently ordered and cyclic of index 2. This value is defined by

$$\omega = \frac{2}{1 + \sqrt{1 - \rho}}, \quad (126)$$

where ρ is the largest eigenvalue in modulus of the iteration matrix $(D - L)^{-1}U$. The block overrelaxation iteration procedure relative to the decomposition defined by Eq. 124 is given by

$$\phi^{(n+1)} = (D - \omega L)^{-1} \{ [(1 - \omega) D + \omega U] \phi^{(n)} + \omega S \}, \quad (127)$$

or, as actually performed,

$$\left. \begin{aligned} D\bar{\phi}^{(n+1)} &= L\phi^{(n+1)} + U\phi^{(n)} + S; \\ \phi^{(n+1)} &= \phi^{(n)} + \omega(\bar{\phi}^{(n+1)} - \phi^{(n)}). \end{aligned} \right\} \quad (128)$$

In more explicit terms, it is defined by

$$\left. \begin{aligned} \bar{A}_g \bar{\phi}_g^{(n+1)} &= \sum_{g' < g} (B g' g + F g' g) \phi_{g'}^{(n+1)} + \sum_{g' > g} (B g' g + F g' g) \phi_{g'}^{(n)} + S_g; \\ \phi_g^{(n+1)} &= \phi_g^{(n)} + \omega(\bar{\phi}_g^{(n+1)} - \phi_g^{(n)}) \quad \text{for } g = 1, 2, \dots, G. \end{aligned} \right\} \quad (129)$$

For $\omega = 1$, we have the basic Gauss-Seidel iteration scheme defined by Eq. 125.

There remains the problem of estimating the largest eigenvalue ρ of $R = (D - L)^{-1} U$. This is estimated in the following manner. Since R is a nonnegative irreducible matrix, it has a unique largest eigenvalue in modulus which is positive and simple.² Thus, we form

$$\delta^{(n+1)} = \left\| \phi^{(n+1)} - \phi^{(n)} \right\|_1 = \sum_g \sum_i \left| \phi_{ig}^{(n+1)} - \phi_{ig}^{(n)} \right| \quad (130)$$

then

$$\rho_{n+1} = \frac{\delta^{(n+1)}}{\delta^{(n)}} \approx \rho \text{ as } n \rightarrow \infty. \quad (131)$$

The disadvantage of this method for estimating ρ is that it does not provide upper and lower estimates for ρ . It has, however, the advantage that we are iterating towards the solutions while the estimates are being made. An alternative procedure,⁴ which takes full advantage of the power iteration method for finding the largest eigenvalue of a nonnegative, irreducible matrix, provides upper and lower estimates, but does not iterate toward the solution as the estimate is being made, since the source term is put equal to zero.

An alternative acceleration procedure is provided for source calculations. Recall that in terms of the block Gauss-Seidel splitting $E - F = (D - L) - U$, the basic iterative procedure can be written in the form

$$\phi^{(n+1)} = R\phi^{(n)} + f, \quad (132)$$

where $R = (D - L)^{-1} U$ and $f = (D - L)^{-1} S$. If it is assumed that the matrix R has only real eigenvalues, then Chebyshev acceleration can be applied to the above procedure.² Suppose that the eigenvalues lie in the interval $[a, \lambda]$, where $|a| \leq \lambda < 1$. Suppose that beginning with $\phi^{(n)}$ we wish to accelerate the sequence of iterates. If $\hat{\phi}$ denotes the extrapolated flux, the procedure can be represented in the form

$$\hat{\phi}^{(n+p)} = \hat{\phi}^{(n+p-1)} + \alpha_p \left(\phi^{(n+p)} - \hat{\phi}^{(n+p-1)} \right) + \beta_p \left(\hat{\phi}^{(n+p-1)} - \hat{\phi}^{(n+p-2)} \right). \quad (133)$$

The coefficients α_p and β_p are defined just as they were in Eq. 110, except that now the estimate λ for the largest eigenvalue in modulus of R replaces the estimate for the dominance ratio σ of the matrix T . Note that the unextrapolated flux $\phi^{(n+p)}$ is defined by

$$\phi^{(n+p)} = R\hat{\phi}^{(n+p-1)} + f \quad \text{for } p \geq 1, \quad (134)$$

with $\hat{\phi}^{(n)} \equiv \phi^{(n)}$. Again just as in the power iteration case, the estimation of acceleration parameters is the most important aspect of the procedure.

In this case the relevant parameter is the estimate λ of the largest eigenvalue of R . The other parameter, a , is an input quantity. We use the same technique that is used in the power iteration case for estimating and updating the estimate of the largest eigenvalue of R .

(6) Kinetics Options

This module provides two calculation options which can be used in spatial kinetic systems.⁴ The first is simply to permit the external source density to be that due to delayed neutrons. Thus if there are m delayed-neutron families, the module forms an external delayed-neutron source $S_g(r)$ for each point and into each energy group, where this source density is defined by

$$S_g(r) = \sum_{i=1}^m \chi_i^g \lambda_i \xi_i(r). \quad (135)$$

Here $\xi_i(r)$ is the delayed-neutron distribution, λ_i the release constants, and χ_i^g the spectrum. The module forms this distributed source and performs a source calculation. The second option is a special case of an α calculation in which delayed neutrons are taken into account. The spatial kinetics equations can be written in the form⁵

$$\left. \begin{aligned} v_g^{-1} \frac{\partial \Phi_g}{\partial t} &= (F_p \Phi)_g - (E \Phi)_g + \sum_{i=1}^m \lambda_i \chi_i^g \xi_i, \\ \frac{\partial \xi_i}{\partial t} &= \sum_{g'=1}^G (\nu_p \Sigma_f^{g'}) \chi_i^{g'} \Phi_{g'} - \lambda_i \xi_i, \end{aligned} \right\} \quad (136)$$

where

$$(F_p \Phi)_g = \sum_{g'=1}^G \chi^{g'g} (\nu_p \Sigma_f)^{g'} \Phi_{g'}, \quad (137)$$

and

$$(E \Phi)_g = A_g \Phi_g - \sum_{g' \neq g} B^{g'g} \Phi_{g'}. \quad (138)$$

If the flux and precursor concentration are assumed to be separable in space and time, so that $\Phi = \phi e^{\alpha t}$ and $\xi_i = \zeta_i e^{\alpha t}$, then the above equations take the form

$$\left. \begin{aligned} v_g^{-1} \alpha \phi_g &= (F_p \phi)_g - (E \phi)_g + \sum_{i=1}^m \lambda_i \chi_i^g \zeta_i \\ \alpha \zeta_i &= -\lambda_i \zeta_i + \sum_{g'=1}^G \chi^{g'i} (\nu_p \Sigma_f)^{g'} \phi_{g'} \end{aligned} \right\} \quad (139)$$

Eliminating the spatial precursors ζ_i , we arrive at the single equation

$$[(E + \alpha v^{-1}) \phi]_g = \sum_{g'=1}^G \left[\chi^{g'g} + \sum_{i=1}^m \lambda_i (\lambda_i + \alpha)^{-1} \chi^{g'i} \chi_i^g \right] (\nu_p \Sigma_f)^{g'} \phi_{g'}. \quad (140)$$

The assumption of separability implies that we are interested in the time behavior of the flux after the transients have died out. Thus we seek the largest value of α and the corresponding nonnegative flux that satisfy Eq. 140. This is simply a generalized α calculation that the module performs. Thus for each α , the module solves the system

$$[(E + \alpha v^{-1}) \phi]_g = \frac{1}{k_\alpha} \sum_{g'=1}^G \left[\chi^{g'g} + \sum_{i=1}^m \lambda_i (\lambda_i + \alpha)^{-1} \chi_i^g \chi^{g'i} \right] (\nu_p \Sigma_f)^{g'} \phi_{g'}(\alpha) \quad (141)$$

and then searches on α to achieve $k_\alpha = 1$. A special case of this procedure is to seek the solution of Eq. 141 when $\alpha = 0$. This solution is used in spatial kinetics.

c. References

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d. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
A.DIFF1D	Module-dependent data. Iteration limits. Convergence criteria.
SP.CICN	Module-independent data.
GEOM	General descriptive data on mesh structure. Region-to-mesh correspondence. Composition-to-mesh correspondence. Buckling.
BC	Definitions of external and internal boundary conditions.
XS.C.MIN	Composition cross sections Σ_{tr} , Σ_R , Σ_S , $\nu\Sigma_f$, χ .
FR.D1 (or FA.D1)	Eigenvalue (k_{eff}). One-dimensional real (or adjoint) flux guess.
ES.D1D	One-dimensional distributed external service if doing an external source calculation.
XS.DELAY	Delayed data (if doing a kinetics option) delayed-neutron spectrum, decay constants, and delayed-neutron distributions.
XS.C.AUX	Prompt $\nu\Sigma_f$, delayed χ (if doing a kinetics option).
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
FR.D1 (or FA.D1)	Eigenvalue (k_{eff}). One-dimensional real (or adjoint) flux vector.

17. 1D-Transport NUC003

Prepared by: G. J. Duffy

a. Nature of Physical Problem Solved

This module solves the time-independent transport equation in one dimension for many groups, allowing up to linear anisotropic scattering. Geometries include those that describe the sphere, cylinder, and slab. A fixed isotropic source (or a shell source) is allowed in the solution of an inhomogeneous system. A homogeneous system can be solved to obtain a value of k_{eff} , or geometry, concentration, or α can be varied until criticality is reached. Density factors may be used to modify cross sections by interval. A consistent P1 calculation may be used in lieu of the iterative, SN, difference solution. A real or adjoint system can be solved. Left and right boundary conditions can be free, reflective, or periodic; the right boundary can be white for curved geometries. Fission sources and/or fluxes may be used to start the calculation. Provision for the leakage correction in transverse buckling is available. A fixed value of k_{eff} or α is allowed. A workable negative flux fixup has been incorporated, as has scaling necessary to accelerate convergence when up-scattering is present.

b. Method of Solution

Let $\vec{x}$ be a position vector, $\vec{\Omega}$ a point on the unit direction sphere associated with the point $\vec{x}$, and v_j the neutron speed in energy group j . Then the equation for the angular flux in group j , $\bar{\phi}_j(t, \vec{x}, \vec{\Omega})$ is

$$\frac{1}{v_j} \frac{\partial \bar{\phi}_j}{\partial t} + \vec{\Omega} \cdot \vec{\nabla} \bar{\phi}_j + \sigma_j(\vec{x}) \bar{\phi}_j = \bar{S}_j(t, \vec{x}, \vec{\Omega}), \quad (142)$$

where $\sigma_j(\vec{x})$ is the total cross section and $\bar{S}_j$ the source for group j .

Furthermore, assume that the angular flux is separable into a product $T\phi$, where T only is time-dependent and equal to $e^{\alpha t}$; let S_j be separable in the same way:

Equation 142 becomes

$$\vec{\Omega} \cdot \vec{\nabla} \phi_j + \left(\sigma_j(\vec{x}) + \frac{\alpha}{v_j} \right) \phi_j = S_j(\vec{x}, \vec{\Omega}),$$

where

$$\phi_j = \phi_j(\vec{x}, \vec{\Omega}). \quad (143)$$

Equation 143 now represents the time-independent transport equation.

The angular variable in Eq. 142 is discretized into $\{\vec{\Omega}_m\}$, and integration is performed by using weights, W_m , and direction cosines, μ_m , which satisfy the relations

$$\sum_{m=1}^M W_m = 1, \quad (144)$$

$$\sum_{m=1}^M \mu_m W_m = 0, \quad (145)$$

and

$$\sum_{m=1}^M \mu_m^2 W_m = \frac{1}{3}, \quad (146)$$

where M is the total number of directions on the octant of the unit sphere.

A neutron balance equation is written for an arbitrary cell enclosing the point $(\vec{x}, \vec{\Omega}_m)$ and becomes Eq. 143 as the cell size shrinks.

Let i be the index specifying the mesh structure along the x axis, and m the direction index; x stands for the space coordinate in slab, sphere, or cylinder geometry. The cell-face area perpendicular to x at i is denoted by A_i .

The balance equation for any of these geometries for group j is then

$$\begin{aligned} & \frac{\mu_m}{V_{i+\frac{1}{2}}} (A_{i+1} \phi_{m,i+1,j} - A_i \phi_{m,i,j}) \\ & + \frac{(A_{i+1} - A_i)}{V_{i+\frac{1}{2}} W_m} (\beta_{m+\frac{1}{2}} \phi_{m+\frac{1}{2},i+\frac{1}{2},j} - \beta_{m-\frac{1}{2}} \phi_{m-\frac{1}{2},i+\frac{1}{2},j}) \\ & + \sigma_{i+\frac{1}{2},j} \phi_{m,i+\frac{1}{2},j} = S_{m,i+\frac{1}{2},j} \end{aligned} \quad (147)$$

with

$$\phi_{m,i+\frac{1}{2},j} = \frac{1}{2} (\phi_{m,i+1,j} \pm \phi_{m,i,j}), \quad (148)$$

the index $i + \frac{1}{2}$ denoting the midpoint of the interval between x_i and x_{i+1} .

The first term in Eq. 147 represents the flow through the geometric face area of the cell; the second term represents flow across the direction intervals; $V_{i+\frac{1}{2}}$ is the geometric volume of the cell.

The β 's satisfy the relation

$$\beta_{m+\frac{1}{2}} - \beta_{m-\frac{1}{2}} = -W_m \mu_m. \quad (149)$$

Define the curvature as

$$GC_{m,i} = (A_{i+1} - A_i) \left\{ \frac{2\beta_{m+\frac{1}{2}}}{W_m} + \mu_m \right\}. \quad (150)$$

Use Eq. 149 to eliminate the β 's and obtain

$$GC_{m,i} = \frac{GC_{m-1,i} \cdot W_{m-1} - (A_{i+1} - A_i) (W_m \mu_m - W_{m-1} \mu_{m-1})}{W_m} \quad \text{if } W_m \neq 0 \quad (151)$$

for cylinders and spheres ($GC_{m,i} = 0$ if $W_m = 0$), and $GC_{m,i} = 0$ for slab.

Equation 147 is put in recursive form to give

(for decreasing $i, \mu_m < 0$)

$$\phi_{m,l,j} = \frac{V_l S_{m,l,j} + |\mu_m| (A_{i+1} + A_i) \phi_{m,i+1,j} + GC_{m,i} \phi_{m-\frac{1}{2},l,j}}{GC_{m,i} + |\mu_m| (A_{i+1} + A_i) + V_l \sigma_{l,j}}, \quad (152)$$

and

(for increasing $i, \mu_m > 0$)

$$\phi_{m,l,j} = \frac{V_l S_{m,l,j} + |\mu_m| (A_{i+1} + A_i) \phi_{m,i,j} + GC_{m,i} \phi_{m-\frac{1}{2},l,j}}{GC_{m,i} + |\mu_m| (A_{i+1} + A_i) + V_l \sigma_{l,j}}, \quad (153)$$

where

$$\left. \begin{aligned} \phi_{m,l,j} &= \phi_{m,i+\frac{1}{2},j}, \\ S_{m,l,j} &= S_{m,i+\frac{1}{2},j}, \end{aligned} \right\} \quad (154)$$

(Contd.)

and

$$\left. \phi_{m,l,j} = \frac{1}{2} \left(\phi_{m+\frac{1}{2},i+\frac{1}{2},j} + \phi_{m-\frac{1}{2},i+\frac{1}{2},j} \right) \right\} \quad \begin{array}{l} \text{(Contd.)} \\ (154) \end{array}$$

The following relations define elements as used in the formula set description:

$$V_l S_{m,l,j} = \mu_m SL_{l,j} + S_{l,j},$$

where $SL_{l,j} = SA_{l,j} + (\nu \sigma_f)_{l,j} J_{l,j}$ calculates the anisotropic component, where

$$SA_{l,j} = \sum_{\substack{k \\ k \neq j}} V_l \sigma_l^{(1)}(k \rightarrow j) J_{l,k}^\rho + V_l \sigma_l^{(1)}(j \rightarrow j) J_{l,j}^\pi,$$

$$J_{l,k}^\rho = 3 \sum_m W_m \mu_m \phi_{m,l,k}^\rho,$$

$$J_{l,j}^\pi = 3 \sum_m W_m \mu_m \phi_{m,l,k}^\pi,$$

$\phi_{m,l,k}^\pi$ is the flux for direction m , interval l , and group k for the π th inner iteration, or ρ th outer iteration,

$\sigma_l^{(1)}(k \rightarrow j)$ is the anisotropic component of scattering,

V_l is the volume for interval l ;

and

$$S_{l,j} = V_l \sigma_l^{(0)}(j \rightarrow j) \phi_{l,j}^\pi + SI_{l,j}$$

calculates the isotropic component, where

$$\phi_{l,j}^\pi = \sum_m W_m \phi_{m,l,k}^\pi$$

is the scalar flux for interval l , group j and the π th inner iteration.

$$SI_{l,j} = \sum_{\substack{k \\ k \neq j}} V_l \sigma_l^{(0)}(k \rightarrow j) \phi_{l,k} + FI_{l,j} + V_l Q_{l,j},$$

$\sigma_{\ell}^{(0)}(k \rightarrow j)$ is the isotropic component of scattering,

$$FI_{\ell,j} = \left\{ \begin{array}{l} V_{\ell} \sum_k \chi_{\ell}(k,j) (\nu \sigma_f)_{\ell,k} \phi_{\ell,k} \text{ for the real case} \\ V_{\ell} (\nu \sigma_f)_{\ell,j} \sum_k \chi_{\ell}(j,k) \phi_{\ell,k} \text{ for the adjoint case} \end{array} \right\},$$

$\phi_{\ell,k}$ is the scalar flux for the previous outer iteration,

$$Q_{\ell,j} = Q_{\ell,j}^* \cdot NF / \overline{QG},$$

where

NF is the normalization factor (input),

$Q_{\ell,j}^*$ is the distributed source (input),

and

$$\overline{QG} = \sum_j \sum_{\ell} V_{\ell} Q_{\ell,j}^*,$$

$$|\mu_m| (A_{i+1} + A_i) = GA_{m,i},$$

$$GC_{m,i} + GA_{m,i} = G_{m,i},$$

$$\phi_{m-\frac{1}{2},\ell,j} = E_{m,\ell},$$

$$V_{\ell} \sigma_{\ell,j} = \sigma_{t,\ell,j},$$

$$\phi_{m,\ell,j} = V3_{\ell}, \quad \text{for } \mu < 0,$$

$$\phi_{m,\ell,j} = V3_{\ell+1}, \quad \text{for } \mu > 0.$$

The value of k_{eff} is determined as

$$k_{\text{eff}}^{\rho} = \lambda_{\rho} \cdot k_{\text{eff}}^{\rho-1},$$

where ρ is the outer iteration count,

and

$$\lambda_\rho = \frac{FG^\rho}{N},$$

where N is the input normalization factor and

$$FG^\rho = \sum_j \sum_\ell FI_{\ell,j}^\rho.$$

In criticality searches, the search parameter, EV_p , is determined from previous values of EV and λ by linear interpolation. The current value, EV_p , is then used to determine new elements in the various type searches in the following ways:

(1) Radius Search

$$x_{i+1}^\rho = x_i^\rho + (1 + EV_p \cdot RZ_i) \Delta_\ell,$$

where

$$\Delta_\ell = x_{i+1}^0 - x_i^0, \quad \text{and } RZ_i$$

are input radius modifiers, constant within each region.

(2) Inverse Reactor Period α . The element t_j is computed and added to the total cross section for each group j for each outer iteration.

$$t_j = \begin{cases} (EV_p + \alpha_0)/v_j & \text{for } \alpha \text{ calculation with fixed } \alpha_0, \\ EV_p/v_j & \text{for } \alpha \text{ calculation,} \\ \alpha_0/v_j & \text{for fixed } \alpha_0 \text{ for any problem type.} \end{cases}$$

(3) Concentration Search. The input module prepares a pseudo-composition cross section, $\sigma_{x,j}^{c'}$, for each composition c to be modified. The input module provides "volume fraction modifiers" that are used as coefficients in forming the linear combination of isotopes or materials used to generate c' , the pseudocomposition for each group j and reaction type x .

For each value of EV_p , the new composition cross sections are computed as

$$\sigma_{x,j}^{c,p} = \sigma_{x,j}^{c,p-1} + (EV_p - EV_{p-1}) \cdot \sigma_{x,j}^{c'}.$$

c. References

G. J. Duffy, H. Greenspan, S. D. Sparck, J. V. Zapatka, and M. K. Butler, SNARG-1D, A One-dimensional, Discrete-ordinate, Transport-theory Program for the CDC-3600, ANL-7221 (June 1966).

R. Avery, M. K. Butler, and H. Greenspan, ANL-CDC Reprogramming Series I, Cross Section Nomenclature for ANL Reactor Codes, ANL, AMD Technical Memorandum 92 (Jan. 5, 1965).

d. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
BC	Left and right boundary conditions.
ES.DISH	Anisotropic and isotropic component of shell source by group.
FR.D1	Fluxes by interval and group.
FR.RB	Angular flux for right boundary by group.
FSA.D1	Adjoint fission source by interval and group.
FSR.D1	Real fission source by interval and group.
GEOM	Composition-region correspondence. Number of regions in reactor. Mesh points. Region-mesh correspondence.
SP.CRIT	Criticality search parameters.
SP.NEUT1	Direction cosines and weights for integration. Density factors by interval. Groups for which consistent P1 calculation is used. Groups to be skipped. Source normalization factor. Maximum number of inner and outer iterations. SN order.
XS.C.MIN	Number of compositions, groups, and fissionable compositions. Order of anisotropy for each composition. Compositions that are fissionable. Number of groups of upscattering and downscattering in each

Upper-interface Data ModulesQuantities Used

XS.C.MIN (Contd.)

composition. Total cross section. Total isotropic component of scattering, $\Sigma_{\ell,j \rightarrow k}$, for composition ℓ . Fission composition cross sections, Σ_f, ν, χ .

XS.VEL

The average velocity for each group.

XS.C.ANI

Anisotropic scattering cross-section components for composition ℓ ,
 $\Sigma_{\ell,j \rightarrow k}^{(L)}$.

ES.D1D

External distributed source by interval and group.

FA.D1

Adjoint fluxes by interval and group.

OUT.TR1

Convergence and error data.

SP.CICN

Module-independent data.

Lower-interface Data ModulesQuantities Produced

FR.D1

Fluxes by interval and group.

FR.D1A

Angular fluxes by interval and group.

FA.D1

Adjoint fluxes by interval and group.

FA.D1A

Adjoint angular fluxes by interval and group.

FSA.D1

Adjoint fission source by interval and group.

FSR.D1

Real fission source by interval and group.

OUT.TR

Convergence and error statistics. Current eigenvalue or k_{eff} value. Current fission ratio. Loop counts.

XS.C.MIN

Fission fractions for compositions. New cross sections if compositions are modified.

Lower-interface Data ModulesQuantities Produced

GEOM

New radii if radii are modified.

XS.C.ANI

New cross sections if compositions are modified.

FR.RB

Angular flux for right boundary by group.

JR.D1

Real current by interval and group.

JA.D1

Adjoint current by interval and group.

18. 2D-Diffusion NUC004

Prepared by: G. K. Leaf and A. S. Kennedy

a. Nature of Physical Problem

The two-dimensional, multigroup, diffusion approximation to the transport equation for the cases of real, adjoint, and external source problems.

b. Method of Solution

(1) Introduction. This module is concerned with the solution of the finite-difference approximation to the multigroup diffusion equation. Three basic types of calculations can be made: real k_{eff} , adjoint k_{eff} , and, in the presence of external sources or inhomogeneous boundary conditions, a source calculation. These calculations can be made in any of the three geometries xy , rz , and $r\theta$, including the periodic case. The permissible form of the external boundary conditions is linear and homogeneous for k_{eff} calculations, and linear and inhomogeneous for source calculations. Interface conditions across regional boundaries can be specified by the logarithmic derivative condition for black regions or the usual continuity of flux and current for all other cases. Scattering between energy groups is unrestricted in form so that full up and down scattering can be present.

(2) Derivation of the Difference Equations. The method used to derive the finite-difference approximation to the diffusion equation in this module is the same as that used by Hassitt in CRAM^{†1} and later by Sangren in CANDID.² For completeness we shall carry through the derivation rz geometry and simply exhibit the results for xy and $r\theta$ geometry.

Let a reactor be given with outer radius R and height H such that the boundary surfaces of the regions making up this reactor are perpendicular to the z axis and the radial axis. The multigroup diffusion system can then be written in the form

$$\begin{aligned}
 -\text{div}(D_g(\bar{r}) \nabla \phi_g(\bar{r})) + \sigma_R^g(\bar{r}) \phi_g(\bar{r}) &= \sum_{g' \neq g} \sigma_{(\bar{r})}^{g' \rightarrow g} \phi_{g'}(\bar{r}) \\
 + \frac{1}{k} \sum_{g'=1}^G \chi_{(\bar{r})}^{g'g} (\nu \sigma_f)_{g'}(\bar{r}) \phi_{g'}(\bar{r}), \quad \text{for } g = 1, 2, \dots, G. \quad (155)
 \end{aligned}$$

[†]For this and other references in this portion of Appendix B, see references listed on page 122.

Here $\phi_g(\bar{r})$ denotes the neutron flux in the g th energy group at the spatial point $\bar{r} = (r, z)$.

The macroscopic cross sections $D_g(\bar{r})$, $\sigma_R^g(\bar{r})$, $\sigma_{g' \rightarrow g}^g(\bar{r})$, $\chi_{g' \rightarrow g}^g(\bar{r})$, and $(\nu\sigma_f)_{g'}(\bar{r})$ are presumed to be constant within any given region. At the exterior boundary surfaces, we shall assume the boundary conditions are of the form

$$A_g(\bar{r}) \nabla \phi_g(\bar{r}) \cdot \hat{n} + B_g(\bar{r}) \phi_g(\bar{r}) = 0, \quad \text{for } g = 1, 2, \dots, G. \quad (156)$$

Again we assume that $A_g(\bar{r})$ and $B_g(\bar{r})$ are constant within a given region. The object in a real k_{eff} calculation is to find the largest value of k and the corresponding set of nonnegative fluxes $\{\phi_g(\bar{r})\}$ satisfying Eqs. 155 and 156. In the adjoint case, we seek the solution to the adjoint system associated with Eqs. 155 and 156. A source-type problem can arise in two ways. If an external source term $S_g(\bar{r})$ is added to the right-hand side of Eq. 155, and if the boundary conditions expressed by Eq. 156 are either left in their homogeneous form or modified to a nonhomogeneous form by replacing the right-hand side by a term $C_g(\bar{r})$, then a source-type problem arises. The second way in which a source-type problem can arise is by inserting the term $C_g(\bar{r})$ on the right-hand side of Eq. 156, but without the addition of an external source in Eq. 155. In either case, there is no determination of k . It is either specified or put equal to one. The sole object is to find the nonnegative flux satisfying Eqs. 155 and 156.

To approximate the solution of the system by means of finite differences, we lay down a mesh structure on the reactor so that all region boundaries lie on mesh lines. Let the abscissas of the vertical mesh lines be denoted by $0 = R_0 < R_1 < \dots < R_I = R$, and the ordinates of the horizontal mesh lines by $0 = Z_0 < Z_1 < \dots < Z_J = H$. The region defined by $R_{i-1} \leq r \leq R_i$; $Z_{j-1} \leq Z \leq Z_j$ with center at (r_i, z_j) will be called by the (i, j) th mesh cell. The vertical set of points $\{(i, j)\}_{j=1}^J$ is called a channel. Consider the differential Eq. 155 in the (i, j) th cell; then integrate the equation over the volume of that cell. Since regional boundaries lie on mesh lines, each cross section is constant within the cell. Thus Eq. 155 becomes

$$\begin{aligned} & - \int_{V_{ij}} \int \text{div} (D_{ijg} \nabla \phi_g(\bar{r})) dV + (\sigma_R)_{ijg} \int_{V_{ij}} \int \phi_g(\bar{r}) dV \\ & = \sum_{g' \neq g} \sigma_{ij}^{g' \rightarrow g} \int_{V_{ij}} \int \phi_{g'}(\bar{r}) dV + \frac{1}{k} \sum_{g'=1}^G \chi_{ij}^{g' \rightarrow g} (\nu\sigma_f)_{ijg'} \int_{V_{ij}} \int \phi_{g'}(\bar{r}). \end{aligned} \quad (157)$$

Here we have used the subscripts ij to denote the constant value of the cross sections in the mesh cell. Let $\phi_{ijg} = \phi_g(r_i, z_j)$; then we make the approximation

$$\int_{V_{ij}} \int \sigma_g(\bar{r}) dV \cong \phi_{ijg} V_{ij}. \quad (158)$$

To the term involving the Laplacian, we apply Green's identity to obtain

$$\int_{V_{ij}} \int \text{div}(D_{ijg} \nabla \phi_g(\bar{r})) dV = - \int_{B_{ij}} D_{ijg} \nabla \phi_g(\bar{r}) \cdot \hat{n} ds, \quad (159)$$

where B_{ij} denotes the boundary of the cell and $\hat{n}$ denotes the unit normal to this boundary. There are three cases to consider in the approximation of the right-hand side of Eq. 159:

- (a) The (ij)th cell is a "normal" interior cell, i.e., one for which the ordinary conditions of continuity of flux and current can be applied across its boundaries.
- (b) The cell is "abnormal" in the sense that it is adjacent to the black cell.
- (c) The cell is an exterior cell, so that at least one of its boundaries is part of the external boundary of the reactor.

Fig. 5 Interior Mesh Cell for 2D-Diffusion Module

We shall consider case (a) first. The energy subscript will be dropped. Referring to Fig. 5, we shall consider the portion of B_{ij} that extends from 1 to 2. We assume first that variations in the flux with respect to Z along the boundary from 1 to 2 can be neglected. In this case, the interface conditions take the form

$$\left. \begin{aligned} \phi(R_i^-) &= \phi(R_i^+); \\ D_{ij} \frac{\partial \phi}{\partial r} \Big|_{r=R_i^-} &= D_{i+1,j} \frac{\partial \phi}{\partial r} \Big|_{r=R_i^+} \end{aligned} \right\} \quad (160)$$

If we expand the flux and its first derivative in the r -direction about the points (i,j) and (i+1,j), we obtain

$$\begin{aligned} \phi(R_i^-) &= \phi_{ij} + \frac{1}{2} \Delta R_i \phi'_{ij} + \dots; \\ \phi(R_i^+) &= \phi_{i+1,j} - \frac{1}{2} \Delta R_{i+1} \phi'_{i+1,j} + \dots; \\ \phi'(R_i^-) &= \phi'_{ij} + 2(\frac{1}{2} \Delta R_i) \phi''_{ij} + \dots; \\ \phi'(R_i^+) &= \phi'_{i+1,j} - 2(\frac{1}{2} \Delta R_{i+1}) \phi''_{i+1,j} + \dots \end{aligned}$$

Solving the first set for ϕ_{ij} and $\phi_{i+1,j}$ and using the second set to solve for ϕ'_{ij} and $\phi'_{i+1,j}$, we obtain

$$\phi_{ij} = \phi(R_i^-) - \frac{1}{2} \Delta R_i \phi'(R_i^-) + \text{higher-order terms};$$

$$\phi_{i+1,j} = \phi(R_i^+) + \frac{1}{2} \Delta R_{i+1} \phi'(R_i^+) + \text{higher-order terms}.$$

Using the interface conditions $\phi(R_i^-) = \phi(R_i^+)$ and $D_{ij} \phi'(R_i^-) = D_{i+1,j} \phi'(R_i^+)$, we multiply the first equation by $\frac{1}{2} \Delta R_{i+1} D_{ij}$ and the second by $\frac{1}{2} \Delta R_i D_{i+1,j}$, then add to obtain, after neglecting terms of order higher than the first,

$$\phi(R_i) \cong \frac{\frac{1}{2} \Delta R_i D_{i+1,j} \phi_{i+1,j} + \frac{1}{2} \Delta R_{i+1} D_{ij} \phi_{ij}}{\frac{1}{2} \Delta R_i D_{i+1,j} + \frac{1}{2} \Delta R_{i+1} D_{ij}}. \quad (161)$$

Putting this expression for $\phi(R_i)$ into the equation for ϕ_{ij} and solving the resulting equation for $D_{ij} \phi'(R_i^-)$, we obtain

$$D_{ij} \phi'(R_i^-) \cong \frac{D_{ij} D_{i+1,j}}{\frac{1}{2} \Delta R_i D_{i+1,j} + \frac{1}{2} \Delta R_{i+1} D_{ij}} (\phi_{i+1,j} - \phi_{ij}). \quad (162)$$

Thus,

$$\int_1^2 D_{ij} \nabla \phi \cdot \hat{n} ds \cong \frac{D_{ij} D_{i+1,j}}{\frac{1}{2} \Delta R_i D_{i+1,j} + \frac{1}{2} \Delta R_{i+1} D_{ij}} (\phi_{i+1,j} - \phi_{ij}) 2R_i \Delta Z_j. \quad (163)$$

The factor π has been left out of the area since it will appear in every term of the finite difference equation. The remaining three sides of the boundary B_{ij} are handled in a similar manner. Hence for a normal interior cell we can make the following definitions:

$$\left. \begin{aligned} a_{ij} &= \frac{D_{ij} D_{i+1,j}}{\frac{1}{2} \Delta R_i D_{i+1,j} + \frac{1}{2} \Delta R_{i+1} D_{ij}} \cdot 2R_i \Delta Z_j, \\ b_{ij} &= \frac{D_{ij} D_{i,j+1}}{\frac{1}{2} \Delta Z_j D_{i,j+1} + \frac{1}{2} \Delta Z_{j+1} D_{ij}} (R_i^2 - R_{i-1}^2), \\ c_{ij} &= a_{i-1,j}, \\ d_{ij} &= b_{i,j-1}, \\ e_{ij} &= a_{ij} + b_{ij} + c_{ij} + d_{ij} + (\sigma_R)_{ij} V_{ij}, \end{aligned} \right\} \quad (164)$$

and

where

$$V_{ij} = (R_i^2 - R_{i-1}^2) \Delta Z_j.$$

We shall consider the case of an external cell next. For convenience, assume that the portion of the boundary from points 1 to 2 is an external boundary on which a boundary condition of the form $A \nabla \phi \cdot \hat{n} + B\phi = C$ is imposed. A , B , and C are constant within the cell. We again neglect the dependence of the flux on z , and expand the flux and its r -derivative in a Taylor series:

$$\phi(R_i) = \phi_{ij} + \frac{1}{2} \Delta R_i \phi'_{ij} + \left(\frac{1}{2} \Delta R_i\right)^2 \phi''_{ij} + \dots;$$

$$\phi'(R_i) = \phi'_{ij} + 2\left(\frac{1}{2} \Delta R_i\right) \phi''_{ij} + \dots$$

Using the relation $A\phi'(R_i) + B\phi(R_i) = C$, we obtain

$$C = B\phi_{ij} + \left(A + \frac{1}{2} \Delta R_i B\right) \phi'_{ij} + \left[2A\left(\frac{1}{2} \Delta R_i\right) + B\left(\frac{1}{2} \Delta R_i\right)^2\right] \phi''_{ij} + \dots$$

Thus, eliminating ϕ'_{ij} between this equation and the expansion for $\phi'(R_i)$, we have

$$(C - B\phi_{ij}) - \left(A + \frac{1}{2} \Delta R_i B\right) \phi'(R_i) = -\left(\frac{1}{2} \Delta R_i\right)^2 B\phi''_{ij} + \dots$$

Neglecting terms of order higher than the first, we obtain

$$\phi'(R_i) \approx \frac{C - B\phi_{ij}}{A + \frac{1}{2} \Delta R_i B}.$$

Finally, we have

$$\int_1^2 D_{ij} \phi'(R_i) ds \approx \frac{D_{ij}(C - B\phi_{ij})}{A + \frac{1}{2} \Delta R_i B} \cdot 2R_i \Delta Z_j. \quad (165)$$

Here we see how inhomogeneous terms

$$\frac{D_{ij} \cdot 2R_i^2 \Delta Z_j}{A + \frac{1}{2} \Delta R_i B}$$

arise in the difference equation when inhomogeneous boundary conditions are imposed. Finally we see that for an external boundary on the right side of the (i,j) th cell, the coefficients a_{ij} are defined by

$$\left. \begin{aligned} a_{ij} &= 0; \\ e_{ij} &= b_{ij} + c_{ij} + d_{ij} + \frac{D_{ij} B 2 R_i \Delta Z_j}{A + \frac{1}{2} \Delta R_i B} + (\sigma_R)_{ij} V_{ij}. \end{aligned} \right\} \quad (166)$$

Similar results hold for each of the other boundaries.

The last case to consider is that of an abnormal cell. Suppose that the $(i+1, j)$ cell is "black" with respect to the flux in a given energy group. Then the region interior to this cell is exterior to the domain of the differential equation for the group; moreover, on the boundary a condition of the form $D \nabla \phi \cdot \hat{n} + \Lambda \phi = 0$ is imposed. Thus for any cell adjacent to this "black" cell we apply the above boundary condition. For example, in the $(i, j)^{\text{th}}$ cell we have

$$a_{ij} = 0,$$

and

$$e_{ij} = b_{ij} + c_{ij} + d_{ij} + \frac{D_{ij} \Lambda 2 R_i \Delta Z_j}{D_{ij} + \frac{1}{2} \Delta R_i \Lambda} + (\sigma_R)_{ij} V_{ij}.$$

Note that all remarks apply to that energy group for which the cell appears "black." The same cell may be normal for other energy groups. Since there is no diffusion in the black cell, we set $D_{i+1, j} = 0$; this gives $a_{i+1, j} = b_{i+1, j} = c_{i+1, j} = d_{i+1, j} = 0$ and $e_{i+1, j} = (\sigma_R)_{i+1, j} V_{i+1, j}$. Having completed the approximation of the right-hand side of Eq. 159 we can write the difference equation obtained from Eq. 157:

$$\begin{aligned} & (a_{ijg} \phi_{i+1, jg} + b_{ijg} \phi_{i, j+1, g} + c_{ijg} \phi_{i-1, j, g} + d_{ijg} \phi_{i, j-1, g} + e_{ijg} \phi_{ijg}) \\ & + e_{ijg} \phi_{ijg} = \sum_{g' \neq g} V_{ij} \sigma_{ij}^{g' \rightarrow g} \phi_{ijg'} + \frac{1}{k} \sum_{g'=1} \chi_{ij}^{g'g} (\nu \sigma_f)_{ijg} V_{ij} \phi_{ijg'} \end{aligned} \quad (167)$$

for $g = 1, 2, \dots, G$, $i = 1, 2, \dots, I$, and $j = 1, 2, \dots, J$.

Note that introducing black regions has not destroyed the symmetry of the coefficient matrix, i.e., $a_{ijg} = c_{i+1, jg}$ and $b_{ijg} = d_{i, j+1, g}$. What it has done is to permit the possibility that some of the coefficients a_{ijg} and b_{ijg} are zero. We shall, however, continue to treat the matrix as unsymmetric,

since more general interface conditions would lead to this situation. The computational part of the code is capable of handling either case.

(3). Solution of the Difference Equations. To derive a method of solution for the system expressed by Eq. 167, we shall order and group the space in a certain way. The equations are first ordered with respect to channels running from 1 through I. Then, within each channel, they are ordered with respect to energy groups beginning with $g = 1$ through $g = G$. Finally, within a given energy group, the ordering is with respect to the points in a channel from $j = 1$ to $j = J$. With this order in mind, we define the following matrices:

$$\left. \begin{aligned} \text{a) } A_{ig} &= \text{diag}[a_{i1g}, a_{i2g}, \dots, a_{iJg}]; \\ \text{b) } C_{ig} &= \text{diag}[c_{i1g}, c_{i2g}, \dots, c_{iJg}]; \\ \text{c) } J_{ig} &= \begin{bmatrix} e_{i1g} & -b_{i1g} & & & \\ -d_{i2g} & e_{i2g} & -b_{i2g} & & 0 \\ & & & \ddots & \\ & & & & -d_{iJg} e_{iJg} \\ 0 & & & & \end{bmatrix}; \\ \text{d) } B_i^{g'g} &= \text{diag}[V_{i1}\sigma_{i1}^{g'g}, \dots, V_{iJ}\sigma_{iJ}^{g'g}]; \\ \text{e) } F_i^{g'g} &= \text{diag}[V_{i1}\chi_{i1}^{g'g}(\nu\sigma_f)_{i1g}, \dots, V_{iJ}\chi_{iJ}^{g'g}(\nu\sigma_f)_{iJg}]. \end{aligned} \right\} \quad (168)$$

Since $e_{ijg} > a_{ijg} + b_{ijg} + c_{ijg} + d_{ijg}$, we see that J_{ig} is positive definite and $J_{ig}^{-1} > 0$.

We next group the above $J \times J$ matrices into blocks of dimension $G \times G$. Thus we define

$$\left. \begin{aligned}
 &\text{a) } A_i = \text{diag}[A_{i1}, A_{i2}, \dots, A_{iG}]; \\
 &\text{b) } C_i = \text{diag}[C_{i1}, C_{i2}, \dots, C_{iG}]; \\
 &\text{c) } J_i = \text{diag}[J_{i1}, J_{i2}, \dots, J_{iG}]; \\
 &\text{d) } B_i = \begin{bmatrix} 0 & B_i^{21} & \dots & B_i^{G1} \\ B_i^{12} & 0 & B_i^{32} & \dots & B_i^{G2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ B_i^{1G} & \dots & \dots & \dots & 0 \end{bmatrix}; \\
 &\text{e) } F_i = \begin{bmatrix} F_i^{11} & F_i^{21} & \dots & F_i^{G1} \\ F_i^{12} & F_i^{22} & \dots & \vdots \\ \vdots & \vdots & \ddots & \vdots \\ F_i^{1G} & \dots & \dots & F_i^{GG} \end{bmatrix}
 \end{aligned} \right\} \quad (169)$$

Since e_{ijg} contains the term $V_{ij}(\sigma_R)_{ig'g}$, where

$$(\sigma_R)_{ijg} = (\sigma_c)_{i,g} + (\sigma_f)_{ijg} + \sum_{g' \neq g} \sigma_{ij}^{gg'} \geq \sum_{g' \neq g} \sigma_{ij}^{gg'},$$

we see that $J_i - B_i$ is diagonally dominant with negative off-diagonal elements. Thus $(J_i - B_i)^{-1}$ exists and is nonnegative.

We now define the last set of block matrices in terms of which the problem as well as the iteration methods can be formulated. Hence we define the following $I \times I$ block matrices:

$$\begin{aligned}
 \text{a) } M &= \left[\begin{array}{cccc} J_1 - B_1 & -A_1 & 0 & 0 \\ -C_2 & J_2 - B_2 & -A_2 & \\ & & & \\ & & & -A_{I-1} \\ 0 & -C_I & J_I - B_I & \end{array} \right]; \\
 \text{b) } F &= \text{diag}[F_1, F_2, \dots, F_I].
 \end{aligned} \tag{170}$$

If we set $\phi_{ig} = (\phi_{i1g}, \dots, \phi_{iJg})^T$, $\phi_i = (\phi_{i1}, \dots, \phi_{iG})^T$, and $\phi = (\phi_1, \phi_2, \dots, \phi_I)^T$, then the finite-difference equation (167) can be written in the form

$$M\phi = \frac{1}{k} F\phi. \tag{171}$$

Since each matrix $(J_i - B_i)^{-1} \geq 0$ and $A_i + C_i \leq J_i - B_i$, we know that M^{-1} exists and $M^{-1} \geq 0$. The matrix F is nonnegative. Hence, if we write $T = M^{-1}F$, we have Eq. 171 in the form

$$T\phi = k\phi, \tag{172}$$

where $T \geq 0$. The problem then is to find the largest real eigenvalue in modulus and the corresponding positive eigenvector of the matrix T . Using the method of power iterations³ to obtain the dominant eigenvalue and eigenvector, we would define the following sequence. Starting with an arbitrary nonnegative guess $\phi^{(n)}$ for the flux and a positive number $\lambda^{(n)}$, we form successively

$$\frac{1}{\lambda^{(n)}} T\phi^{(n)} = \phi^{(n+1)}; \quad \lambda^{(n+1)} = \lambda^{(n)} \frac{(\phi^{(n+1)}, \phi^{(n+1)})}{(\phi^{(n+1)}, \phi^{(n)})}, \tag{173}$$

where

$$(\phi^{(n+1)}, \phi^{(n)}) = \sum_{ijg} \phi_{ijg}^{(n+1)} \phi_{ijg}^{(n)}.$$

Because T has the form $M^{-1}F$, forming $\phi^{(n+1)}$ is equivalent to solving the equation

$$M\phi^{(n+1)} = \frac{1}{\lambda^{(n)}} F\phi^{(n)}. \tag{174}$$

This solution must be achieved by iteration since M is a large scale matrix. We recall from Eq. 170a that M is a block tridiagonal matrix with non-singular diagonal blocks. Thus the Gauss-Seidel³ method of iteration can be applied to achieve the solution of Eq. 174. If we define the matrix D by $D = \text{diag}[J_1 - B_1, \dots, J_I - B_I]$, and L and U to be, respectively, the lower and upper triangular matrices associated with M , i.e., $M = D - L - U$, then the Gauss-Seidel scheme applied to Eq. 174 yields

$$(D - L)X_{(n)}^{(m)} = UX_{(n)}^{(m-1)} + \frac{1}{\lambda^{(n)}} F\phi^{(n)}, \quad m = 1, 2, \dots, \quad (175)$$

where

$$X_{(n)}^{(0)} = \phi^{(n)}.$$

If we drop the power iteration index n , and write Eq. 175 channel by channel, we have

$$(J_i - B_i)X_i^{(m)} = C_i X_{i-1}^{(m)} + A_i X_{i+1}^{(m-1)} + \frac{1}{\lambda^{(n)}} F_i \phi_i^{(n)} \quad (176)$$

for $i = 1, 2, \dots, I$.

The matrices involved in Eq. 176 are of dimension $GJ \times GJ$ grouped into G blocks each of dimension J . If upscattering is present, Eq. 176 is solved by iterative means. If we set

$$f_{ig} = C_{ig} X_{i-1,g}^{(m)} + A_i X_{i+1,g}^{(m-1)} + \frac{1}{\lambda^{(n)}} \sum_{g'=1}^G F_i^{g'g} \phi_{ig'}^{(n)} \quad (177)$$

for $g = 1, 2, \dots, G$,

then Eq. 176 takes the form

$$\begin{bmatrix} J_{i1} & -B_i^{21} & \dots & -B_i^{G1} \\ -B_i^{12} & J_{i2} & \dots & -B_i^{G2} \\ \vdots & \vdots & \ddots & \vdots \\ -B_i^{1G} & \dots & \dots & J_{ig} \end{bmatrix} X_i^{(m)} = f_i. \quad (178)$$

This system, having nonsingular diagonal blocks J_{ig} for which $J_{ig}^{-1} > 0$ and negative off-diagonal elements, can be solved iteratively by means of a block

Gauss-Seidel procedure. If no upscattering is present, $B_i^{g'g} = 0$ for $g' > g$, the system is lower triangular, and no iteration is necessary. Thus if we denote the approximations to $X_{ig}^{(m)}$ by $Y_{ig}^{(\ell)}$, the iteration procedure is defined by

$$J_{ig} Y_{ig}^{(\ell)} = \sum_{g' < g} B_i^{g'g} Y_{ig'}^{(\ell)} + \sum_{g' > g} B_i^{g'g} Y_{ig'}^{(\ell-1)} + f_{ig} \quad (179)$$

for $g = 1, 2, \dots, G$ and $\ell = 1, 2, \dots$. Here, $Y_{ig}^{(0)} = \phi_{ig}^{(n)}$. The $J \times J$ matrices defined by Eq. 168c are tridiagonal matrices. For this reason, the system defined by Eq. 179 can be solved by a direct method to yield $Y_{ig}^{(\ell)}$. The method used is an adaptation of Gauss elimination to tridiagonal matrices known as Choleski's method.⁴ In the periodic case, the matrices J_{ig} are not tridiagonal since they have nonzero elements in the extreme upper and lower corners. This is a reflection of the fact that in the periodic case, there are at most two external boundaries rather than four. We have developed a direct method for this case based on Choleski's method. This procedure is described on pp. 118-122.

To display Choleski's method in a simple manner, we shall drop the subscripts i and g . Thus we have to solve the following system

$$\begin{bmatrix} e_1 & -b_1 & 0 \\ -d_2 & e_2 & -b_2 \\ 0 & -d_j & e_j \end{bmatrix} X = f. \quad (180)$$

The coefficient matrix J is factored $J = LU$ into lower and upper triangular factors. Letting $\omega = Ux$, we have to solve two systems: $L\omega = f$ and $\omega = Ux$. The matrix U that has the form

$$\begin{bmatrix} 1 & -\gamma_1 & 0 \\ & 1 & -\gamma_2 \\ 0 & & -\gamma_{J-1} \\ & & & 1 \end{bmatrix}$$

is created once and stored. Thus the $\{\gamma_j\}_1^J$ are stored rather than the sequence $\{e_j\}_{j=1}^J$. The matrix L is not created explicitly; instead the

sequence $\{\omega_j\}$ is created each time that the system is solved. The sequence $\{\gamma_j\}_{j=1}^J$ is generated in the following manner:

$$\gamma_1 = \frac{b_1}{e_1}, \quad \gamma_j = \frac{b_j}{e_j - d_j \gamma_{j-1}} \quad \text{for } j = 2, 3, \dots, J, \quad \text{using } b_J = 1. \quad (181)$$

If a black cell is present for some point j_0 , then $b_{j_0-1} = d_{j_0} = 0$ and $b_{j_0} = d_{j_0+1} = 0$. Thus Eq. 181 yields $\gamma_{j_0-1} = \gamma_{j_0} = 0$. The sequence $\{\omega_j\}$ is generated by

$$\omega_1 = \frac{f_1}{e_1}, \quad \omega_j = \frac{f_j + d_j \omega_{j-1}}{e_j - d_j \gamma_{j-1}}, \quad j = 2, \dots, J. \quad (182)$$

Since the sequence $\{\gamma_j\}$ is stored, rather than $\{e_j\}$, Eq. 182 can be written in the following form, provided $\gamma_j \neq 0$ for all j :

$$\omega_1 = \frac{\gamma_1 f_1}{b_1}, \quad \omega_j = \frac{\gamma_j}{b_j} [f_j + d_j \omega_{j-1}], \quad j = 2, 3, \dots, J. \quad (183)$$

As we have seen, black cells do give rise to $\gamma_{j_0-1} = \gamma_{j_0} = 0$. Thus we shall use Eq. 183 for those i such that $a_i \neq 0$, and if $a_i = 0$, we shall use Eq. 182. This means we shall have to store $\{e_i : a_i = 0\}$. Having made the forward sweeps, we make a backward sweep that generates the solution. This corresponds to solving the system $\omega = Ux$,

$$x_J = \omega_J, \quad x_j = \omega_j + \gamma_j x_{j+1}, \quad \text{for } j = J-1, \dots, 1. \quad (184)$$

Since $e_j > b_j + d_j$ (recall that $e_j = a_j + b_j + c_j + d_j + \sigma_R V$), we have $0 \leq \gamma_j < 1$ for all j . This condition is sufficient to ensure stability of the Choleski method with respect to local round-off error.

Returning now to system 179, iterations are continued until

$$\sum_{g=1}^G \sum_{j=1}^J \left| Y_{ijg}^{(\ell)} - Y_{ijg}^{(\ell-1)} \right| < \delta_n \sum_{g=1}^G \sum_{j=1}^J \left| Y_{ijg}^{(1)} - \phi_{ijg}^{(n)} \right| \quad (185)$$

is satisfied. At this point we set $X_{ijg}^{(m)} = Y_{ijg}^{(\ell)}$ and continue on to the next channel. Note that the number of iterations as determined by inequality Eq. 185 varies with the channel.

The inner (or channel) iterations are continued until

$$\sum_{i=1}^I \sum_{g=1}^G \sum_{j=1}^J \left| X_{ijg}^{(m)} - X_{ijg}^{(m-1)} \right| < \epsilon_{\phi}, \quad (186)$$

or $m \geq m_{\max}$. At this point $\phi^{(n+1)}$ is defined by $\phi_{ijg}^{(n+1)} = X_{ijg}^{(m)}$ and the following quantities are calculated:

$$\left. \begin{aligned} \text{a) } \lambda^{(n+1)} &= \lambda^{(n)} \frac{(\phi^{(n+1)}, \phi^{(n+1)})}{(\phi^{(n+1)}, \phi^{(n)})}, \\ \text{b) } \bar{\lambda}^{(n+1)} &= \text{MAX}_{ijg} \frac{\phi_{ijg}^{(n+1)}}{\phi_{ijg}^{(n)}}, \quad \underline{\lambda}^{(n+1)} = \text{MIN}_{ijg} \frac{\phi_{ijg}^{(n+1)}}{\phi_{ijg}^{(n)}}, \end{aligned} \right\} \quad (187)$$

where only those $\phi_{ijg}^{(n)}$ for which $\phi_{ijg}^{(n)} \geq \epsilon_{\phi_{\min}}$ are used in the formation of $\bar{\lambda}$ and $\underline{\lambda}$.

The problem is considered to be converged where the following inequalities are satisfied.

$$\left. \begin{aligned} \text{a) } \sum_{i=1}^I \sum_{g=1}^G \sum_{j=1}^J \left| \phi_{ijg}^{(n+1)} - \phi_{ijg}^{(n)} \right| &< \epsilon_{\phi_0} \\ \text{b) } \frac{\bar{\lambda}^{(n+1)} - \underline{\lambda}^{(n+1)}}{2\lambda^{(n+1)}} &< \epsilon_{\lambda} \\ \text{c) } \left| \lambda^{(n+1)} - \lambda^{(n)} \right| &< \epsilon_k. \end{aligned} \right\} \quad (188)$$

It is of interest to note what the actual power iteration procedure is when inner iterations are taken into account. The effect of up-scattering iterations adds another degree of complexity, which for simplicity we shall omit. In addition, we shall assume that a fixed number m of inner iterations are performed for each outer iteration. Then, assuming we have found $\phi^{(n)}$ and $\lambda^{(n)}$, the flux $\phi^{(n+1)}$ is found from Eq. 175 which may be written in the form

$$X^{(m)} = R X^{(m-1)} + \frac{1}{\lambda^{(n)}} (D - L)^{-1} F \phi^{(n)} \quad (189)$$

where

$$R = (D - L)^{-1} U \text{ and } X^{(0)} = \phi^{(n)}.$$

Thus

$$\begin{aligned} \phi^{(n+1)} &= X^{(m)} = (1 - R^m)(1 - R)^{-1} \frac{1}{\lambda^{(n)}} (D - L)^{-1} F \phi^{(n)} + R^m \phi^{(n)} \\ &= (1 - R^m) \frac{T}{\lambda^{(n)}} \phi^{(n)} + R^m \phi^{(n)}, \end{aligned}$$

where

$$T = M^{-1}F = (D - L - U)^{-1} F = (1 - R)^{-1} (D - L)^{-1} F.$$

Thus if we define S_n by

$$S_n = \frac{T}{\lambda^{(n)}} + R^m \left(1 - \frac{T}{\lambda^{(n)}} \right), \quad (191)$$

the actual iteration procedure is defined by

$$\phi^{(n+1)} = S_n \phi^{(n)} = \prod_{k=0}^n S_k \phi^{(0)}; \quad \lambda^{(n+1)} = \lambda^{(n)} \frac{\left(\phi^{(n+1)}, \phi^{(n+1)} \right)}{\left(\phi^{(n+1)}, \phi^{(n)} \right)} \quad (192)$$

This is a nonstationary, nonhomogeneous iteration procedure, which, for m sufficiently large, approximates the stationary, homogeneous procedure described by Eq. 173. There are significant differences in the behavior of the iterates $\phi^{(n)}$ and $\lambda^{(n)}$ for various fixed values of m . For example, if $m = 1$, $\phi^{(n)}$ and $\lambda^{(n)}$ converge at about the same rate; whereas, as m increases, $\lambda^{(n)}$ tends to converge more rapidly than $\phi^{(n)}$. This observation has important consequences in the iteration strategy and acceleration technique employed in this module.

(4) Adjoint Calculation. The differential operator associated with the partial differential system 155 and 156, when viewed in the space L^2 over the reactor, has an adjoint operator in this space. Since the boundary conditions are homogeneous, the domain of the adjoint operator coincides with that of the real operator. Hence functions in the domain of the adjoint satisfy the same boundary conditions as the functions that lie in the domain of the real operator. Thus in this case the adjoint coincides with the formal adjoint. Finally, then, the finite-difference approximation to the adjoint operator can be found by taking the transpose of the matrices that result from the finite-difference approximation to the real operator.

The transposed system corresponding to the real system 171 has one disagreeable aspect. Because of the preponderance of problems involving only downscattering the scattering matrices tend to be lower triangular. The algorithms and indexing schemes are designed to take advantage of this. The adjoint system, on the other hand, then tends to be upper triangular. To avoid this, the transposed system is reordered for the calculation. The reordering is with respect to the energy groups that are now ordered from the highest group to the lowest. With this reordering, the adjoint scattering matrices tend to be lower triangular, and the algorithms designed for the real calculation can be used efficiently.

(5) Acceleration Techniques. We have seen in Section 3 that a k calculation involves two and possibly three, levels of iteration: the power (outer) iteration, the channel (inner) iterations, and for upscattering, the scattering iterations. The scattering iterations are not accelerated for several reasons. First, they occur very infrequently. Second, the number of iterations required is typically of order of 3 or 4 at the beginning of the problem and range down to 2 at the end of the problem. With such a small number of iterations, acceleration techniques are ineffective. However, since these iterations occur at the lowest level, they add significantly to the time required to complete a problem. To reduce this time, we take advantage of the fact that when upscattering occurs, it is among the lowest energy groups. Thus if there is no scattering higher than group g' , the iteration is performed over the groups g for which $G \leq g \leq g'$. This cuts down on data handling; thereby reducing the time.

The outer or power iterations are extrapolated using three-term Chebyshev extrapolation.³ The inner or channel iterations are also accelerated by means of three-term Chebyshev extrapolations. In addition, the equations are periodically rebalanced with respect to energy groups and regions.

(6) A Method for the Direct Solutions of Certain Linear Systems. Linear systems of the form $Ax = f$, when A is a tridiagonal matrix, arise in many fields, both pure and applied. For example, the finite-difference approach to linear second-order differential equations leads to matrices of the above form. A popular method used in solving such systems is based on an adaptation of Gauss elimination to tridiagonal matrices. This factorization method is sometimes referred to as line inversion, or Choleski's method (Ralston and Wilf, Fox, Henrici). The factorization method has also been applied directly to second-order differential equations in connection with two-point boundary-value problems; here the method is known as the method of sweeps (Gelfand). An excellent account of this method and its applications can be found in a discussion by J. M. Cook in Computational Methods in Reactor Physics.

If we seek approximations to periodic solutions of second-order differential equations by means of finite differences, the tridiagonal

character of the matrix A is altered by the inclusion of two nonzero elements, one at each of the extreme corners of the matrix. We will show how the method of line inversion can be used in the solution of this linear system.

Let the following system be given:

$$\hat{A}\hat{x} = f, \quad (193)$$

where

$$\hat{A} = \begin{bmatrix} e_1 & -c_1 & & -c \\ -a_2 & e_2 & -c_2 & \\ & & & -c_{p-1} \\ -a & -a_p & & e_p \end{bmatrix}, \quad (194)$$

where $e_j > a_j + c_j$, and a_j, c_j are positive. Let A denote the matrix that results when $a = c = 0$. The method of line inversion applied to the system $Ax = f$ yields the pair of systems $L\omega = f$ and $Ux = \omega$, where the last system has the form

$$\begin{bmatrix} 1 & -\gamma_1 & & \\ 0 & 1 & -\gamma_2 & 0 \\ & 0 & & -\gamma_{p-1} \\ & & & 1 \end{bmatrix} x = \omega.$$

The forward sweep gives the sequences $\{\gamma_j\}$ and $\{\omega_j\}$, and the backward sweep yields the solution $\{x_j\}$.

$$\gamma_1 = c_1/e_1, \quad \omega_1 = f_1/e_1,$$

$$\gamma_j = \frac{c_j}{e_j - a_j \gamma_{j-1}}, \quad j = 2, 3, \dots, p \text{ with } c_p = 1,$$

and

$$\omega_j = \frac{\gamma_j}{c_j} (f_j + a_j \omega_{j-1}) \quad \text{for } j = 2, 3, \dots, p.$$

(195)

Then

$$x_p = \omega_p,$$

and

$$x_j = \omega_j + \gamma_j x_{j+1} \quad \text{for } j = p-1, \dots, 1.$$

We would like to have a method similar to Eq. 195 in the periodic case, especially when we must solve the system repeatedly, each time varying only the inhomogeneous terms.

The basic idea of the method is to perform a forward sweep on the original system, then a forward sweep on a system obtained by reversing the order of the equations. This leads to a pair of equations determining x_1 and x_p . We then perform a backward sweep to determine $x_{p-1}, \dots, x_2$.

A forward sweep on the system

$$\begin{bmatrix} e_p & -a_p & & 0 \\ -c_{p-1} & e_{p-1} & -a_{p-1} & \\ & & & -a_2 \\ & 0 & -c_1 & e_1 \end{bmatrix} \begin{bmatrix} x_p \\ x_{p-1} \\ \vdots \\ x_2 \\ x_1 \end{bmatrix} = \begin{bmatrix} f_p \\ f_{p-1} \\ \vdots \\ f_2 \\ f_1 \end{bmatrix} \quad (196)$$

would lead to the generation of $\{\bar{\gamma}_j\}$ and $\{\bar{\omega}_j\}$ given by

$$\left. \begin{aligned} \bar{\gamma}_1 &= a_p/e_p, \quad \bar{\omega}_1 = f_p/e_p, \\ \bar{\gamma}_j &= \frac{a_{p-j+1}}{e_{p-j+1} - c_{p-j+1}\bar{\gamma}_{j-1}}, \quad j = 2, 3, \dots, p, \quad \text{where } a_1 = 1, \\ \bar{\omega}_j &= \frac{\bar{\gamma}_j}{a_{p-j+1}} (f_{p-j+1} + c_{p-j+1}\bar{\omega}_{j-1}) \quad \text{for } j = 2, 3, \dots, p. \end{aligned} \right\} (197)$$

and

$$\bar{\omega}_j = \frac{\bar{\gamma}_j}{a_{p-j+1}} (f_{p-j+1} + c_{p-j+1}\bar{\omega}_{j-1}) \quad \text{for } j = 2, 3, \dots, p.$$

Let the periodic system be written in the form

$$\begin{bmatrix} e_1 & -c_1 & & 0 \\ -a_2 & e_2 & -c_2 & \\ 0 & & & \\ & & -a_p & e_p \end{bmatrix} \begin{bmatrix} \hat{x}_1 \\ \hat{x}_2 \\ \vdots \\ \hat{x}_{p-1} \\ \hat{x}_p \end{bmatrix} = \begin{bmatrix} f_1 + c\hat{x}_p \\ f_2 \\ \vdots \\ f_{p-1} \\ f_p + a\hat{x}_1 \end{bmatrix} \quad (198)$$

Let $\{\gamma_j\}$ and $\{\omega_j\}$ denote the result of a forward sweep on the system obtained from Eq. 198 by setting $a = c = 0$. Then if $\{\hat{\gamma}_j\}$ and $\{\hat{\omega}_j\}$ are the result of a forward sweep on system 198, we have the following relations:

$$\left. \begin{aligned} \hat{\omega}_1 &= \omega_1 + \frac{c}{e_1} \hat{x}_p, \\ \hat{\omega}_j &= \omega_j + c g_j \hat{x}_p, \quad \text{for } j = 2, 3, \dots, p-1, \\ \hat{\omega}_p &= \omega_p + a \gamma_p \hat{x}_1 + c g_p \hat{x}_p, \end{aligned} \right\} \quad (199)$$

where $g_j = (\gamma_j a_j / c_j) g_{j-1}$ for $j = 2, 3, \dots, p$, $g_1 = 1/e_1$, and $c_p = 1$. Furthermore, $\hat{\gamma}_j \equiv \gamma_j$.

By performing a forward sweep on the systems obtained from Eq. 198 by reversing the order, we will generate sequences

$$\left. \begin{aligned} \{\hat{\bar{\gamma}}_j\} \text{ and } \{\hat{\bar{\omega}}_j\} \text{ where } \hat{\bar{\gamma}}_j &\equiv \bar{\gamma}_j \text{ and } \hat{\bar{\omega}}_1 = \bar{\omega}_1 + \frac{a}{e_p} \hat{x}_1 \\ \hat{\bar{\omega}} &= \bar{\omega}_j + \bar{g}_j a \hat{x}_1 \quad \text{for } j = 2, 3, \dots, p-1 \\ \hat{\bar{\omega}}_p &= \bar{\omega}_p \bar{\gamma}_p c \hat{x}_p + \bar{g}_p a \hat{x}_1. \end{aligned} \right\} \quad (200)$$

Here $\bar{g}_j = (\bar{\gamma}_j / a_{p-j+1})$, $c_{p-j+1} \bar{g}_{j-1}$ for $j = 2, \dots, p$ with $\bar{g}_1 = 1/e_p$ and $a_1 = 1$.

Now starting the backward sweep with systems 198, we have $\hat{x}_p = \hat{\omega}_p$; moreover, starting the backward sweep with the reversed systems, we have $\hat{x}_1 = \hat{\bar{\omega}}_p$. Thus,

$$\left. \begin{aligned} (1 - c g_p) \hat{x}_p - a \gamma_p \hat{x}_1 &= \omega_p; \\ -c \bar{\gamma}_p \hat{x}_p + (1 - a \bar{g}_p) \hat{x}_1 &= \bar{\omega}_p. \end{aligned} \right\} \quad (201)$$

With the solution of Eq. 201, we are in a position to perform the backward sweep:

$$\hat{x}_p = \hat{x}_p,$$

$$\hat{x}_u = \hat{\omega}_j + \gamma_j \hat{x}_{j+1} = \omega_j + c g_j \hat{x}_p + \gamma_j \hat{x}_{j+1},$$

for $j = p - 1, p - 2, \dots, 1$.

c. References

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d. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
A.DIF2D	Module-dependent data. Includes iteration limits, convergence criteria, etc.
SP.CICN	Module-independent data.
GEOM	General descriptive data on mesh structure. Region-to-mesh correspondence. Composition-to-mesh correspondence. Buckling.
BC	Definitions of external and internal boundary conditions.
XS.C.MIN	Composition cross sections Σ_{tr} , Σ_R , Σ_S , $\nu\Sigma_f$, χ .
FR.D2 (or FA.D2)	Eigenvalue (k_{eff}). Two-dimensional real (or adjoint) flux guess.

Upper-interface Data ModulesQuantities Used

ES.D2D

Two-dimensional distributed external source, if doing an external source calculation.

XS.DELAY

Delayed data (if doing a kinetics option). Delayed-neutron spectrum. Decay constants, and delayed-neutron distributions.

XS.C.AUX

Prompt $\nu\Sigma_f$, delayed χ (if doing a kinetics option).

Lower-interface Data ModuleQuantities Produced

FR.D2 (or FA.D2)

Eigenvalue (k_{eff}). Two-dimensional real (or adjoint) flux vector.

19. 2D-Transport NUC005

Prepared by: G. J. Duffy

a. Nature of Physical Problem Solved

This module solves the S_N difference equations for the two-dimensional transport problem for many groups, allowing up to linear anisotropic scattering. Geometries include xy, rz, and r θ . A fixed isotropic source is allowed in the solution of an inhomogeneous system. A homogeneous system can be solved to obtain a value of k_{eff} or to obtain the correct concentration, geometry, or α to achieve criticality. Density factors may be used to modify cross sections by interval. A real or adjoint system can be solved. Left, right, bottom, and top boundaries can be free, reflective, or periodic. Right and top boundaries can be white for curved geometries. Fission sources and/or fluxes may be used to start the calculation. A fixed value of k_{eff} or α is allowed.

b. Method of Solution

Here we briefly summarize the mathematical basis of the SNARG-2D program.

If $\vec{x}$ is a positive vector, $\vec{\Omega}$ a point on the unit direction sphere associated with the point $\vec{x}$, and v_j is the neutron speed in energy group j , then the equation for the angular flux in group j , $\bar{\phi}_j(t, \vec{x}, \vec{\Omega})$ is

$$\frac{1}{v_j} \frac{\partial \bar{\phi}_j}{\partial t} + \vec{\Omega} \cdot \vec{\nabla} \bar{\phi}_j + \sigma_j(\vec{x}) \bar{\phi}_j = \bar{S}_j(t, \vec{x}, \vec{\Omega}), \quad (202)$$

where $\sigma_j(\vec{x})$ is the total cross section and $\bar{S}_j$ the source for group j .

Before proceeding with the finite-difference form of Eq. 202, we consider the time dependence. Assume that the angular flux and the source are separable in the same way into the product of a time-independent function of position and direction and a time-dependent function $e^{\alpha t}$. Equation 202 becomes

$$\vec{\Omega} \cdot \vec{\nabla} \phi_j + \left(\sigma_j(\vec{x}) + \frac{\alpha}{v_j} \right) \phi_j = S_j(\vec{x}, \vec{\Omega}), \quad (203)$$

where

$$\phi_j = \bar{\phi}_j(\vec{x}, \vec{\Omega}).$$

Equation 203 represents the time-independent transport equation.

The angular variable in Eq. 202 is discretized into $\{\vec{\Omega}_m\}$ and integration is performed by using weights, W_m and direction cosines, μ_m and η_m , which satisfy the relations

$$\sum_{m=1}^M W_m = 1, \quad (204)$$

$$\sum_{m=1}^M W_m \mu_m \eta_m = 0, \quad (205)$$

and

$$\sum_{m=1}^M W_m \mu_m^2 = \sum_{m=1}^M W_m \eta_m^2 = \frac{1}{3}, \quad (206)$$

where M is the total number of directions on the octant of the unit sphere.

A neutron balance equation, which is written for an arbitrary cell enclosing the point $(\vec{x}, \vec{\Omega})$, becomes Eq. 203 as the cell size shrinks.

Let i and h be the indices specifying the mesh structure along the x and y axes, and m the direction index, x and y standing for the space coordinates in xy , rz and $r\theta$ geometries. The cell-face area perpendicular to x at i is denoted by A_i . The cell-face area perpendicular to y at l (index for interval along x axis between x_i and x_{i+1}) is denoted by B_l .

The balance equation for any of these geometries for group j is then

$$\begin{aligned} & \frac{\mu_m}{V_\ell} \left(A_{i+1} \phi_{m,i+1,q,j} - A_i \phi_{m,i,q,j} \right) + \frac{\eta_m}{V_\ell} \left(B_l \phi_{m,l,h+1,j} - B_l \phi_{m,l,h,j} \right) \\ & + \frac{1}{V_\ell W_m} \left(\alpha_{m+\frac{1}{2},l,q,j} \phi_{m+\frac{1}{2},l,q,j} - \alpha_{m-\frac{1}{2},l,q,j} \phi_{m-\frac{1}{2},l,q,j} \right) \\ & + \sigma_{l,q,j} \phi_{m,l,q,j} = S_{m,l,q,j}, \end{aligned} \quad (207)$$

where q is the index for the interval along the y axis between y_h and y_{h+1} . Then,

$$\phi_{m,l,q,j} = \frac{1}{2} \left(\phi_{m,i+1,q,j} + \phi_{m,i,q,j} \right) = \frac{1}{2} \left(\phi_{m,l,h+1,j} + \phi_{m,l,h,j} \right). \quad (208)$$

The first two terms in Eq. 207 represent the flow through the geometric faces of the cell; the third term represents flow across the direction intervals; V_ℓ is the geometric volume of the cell.

The α 's satisfy the relations

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = -W_m \mu_m. \quad (209)$$

Define the curvature as

$$\bar{\mu}_m = \frac{2\alpha_{m+\frac{1}{2}}}{W_m} + \mu_m. \quad (210)$$

Use Eq. 209 to eliminate the α 's and obtain

$$\bar{\mu}_m = \frac{W_{m-1} \bar{\mu}_{m-1} - (W_m \mu_m + W_{m-1} \mu_{m-1})}{W_m}, \quad \text{if } W_m \neq 0, \quad (211)$$

where $\bar{\mu}_m = 0$ for $W_m = 0$.

Equation 207 is put in recursive form. Define

$$\begin{aligned} \text{DENOM} = & (\Delta y_q) |\bar{\mu}_m (A_{i+1} - A_i)| + 2|\eta_m| B_\ell + (\Delta y_q) \bar{\mu}_m (A_{i+1} - A_i) \\ & + V_{\ell, q} \sigma_{t, \ell, q, j}. \end{aligned}$$

for $\eta_m < 0, \mu_m < 0$,

$$\begin{aligned} \phi_{m-\frac{1}{2}, \ell, q, j} = & \frac{V_{\ell, q} S_{m, \ell, q, j} + (\Delta y_q) \bar{\mu}_m (A_{i+1} - A_i) \phi_{m-1, \ell, q, j}}{\text{DENOM}} \\ & + \frac{(\Delta y_q) |\mu_m (A_{i+1} + A_i)| \phi_{m, i+1, q, j} + 2|\eta_m| B_\ell \phi_{m, \ell, h+1, j}}{\text{DENOM}}, \end{aligned} \quad (212)$$

For $\eta_m > 0, \mu_m < 0$,

$$\begin{aligned} \phi_{m-\frac{1}{2}, \ell, q} = & \frac{V_{\ell, q} S_{m, \ell, q, j} + (\Delta y_q) \bar{\mu}_m (A_{i+1} - A_i) \phi_{m-1, \ell, q, j}}{\text{DENOM}} \\ & + \frac{(\Delta y_q) |\mu_m (A_{i+1} + A_i)| \phi_{m, i+1, q, j} + 2|\eta_m| B_\ell \phi_{m, \ell, h, j}}{\text{DENOM}}. \end{aligned} \quad (213)$$

For $\eta_m < 0$, $\mu_m > 0$,

$$\phi_{m-\frac{1}{2}, l, q} = \frac{V_{l, q} S_{m, l, q, j} + (\Delta y_q) \bar{\mu}_m (A_{i+1} - A_i) \phi_{m-1, l, q, j}}{\text{DENOM}} + \frac{(\Delta y_q) \left| \mu_m (A_{i+1} + A_i) \right| \phi_{m, i, q, j} + 2 \left| \eta_m \right| B_l \phi_{m, l, h+1, j}}{\text{DENOM}}, \quad (214)$$

for $\eta_m > 0$, $\mu_m > 0$,

$$\phi_{m-\frac{1}{2}, l, q} = \frac{V_{l, q} S_{m, l, q, j} + (\Delta y_q) \bar{\mu}_m (A_{i+1} - A_i) \phi_{m-1, l, q, j}}{\text{DENOM}} + \frac{(\Delta y_q) \left| \mu_m (A_{i+1} + A_i) \right| \phi_{m, i, q, j} + 2 \left| \eta_m \right| B_l \phi_{m, l, h, j}}{\text{DENOM}}. \quad (215)$$

where

$$\left. \begin{aligned} \text{a) } \phi_{m, l, q, j} &= \phi_{m, i+\frac{1}{2}, h+\frac{1}{2}, j} \\ \text{b) } S_{m, l, q, j} &= S_{m, i+\frac{1}{2}, h+\frac{1}{2}, j} \\ \text{c) } \phi_{m, l, q, j} &= \frac{1}{2} (\phi_{m+\frac{1}{2}, i+\frac{1}{2}, h+\frac{1}{2}, j} + \phi_{m-\frac{1}{2}, i+\frac{1}{2}, h+\frac{1}{2}, j}) \\ \text{d) } \phi_{m, l, q, j} &= 2\phi_{m-\frac{1}{2}, l, q, j} - \phi_{m-1, l, q, j} \quad \text{for } W_m \neq 0. \end{aligned} \right\} \quad (216)$$

and

The source term is defined as (for outer iteration ρ , inner iteration π)

$$V_{l, q} S_{m, l, q, j} = \mu_m SH_{l, q, j} + \eta_m SV_{l, q, j} + S_{l, q, j}, \quad (217)$$

where

$$SH_{l, q, j} = 3 \sum_{\substack{k \\ k \neq j}} V_{l, q} \sigma_{l, q}^{(1)}(k \rightarrow j) J_{l, q, j}^{H, \rho} + 3 V_{l, q} J_{l, q, j}^{H, \pi} \sigma_{l, q}^{(1)}(j \rightarrow j), \quad (218)$$

$$SV_{l, q, j} = 3 \sum_{\substack{k \\ k \neq j}} V_{l, q} \sigma_{l, q}^{(1)}(k \rightarrow j) J_{l, q, j}^{V, \rho} + 3 V_{l, q} J_{l, q, j}^{V, \pi} \sigma_{l, q}^{(1)}(j \rightarrow j), \quad (219)$$

$$S_{l,q,j} = \sum_{k \neq j} V_{l,q} \sigma_{l,q}^{(0)}(k \rightarrow j) \phi_{l,q,j}^{\rho} + V_{l,q} \phi_{l,q,j}^{\pi} \sigma_{l,q}^{(0)}(j \rightarrow j) + FI_{l,q,j} + V_{l,q} Q_{l,q,j}, \quad (220)$$

$$\left. \begin{aligned} \text{a) } J_{l,q,j}^{H,\pi} &= \sum_m W_m \mu_m \phi_{m,l,q,j}^{\pi} \\ \text{b) } J_{l,q,j}^{V,\pi} &= \sum_m W_m \eta_m \phi_{m,l,q,j}^{\pi} \end{aligned} \right\} \quad (221)$$

and

$\phi_{m,l,q,j}^{\pi}$ is the flux for direction m , interval (l,q) and group j in inner iteration π ,

$\phi_{l,q,j}^{\rho}$ is the scalar flux for interval (l,q) for group j in outer iteration ρ defined by

$$\phi_{l,j}^{\pi} = \sum_m W_m \phi_{m,l,j}^{\pi} \quad (222)$$

$$\sigma_{l,q}^{(0)}(k \rightarrow j)$$

and

$$\sigma_{l,q}^{(1)}(k \rightarrow j)$$

are the isotropic and anisotropic components of scattering.

The fission source $FI_{l,q,j}$ is defined as

$$FI_{l,q,j} = \begin{cases} V_{l,q} \sum_k \chi_{l,q}(k,j) (\nu \sigma_f)_{l,q,k} \phi_{l,k} & \text{for the real case;} \\ V_{l,q} (\nu \sigma_f)_{l,q,j} \sum_k \chi_l(j,k) \phi_{l,k} & \text{for the adjoint case.} \end{cases} \quad (223)$$

$$Q_{l,q,j} = Q_{l,q,j}^* \cdot NF/\overline{QG}, \quad (224)$$

where NF is the normalization factor (input), $Q_{\ell,q,j}^*$ is the input distributed source, and

$$\overline{QG} = \sum_j \sum_{\ell} \sum_q v_{\ell,q} Q_{\ell,q,j}^*$$

The value of k_{eff} is determined as

$$k_{\text{eff}}^{\rho} = \lambda_{\rho} \cdot k_{\text{eff}}^{\rho-1},$$

where ρ is the outer iteration count, and

$$\lambda_{\rho} = \frac{FG^{\rho}}{N},$$

where N is the input normalization factor, and

$$FG^{\rho} = \sum_j \sum_{\ell} \sum_q FI_{\ell,q,j}^{\rho}$$

In criticality searches, the search parameter, EV_p , is determined from previous values of EV and λ by linear or quadratic interpolation. The current value EV_p is then used to determine new elements in the various type searches in the following ways:

(1) Radius Search

$$x_{i+1}^{\rho} = x_i^{\rho} + (1 + EV_p \cdot RZ_i) \Delta x_{\ell}$$

$$y_{h+1}^{\rho} = y_h^{\rho} + (1 + EV_p \cdot RZ_h) \Delta y_q$$

where

$$\left. \begin{aligned} \Delta x_{\ell} &= x_{i+1}^0 - x_i^0 \\ \Delta y_q &= y_{h+1}^0 - y_h^0 \end{aligned} \right\}, \quad \text{and } RZ_i$$

are input radius modifiers, constant within each region.

(2) Inverse Reactor Period α . The element t_j is computed and added to the total cross section for each group j for each outer iteration.

$$t_j = \begin{cases} (EV_p + \alpha_0)/v_j & \text{for } \alpha \text{ calculation with fixed } \alpha_0, \\ EV_p/v_j & \text{for } \alpha \text{ calculation,} \\ \alpha_0/v_j & \text{for fixed } \alpha_0 \text{ for any problem type.} \end{cases}$$

(3) Concentration Search. The input module prepares a pseudocomposition cross section, $\sigma_{x,j}^c$, for each composition c to be modified. The input module provides "volume fraction modifiers" that are used as coefficients in forming the linear combination of isotopes or materials used to generate c' , the pseudocomposition for each group j and reaction type x .

For each value of EV_p , the new composition cross sections are computed as

$$\sigma_{x,j}^{c,p} = \sigma_{x,j}^{c,p-1} + (EV_p - EV_{p-1}) \cdot \sigma_{x,j}^{c'}$$

c. References

G. J. Duffy et al., ANL-CDC Reprogramming Series V, SNARG-2D, ANL, AMD Technical Memorandum No. 96 (1967).

d. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
BC	Left, right, bottom, and top boundary conditions.
FR.D2	Fluxes by interval and group.
FSA.D2	Adjoint fission source by interval and group.
FSR.D2	Real fission source by interval and group.
GEOM	Composition-region correspondence. Number of regions in reactor. Mesh points. Region-mesh correspondence parameters.
SP.NEUT2	Direction cosines, direction mates, and weights for integration and combinations of these. Density factors by interval.

Upper-interface Data Modules

SP.NEUT2 (Contd.)

FR.RB

FR.TB

SP.CRIT

OUT.TR2

SP.CICN

XS.C.MIN

XS.VEL

XS.C.ANI

ES.D2D

ES.D2SH

FA.D2

Lower-interface Data Modules

FR.D2

FR.D2A

Quantities Used

Convergence criterion constant. Source normalization factor. Maximum number of inner and outer iterations. Calculation type and input guess (flux or source). S_N order.

Angular fluxes for right boundary by group.

Angular fluxes for top boundary by group.

Criticality search parameters.

Convergence and error data.

Module-independent data.

Number of compositions, groups, and fissionable compositions. Order of anisotropy for each composition. Compositions that are fissionable. Number of groups of upscattering and downscattering in each composition. Total cross section. Total isotropic component of scattering, $\Sigma_{\ell,j \rightarrow K}$, for composition ℓ . Fission-composition cross sections, Σ_f , ν , χ .

Average velocity for each group.

Anisotropic scattering cross section for composition ℓ , $\Sigma_{\ell,j \rightarrow K}^{(L)}$.

External distributed source by group and interval.

Anisotropic and isotropic component of shell source by group.

Adjoint fluxes by interval and group.

Quantities Produced

Fluxes by interval and group.

Angular fluxes by interval and group.

Lower-interface Data ModulesQuantities Produced

FA.D2	Adjoint fluxes by interval and group.
FA.D2A	Adjoint angular fluxes by interval and group.
FSR.D2	Real fission source by interval and group.
FSA.D2	Adjoint fission source by interval and group.
OUT.TR	Convergence and error statistics. Current eigenvalue or k_{eff} value. Current fission ratio. Loop counts.
XS.C.MIN	Fission fractions for compositions. New cross sections if compositions are modified.
GEOM	New radii if radii are modified.
XS.C.ANI	New cross sections if compositions are modified.
FR.RB	Angular fluxes for right boundary by group.
FR.TB	Angular fluxes for top boundary by group.
JR.D2	Real current by interval and group.
JA.D2	Adjoint current by interval and group.

20. Transport-mesh Refinement NUC007

Prepared by: G. J. Duffy

a. Nature of Problem Solved

This module creates extra mesh intervals as specified, and interpolates and/or extrapolates to find new values of 1D and 2D transport-theory fluxes and fission sources corresponding to the new intervals. The module updates all tables that are functions of the mesh interval space.

b. Method of Solution

Linear and quadratic interpolation and extrapolation is used.

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>		<u>Quantities Used</u>
MR.TN		Specified changes in the mesh structure in table form. Number of dimensions. Type and order of interpolation to be performed on fluxes.
GEOM		Previously defined mesh structure and other interval-dependent tables.
FR.D1	Any one of these.	Real or adjoint fluxes.
FR.D2		
FA.D1		
FA.D2		
FSR.D1	One of these.	Real or adjoint fission sources.
FSR.D2		
FSA.D1		
FSA.D2		
<u>Lower-interface Data Modules</u>		<u>Quantities Produced</u>
GEOM		New mesh structure and tables that are a function thereof.
FR.D1	Any of these.	New fluxes.
FR.D2		
FA.D1		
FA.D2		
FSR.D1	One of these.	New fission sources.
FSR.D2		
FSA.D1		
FSA.D2		

21. Criticality Search NUC008

Prepared by: G. K. Leaf and A. S. Kennedy

a. Nature of Physical Problem

This module adjusts certain parameters to achieve a desired value of k_{eff} . These parameters include material volume fractions, region size, buckling, and alpha.

b. Method of Solution

A general expression describing the search procedure is

$$P_N(X) = P_N(0) + X \cdot \delta P_N, \quad (225)$$

where

P_N are the parameters being varied,

and

δP_N are the parameter modifiers.

For a concentration search,

$$P_N = \text{volume fractions} = VF_m,$$

and

N is the index of material (m).

For a dimension search (one or two dimensions),

$$P_N = \text{mesh increments} = \Delta R_i \text{ (and/or } \Delta Z_j),$$

and

N is the index of mesh interval (i and/or j).

For a buckling search,

$$P_N = B_{r,g}^2,$$

and

N is the index of region (r) and group (g).

For an alpha search,

$$P = \alpha.$$

k_{eff} is considered a function of the single parameter X ; i.e., $K = K(X)$. Thus, given two initial values $X^{(1)}$ and $X^{(2)}$, or one initial value $X^{(1)}$ and a slope dK/dX , the search proceeds as follows: The parameters corresponding to $X^{(1)}$ are calculated by Eq. 225. The appropriate neutronics module calculates $K^{(1)}$. Then $X^{(2)}$ and $K^{(2)}$ are produced in a similar manner. The pairs of points $(X^{(1)}, K^{(1)})$, $(X^{(2)}, K^{(2)})$ are considered to lie on the graph of k_{eff} versus X . Using the method of tangent lines, we find the value of $X^{(3)}$ by finding the intersection of the chord joining these two points with the line $K = K_0$ (K_0 the desired value of k_{eff}). The process continues until

$$|K^{(\ell)} - K_0| \leq \epsilon_{crit},$$

where ϵ_{crit} is a specified convergence criterion.

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
SP.CRIT	Search type. Maximum number of passes. Convergence criterion. Search bounds. Desired k_{eff} . Initial guess $X^{(1)}$. Initial guess $X^{(2)}$ or dK/dX . Search parameter modifiers δP_N .
SP.CICN	Initial value of alpha.
GEOM	Initial values of mesh increments, buckling.
B.HOMOG	Initial values of volume fractions.
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
SP.CRIT	Latest values of X .
SP.CICN	Modified value of alpha.
GEOM	Modified values of mesh increments, or buckling.
B.HOMOG	Modified values of volume fractions.

22. Neutronics Output Manipulation NUE001

Prepared by: J. L. Zeman

a. Nature of Physical Problem Solved

Given general neutronics specifications, fluxes--real and/or adjoint, angular for transport theory, boundary, geometry, and cross-section data, this module computes flux integrals and averages, power, fission density, fission sources, currents, neutron sources and removals, and leakages. All input and computed quantities are edited according to output calculation options requested in data module A.OUTMAN.

b. Method of Solution

The following output quantities are calculated:

(1) Normalized fluxes, if so desired; these will then replace the input fluxes and will be used henceforth.[†]

(a) Normalization to one fission per unit height:

$$\bar{\phi}_{i,g} = \frac{\phi_{i,g}}{\sum_{i,g} \Sigma_{fci,g} \phi_{i,g} dV_i}$$

(b) Power normalization:

$$\bar{\phi}_{i,g}^P = \bar{\phi}_{i,g} \cdot 3.1 \times 10^{10} P,$$

where P is the input power.

(2) Regional flux integrals for real and/or adjoint flux:

$$\Phi_{r,g} = \int_{\text{region}} dV_i \phi_{i,g}$$

(3) Regional averages for real and/or adjoint flux:

$$\bar{\Phi}_{r,g} = \frac{\Phi_{r,g}}{dV_r}$$

[†]Similarly for angular fluxes, used only in transport theory and represented by $\phi_{m,i,g}$.

(4) Power per interval:

$$P_i = \sum_{g=1}^G \Phi_{i,g} \Sigma_{f_{c_i,g}}.$$

(5) Power by regions:

$$P_r = \sum_{g=1}^G \Phi_{r,g} \Sigma_{f_{c_r,g}}.$$

(6) Average power by regions:

$$\overline{P}_r = \frac{P_r}{dV_r}.$$

(7) Total power:

$$P = \sum_r P_r.$$

(8) Fission density by interval and group:

$$FS_{i,g} = \sum_{h=1}^G \phi_{i,h} \chi_{c_i,h \rightarrow g} \nu \Sigma_{f_{c_i,g}}.$$

(9) Fission-source integral by region and group:

$$FS_{r,g} = \int_{\text{region } r} dV_i FS_{i,g}.$$

(10) Average fission source by regions and groups:

$$\overline{FS}_{r,g} = \frac{FS_{r,g}}{dV_r}.$$

(11) Total fission source by region:

$$FS_r = \sum_{g=1}^G FS_{r,g}.$$

(12) Total fission source:

$$FS = \sum_r FS_r.$$

(13) Currents at interfaces

(a) Internal interface

Diffusion theory:

$$J_{i,g} = \frac{-2D_{i,g}D_{i+1,g}}{D_{i,g}(\Delta x)_{i+1} + D_{i+1,g}(\Delta x)_i} (\phi_{i+1,g} - \phi_{i,g})$$

Transport theory:

$$J_{i,g} = \sum_m W_m \mu_m \phi_{m,i,g} (\mu_m < 0)$$

(b) Left boundary

Diffusion theory:

$$J_{1,g} = \frac{D_{1,g}(C_{1,g} - B_{1,g}\phi_{1,g})}{A_{1,g} + 0.5\Delta x_1 B_{1,g}},$$

where A, B, and C are diffusion-theory boundary-value constants defined in the diffusion-theory modules.

Transport theory:

$$J_{1,g} = \sum_m W_m \mu_m \phi_{m,1,g}$$

(c) Right boundary

Diffusion theory:

$$J_{imax,g} = \frac{-D_{imax,g}(C_{imax,g} - B_{imax,g}\phi_{imax,g})}{A_{imax,g} + 0.5\Delta x_{imax} B_{imax,g}}$$

Transport theory:

$$J_{imax,g} = \sum_m W_m \mu_m \phi_{m,imax,g}$$

(14) Neutron source into groups by regions, total, elastic, inelastic, (n,2n):

$$S_{r,g} = \int_{\text{region } r} dV_i \left[FS_{i,g} + \sum_{h=1}^G \left\{ \Sigma_{el(i,h \rightarrow g)} + \Sigma_{in(i,h \rightarrow g)} + 2\Sigma_{n,2n(h \rightarrow g,i)} \right\} \phi_{h,i} \right]$$

(15) Total source into groups:

$$S_g = \sum_r S_{r,g}$$

(16) Neutron removal from group by region, total, elastic, inelastic, (n,2n), capture:

$$R_{r,g} = \int_{\text{region } r} \left[\Sigma_{c,i,g} + \Sigma_{FISS,i,g} + \sum_{h \neq g}^G \left\{ \Sigma_{el(i,g \rightarrow h)} + \Sigma_{in(i,g \rightarrow h)} + \Sigma_{n,2n(i,g \rightarrow h)} \right\} \right] \phi_{i,g}$$

(17) Total removal from group:

$$R_g = \sum_r R_{r,g}$$

(18) Leakage from region by group:

$$L_{r,g} = \int_{\text{boundary of } r} d\vec{a} J_{i,g}$$

(19) Leakage from reactor by group:

$$TL_{\text{reactor boundary},g} = \int_{\text{reactor boundary}} d\vec{a} J_{i,g}$$

(20) Total leakage from reactor:

$$TL_{\text{reactor boundary}} = \sum_{g=1}^G TL_{\text{reactor boundary, g.}}$$

(21) Leakage from region by group calculated from neutron balance:

$$BL_{r, g} = S_{r, g} - R_{r, g}.$$

(22) Total leakage from reactor by group calculated from neutron balance:

$$BL_{\text{reactor boundary, g}} = S_{\text{reactor boundary, g}} - R_{\text{reactor boundary, g}}.$$

All the calculations mentioned above that are performed over regions will be performed over areas and/or zones, if so specified.

All variables having space-point index i will have a second index j , representing the second dimension, for two-dimensional calculations.

The delta areas ($d\vec{a}$) (which are per unit height in cylindrical, rz , and $r\theta$ geometries) and the delta volumes used in the calculations above are as follows:

<u>Dimensions</u>	<u>Geometry</u>	<u>Delta Area</u>	<u>Delta Volume</u>
1	Slab	1	$x_{i+1} - x_i$
1	Cylinder	$2\pi(r_{i+1} - r_i)$	$\pi(r_{i+1}^2 - r_i^2)$
1	Sphere	$4\pi(r_{i+1}^2 - r_i^2)$	$\frac{4\pi}{3}(r_{i+1}^3 - r_i^3)$
2	xy	1	$(x_{i+1} - x_i)(y_{j+1} - y_j)$
2	rz	$2\pi(r_{i+1} - r_i)$	$\pi(r_{i+1}^2 - r_i^2)(z_{j+1} - z_j)$
2	$r\theta$	$r_{i+1} - r_i$	$\frac{1}{2}(r_{i+1}^2 - r_i^2)(\theta_{j+1} - \theta_j)$

If the geometric representations listed above are finite in one or more directions, the above delta volumes are modified by factors ρ_i , which are formed as follows:

$$\text{Finite cylinder } \rho_i = \int_{-H_{Li}}^{H_{Li}} \cos(Bz)_i dz;$$

$$\text{Cylindrical slab } \rho_i = \int_{-R_{Li}}^{R_{Li}} J_0(Br)_i r dr;$$

$$\text{Slab finite in y direction } \rho_i = \int_{-b_{Li}}^{b_{Li}} \cos(By)_i dy;$$

$$\text{Slab finite in both y and z directions } \rho_i = \int_{-b_{Li}}^{b_{Li}} \cos(By)_i dy \int_{-H_{Li}}^{H_{Li}} \cos(Bz)_i dz;$$

$$r\theta \text{ finite in z direction } \rho_i = \int_{-H_{Li}}^{H_{Li}} \cos(Bz)_i dz;$$

$$xy \text{ finite in z direction } \rho_i = \int_{-H_{Li}}^{H_{Li}} \cos(Bz)_i dz;$$

where the limits of integration are given as input and $B = \sqrt{B^2}$, the geometric buckling.

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
A.OUT.NM	Normalization option. Output calculation options. Power values.
GEOM	General descriptive data. Mesh structure. Region-mesh correspondence. Composition-mesh correspondence. Area definitions. Zone definitions. Buckling and integration limits.
XS.C.MIN	Composition cross sections. Σ_{removal} , D , Σ_{fission} , $\nu\Sigma_{\text{fission}}$, χ , $\Sigma_{\text{scattering}}$.

Upper-interface Data ModulesQuantities Used

BC	External and internal boundary condition types and constants.
FR.D1 (or FR.D2)*	Diffusion or transport one- (or two-) dimensional real fluxes.
FR.D1A (or FR.D2A)*	Diffusion or transport one- (or two-) dimensional real angular fluxes.
FA.D1 (or FA.D2)*	One- (or two-) dimensional adjoint fluxes.
SP.CICN	Real and/or adjoint specifications.
JR.D1 (or JR.D2)	Real currents.
JA.D1 (or JA.D2)	Adjoint currents.

Lower-interface Data ModulesQuantities Produced

FR.PN	k_{eff} . Power-normalized regional flux.
Printer output.	User output.

*For two-dimensional geometries.

23... Neutron Inventory Specifications AJI001

Prepared by: D. J. Bingaman

a. Nature of Physical Problem Solved

This module reads the BCD card image data set. A.INVENT, containing the option parameters for a neutron-inventory calculation, and writes the binary data set OUT.NI.

b. Upper- and Lower-interface Data Modules

Upper-interface Data Module

Quantities Used

A.INVENT

Initial and final broad-group numbers defining the coarse groups to be considered.

Labels of isotopes to be inventoried.

Labels of material to be inventoried.

Composition flag.

Interval flag and associated group-structure flag.

Region labels to be inventoried and associated group-structure flag.

Area labels to be inventoried and associated group-structure flag.

Zone labels to be inventoried and associated group-structure flag.

Total reactor flag and associated group-structure flag.

Total power.

Fertile material--mesh correspondence.

Fissile material--mesh correspondence.

Types of inventory to be calculated.

Lower-interface Data Module

Quantities Produced

OUT.NI

Same as above.

24. Transport Perturbation Specifications AJI003

Prepared by: G. J. Duffy

a. Nature of Problem Solved

Module-dependent input will be accepted in the form of

- (1) A BCD data set containing card images; and/or
- (2) A collection of binary data sets.

The input will be collected and translated into a form usable by the module-handling perturbation theory for one- and two-dimensional transport theory.

b. Method of Solution

If only the BCD data set A.INPRTR is given as input, the card images will be processed and translated into the form of the binary data set PT.TIN. If only the PT.TIN data set is given, no processing takes place. If both data sets are input, A.INPRTR is scanned to determine what modifications are to be made in PT.TIN, and these are processed.

c. Upper- and Lower-interface Data ModulesUpper-interface Data ModulesQuantities Used

A.INPRTR

Specified incremental changes in cross sections at isotope and/or composition level.

PT.TIN

Increments previously proposed for cross sections.

Lower-interface Data ModuleQuantities Produced

PT.TIN

Increments for all cross sections.

25. Neutron Inventory AJC001

Prepared by: D. J. Bingaman

a. Nature of Physical Problem Solved

Given flux, geometry, and cross-section data, this module computes for specified isotopes, materials and/or compositions, at each point, region, area, special zone and/or total reactor, for specified groups, the following reaction rates: (n, γ) , (n, α) , (n, p) , fission, total, elastic removal, inelastic removal, $(n, 2n)$ removal, total removal, power, power density, maximum-to-average power density, and/or the following source rates: fission, $(n, 2n)$, scattering. In addition, total or regional leakage rates and breeding and conversion rates may be calculated.

b. Method of Solution

Initially all fluxes for energy group g and space point i , $\phi(g, i)$, are normalized as follows:

$$\bar{\phi}(g, i) = \frac{\phi(g, i)}{\sum_i \sum_g \{[\nu \Sigma_f(g, i) + 2\Sigma_{n, 2n}(g, i)] \phi(g, i) + Q(g, i)\} \Delta \text{Vol}(i)}$$

$$= \frac{\phi(g, i)}{N}$$

The denominator, N , represents the total source of neutrons in the reactor including fission, $(n, 2n)$, and external source, if any. The volume element $\Delta \text{Vol}(i)$ is defined as:

$$x_{i+1} - x_i \quad \text{slab}$$

$$\pi(r_{i+1}^2 - r_i^2) \quad \text{cylinder}$$

$$\frac{4\pi}{3} (r_{i+1}^3 - r_i^3) \quad \text{sphere}$$

$$(x_{i+1} - x_i)(y_{j+1} - y_j) \quad x, y$$

$$\pi(r_{i+1}^2 - r_i^2)(z_{j+1} - z_j) \quad r, z$$

$$\frac{1}{2}(r_{i+1}^2 - r_i^2)(\theta_{j+1} - \theta_j) \quad r, \theta$$

If a finite length is to be estimated in one or more of the unspecified directions, the volume elements are modified by the following ρ_i :

$$2 \int_0^{bL_i} \cos (By)_i dy \quad \text{slab finite in } y \text{ direction}$$

$$4 \int_0^{bL_i} \cos (By)_i dy \int_0^{HL_i} \cos (Bz)_i dz \quad \text{slab finite in both } y \text{ and } z \text{ directions}$$

$$2 \int_0^{RL_i} J_0(Br)_i r dr \quad \text{cylindrical slab}$$

$$2 \int_0^{HL_i} \cos (Bz)_i dz \quad \text{finite cylinder}$$

$$2 \int_0^{HL_i} \cos (Bz)_i dz \quad r, \theta \text{ finite in } z \text{ direction}$$

$$2 \int_0^{HL_i} \cos (Bz)_i dz \quad x, y \text{ finite in } z \text{ direction}$$

where the limits of integration are given as input and $B = \sqrt{B^2}$, the geometric buckling.

Reaction rates for isotope m , at space point i , and for energy group g , are calculated as

$$RR_x^m(g,i) = \sigma_x^m(g,i) \bar{\phi}(g,i) \Delta Vol(i).$$

For materials and compositions, the σ_x^m is replaced by the appropriate macroscopic cross section, Σ_x . The cross-section data for isotopes and materials present in the mix are multiplied by the appropriate number densities and volume fractions. RR_x^m may be summed over requested energy groups and spatial regions; x and $\sigma_x(z,i)$ may be any of the following:

$$(n,\gamma): \quad \sigma_{n,\gamma}(g,i)$$

$$(n,\alpha): \quad \sigma_{n,\alpha}(g,i)$$

$$(n,p): \quad \sigma_{n,p}(g,i)$$

$$\text{Fission:} \quad \sigma_f(g,i)$$

$$\text{Total:} \quad \sigma_a(g,i) + \sum_k [\sigma_{el}^{(0)}(g \rightarrow k,i) + \sigma_{in}^{(0)}(g \rightarrow k,i) + \sigma_{n,2n}^{(0)}(g \rightarrow k,i)]$$

$$\text{where } \sigma_a(g,i) = \sigma_{n,\gamma}(g,i) + \sigma_{n,\alpha}(g,i) + \sigma_{n,p}(g,i) + \sigma_f(g,i)$$

$$\text{Elastic Removal:} \quad \sum_{\substack{k \\ k \neq g}} \sigma_{el}^{(0)}(g \rightarrow k,i)$$

$$\text{Inelastic Removal:} \quad \sum_{\substack{k \\ k \neq g}} \sigma_{inel}^{(0)}(g \rightarrow k,i)$$

$$\text{(n,2n) Removal:} \quad \sum_{\substack{k \\ k \neq g}} \sigma_{n,2n}^{(0)}(g \rightarrow k,i)$$

$$\text{Total Removal:} \quad \sigma_a(g,i) + \sum_{\substack{k \\ k \neq g}} [\sigma_{el}^{(0)}(g \rightarrow k,i) + \sigma_{in}^{(0)}(g \rightarrow k,i) + \sigma_{n,2n}^{(0)}(g \rightarrow k,i)]$$

$$\text{Power:} \quad A\sigma_f(g,i)$$

$$\text{where } A = \frac{\text{Total power}}{\sum_g \sum_i \sigma_f(g,i) \bar{\phi}(g,i) \Delta \text{Vol}(i)}$$

and total power is an input quantity

$$\text{Power Density:} \quad \frac{A\sigma_f(g,i)}{\Delta \text{Vol}(i)}$$

The maximum-to-average power density is computed by finding the maximum power density within a given spatial region and dividing by the average power density within that region.

Source rates for isotope m , at space point i , and for energy group g are calculated as

$$SR_X^m(g,i) = \sum_k \sigma_X^m(k \rightarrow g,i) \bar{\phi}(k,i) \Delta Vol(i).$$

For materials and composition, the σ_X^m is replaced by the appropriate macroscopic cross section, Σ_X . The cross-section data for isotopes and materials present in the mix are multiplied by the appropriate number densities and volume fractions. SR_X^m may be summed over requested energy groups and spatial regions; x and $\sigma_X(k \rightarrow g,i)$ may be any of the following:

$$\text{Fission: } \nu \sigma_f(k,i) \chi(k \rightarrow g) \quad (\chi \text{ matrix})$$

or

$$\nu \sigma_f(k,i) \chi(g) \quad (\chi \text{ vector})$$

$$(n,2n): \quad 2\sigma_{n,2n}^{(0)}(k \rightarrow g,i)$$

$$\text{Scattering: } \sigma_{el}^{(0)}(k \rightarrow g,i) + \sigma_{in}^{(0)}(k \rightarrow g,i).$$

Leakage rates at space point i are calculated as

$$LR(i) = \frac{\sum_g \{[\nu \Sigma_f(g,i) + 2\Sigma_{n,2n}(g,i)] \bar{\phi}(g,i) + Q(g,i)\} \Delta Vol(i)}{N} - \sum_g RR_{\text{absorption}}(g,i),$$

where $RR_{\text{absorption}}(g,i) = \Sigma_a(g,i) \bar{\phi}(g,i) \Delta Vol(i)$, and N is the normalization factor defined above. LR may be summed over requested spatial regions.

Breeding ratios at space point i are defined as

$$BR(i) = \frac{\sum_g \sum_m \Sigma_c^m(g,i) \bar{\phi}(g,i) \Delta Vol(i)}{\sum_i \sum_g \sum_{m'} \left[\Sigma^{m'}(g,i) + \sum_k \Sigma_{n,2n}^{(0)m'}(g \rightarrow k,i) \right] \bar{\phi}(g,i) \Delta Vol(i)}$$

entire
reactor

where the superscript m refers to specified fertile isotopes within the composition at the point i , and the m' refers to specified fissile isotopes at the point i . BR may be summed over requested spatial regions.

Conversion ratios at space point i are calculated as

$$CR(i) = \frac{\sum_g \sum_m \Sigma_c^m(g,i) \bar{\phi}(g,i) \Delta Vol(i)}{\sum_g \sum_{m'} \left[\Sigma_a^{m'}(g,i) + \sum_k \Sigma_{n,2n}^{(0)m'}(g \rightarrow k,i) \right] \bar{\phi}(g,i) \Delta Vol(i)}$$

where m and m' are defined above. CR may be summed over requested spatial regions.

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
GEOM	General descriptive data. Mesh structure. Region-mesh correspondence. Composition-mesh correspondence. Area definitions. Zone definitions. Buckling and integration limits.
FR.D1 (or FR.D2)	One- (or two-) dimensional fluxes.
XS.C.MIN	Composition cross sections Σ_a , Σ_{total} , $\Sigma_{removal}$, Σ_f , $\nu\Sigma_f$, χ .
XS.C.AUX	Composition cross sections, Σ_{el} , Σ_{inel} , $\Sigma_{n,2n}$, $\Sigma_{n,\gamma}$, $\Sigma_{n,\alpha}$, $\Sigma_{n,p}$.
XS.M.MIN	Material cross sections, Σ_a , Σ_{total} , $\Sigma_{removal}$, Σ_f , $\nu\Sigma_f$, χ .
XS.M.AUX	Material cross sections, Σ_{el} , Σ_{inel} , $\Sigma_{n,2n}$, $\Sigma_{n,\gamma}$, $\Sigma_{n,\alpha}$, $\Sigma_{n,p}$.
XS.ISO	Isotope cross sections, $\sigma_{n,\gamma}$, $\sigma_{n,\alpha}$, $\sigma_{n,p}$, σ_f , $\nu\sigma_f$, σ_{inel} , σ_{el} , $\sigma_{n,2n}$.

Upper-interface Data Module

B.HOMOG

ES.D1D (or ES.D2D)

OUT.NI

Quantities Used

Number densities of isotopes in the mix.

Volume fractions of materials in the mix.

One- (or two-) dimensional external sources.

Specifications of requested isotopes, materials, energy group structures, spatial regions, and reaction types to be inventoried.

Lower-interface Data Module

OUT.NI

Quantities Produced

All requested reaction rates, source rates, leakage rates, breeding ratios, and/or conversion ratios.

26. Diffusion Perturbation AJC002

Prepared by: G. K. Leaf and A. S. Kennedy

a. Nature of Physical Problem Solved

This module is concerned with estimating changes in k_{eff} due to changes in the reactor system. The means for estimating these changes is based on first-order perturbation theory applied to the steady-state multigroup diffusion equation. In addition, prompt-neutron lifetime and effective delayed-neutron fractions are found.

b. Method of Solution

The basic method used is to apply first-order perturbation theory to the steady-state multigroup diffusion equation with homogeneous boundary conditions on the external boundaries of the reactor system. Thus in any geometry and any dimension, the steady diffusion, in the absence of external sources, can be written abstractly in the form

$$\frac{1}{k} F \phi - M \phi = 0, \quad (226)$$

where F is the fission operator and M is the operator containing the scattering, absorption, and Laplacian terms. The adjoint flux ϕ^* for this system is defined by

$$\left(\frac{1}{k} F^* - M^* \right) \phi^* = 0, \quad (227)$$

where F^* and M^* are the adjoint operators of F and M in the appropriate space. The system is perturbed, and the resulting system is assumed to be described by the equation

$$\left(\frac{1}{k'} F' - M' \right) \phi' = 0. \quad (228)$$

Let the perturbed quantities M' , F' , ϕ' , and k' be expressed in the form $P' = P + \delta P$, and let the inner product be defined by

$$\langle \phi, \psi \rangle = \sum_{g=1}^G \iiint_{\Omega} \phi_g(r) \psi_g(r) dV, \quad (229)$$

where G is the maximum number of energy groups, and the integration extends over the reactor region Ω . Then, as a result of first-order perturbation theory applied to the above system, we obtain the following expression for the change in $1/k$:

$$\delta\left(\frac{1}{k}\right) = \frac{\left\langle \left(\delta M - \frac{1}{k} \delta F \right) \phi, \phi^* \right\rangle}{\langle F \phi, \phi^* \rangle} \quad (230)$$

It remains then to evaluate the inner products in the above expression. The perturbations allowed include changes in the cross sections at any level of homogenization from isotope to composition. Changes in isotope to material, material to composition, and composition to region assignments are also permitted, as well as changes in densities and volume fractions. Before we discuss the evaluation of Eq. 230, we shall display the flux, volume elements, and inner product for each geometry and dimension.

One Dimension	Two Dimensions
Spherical: $\phi_g(r_i)$, $\Delta V_i = \frac{4\pi}{3}(R_i^3 - R_{i-1}^3)$	RZ: $\phi_g(r_i, z_j)$, $\Delta V_{ij} = \pi(R_i^2 - R_{i-1}^2) \Delta Z_j$
Cylindrical: $\phi_g(r_i) \cos \frac{\pi z}{2H_m}$, $\Delta V_i = \pi(R_i^2 - R_{i-1}^2)$	R θ : $\phi_g(r_i, \theta_j) \cos \frac{\pi z}{2H_m}$, $\Delta V_{ij} = \frac{1}{2}(R_i^2 - R_{i-1}^2) \Delta \theta_j$
Slab: $\phi_g(x_i) \cos \frac{\pi y}{2b_m} \cos \frac{\pi z}{2c_m}$, $\Delta V_i = \Delta x_i$	XY: $\phi_g(X_i, Y_j) \cos \frac{\pi z}{2c_m}$, $\Delta V_{ij} = \Delta X_i \Delta Y_j$

In this tabulation, H_m is the half-height of region m , and b_m and c_m are the half-side lengths of region m .

The inner product

$$\langle \phi, \psi \rangle = \sum_{g=1}^G \iiint \phi_g \psi_g \, dV \quad (231)$$

can then be approximated for each geometry and dimension using the fluxes and volume elements listed above.

For one dimension,

$$\langle \phi, \psi \rangle = \sum_m W_m \sum_g \sum_{i \in m} \phi_{g_i} \psi_{g_i} \Delta V_i, \quad (232)$$

where, if $\pm(H_L)_m$, $\pm(b_L)_m$, $\pm(c_L)_m$, or $\pm(R_L)_m$ are the desired limits of integration,

$$W_m = \begin{cases} 1 \text{ for sphere;} \\ (H_L)_m + \frac{H_m}{\pi} \sin \frac{\pi(H_L)_m}{H_m} \text{ for cylinder;} \\ \left[(b_L)_m + \frac{b_m}{\pi} \sin \frac{\pi(b_L)_m}{b_m} \right] \left[(c_L)_m + \frac{c_m}{\pi} \sin \frac{\pi(c_L)_m}{c_m} \right] \text{ for slab;} \\ \pi \left[(R_L)_m \right]^2 \left\{ J_0^2 \left(\frac{\alpha}{R_m} (R_L)_m \right) + J_1^2 \left(\frac{\alpha}{R_m} (R_L)_m \right) \right\} \text{ for cylindrical slab.} \end{cases}$$

For two dimensions,

$$\langle \phi, \psi \rangle = \sum_m W_m \sum_g \sum_{ij \in m} \phi_{ij,g} \psi_{ij,g} \Delta V_{ij}, \quad (233)$$

where, if $\pm(H_L)_m$ and $\pm(c_L)_m$ are the desired limits of integration,

$$W_m = \begin{cases} 1 \text{ for RZ;} \\ (H_L)_m + \frac{H_m}{\pi} \sin \frac{\pi(H_L)_m}{H_m} \text{ for R}\theta; \\ (c_L)_m + \frac{c_m}{\pi} \sin \frac{\pi(c_L)_m}{c_m} \text{ for XY.} \end{cases}$$

With the inner product defined, the change in $1/k$ can be calculated. Four main terms contribute to this change: leakage, removal, scattering, and fission.

The first step is to approximate the inner product $\langle F\phi, \phi^* \rangle$. This is done in the following manner. Let H be defined by

$$H = \sum_m \hat{W}_m \sum_g \sum_{r \in m} S_{gr} \phi_{gr}^* \Delta V_r, \quad (234)$$

where $\hat{W}_m = W_m$ with $(iH_L)_m = H_m$, $(b_L)_m = b_m$, etc, and the fission-source density S_{gr} is definite by

$$S_{gr} = \sum_{g'=1}^G \chi_m^{g'} g(\nu \sigma_f)_{mg'} \phi_{g'r} \quad \text{for } r \in m.$$

Here we have used the index r as a general index in both one and two dimensions. With the normalization factor thus defined, the various terms contributing to the change in $1/k$ will now be calculated.

Fig. 6

Interior Mesh Cell For Diffusion
Perturbation Module

(1) Leakage. To calculate the leakage contribution we must approximate the gradients of the real and adjoint flux. Consider a typical interior mesh cell centered at O with its four neighboring cells indexed by E , N , S , and W as shown in Fig. 6. Suppose for example we wish to approximate the partial derivative of ϕ at O in the r or x direction in any geometry or dimension. This is done in the following way:

$$(\phi_x)_0 \cong \frac{1}{2} \left[(\phi_x)_E^- + (\phi_x)_W^+ \right], \quad (235)$$

where $(\phi_x)_E^-$ and $(\phi_x)_W^+$ are defined by

$$\left. \begin{aligned} \text{a) } (\phi_x)_E^- &= \frac{D_E}{\frac{1}{2}(\Delta X)_E D_0 + \frac{1}{2}(\Delta X)_0 D_E} (\phi_E - \phi_0); \\ \text{b) } (\phi_x)_W^+ &= \frac{D_W}{\frac{1}{2}(\Delta X)_W D_0 + \frac{1}{2}(\Delta X)_0 D_W} (\phi_0 - \phi_W). \end{aligned} \right\} \quad (236)$$

Here we have dropped the group index, and $D(\)$ represents the diffusion constant associated with the respective mesh cell. If the mesh cell centered at O is a boundary cell; we make the following definitions:

Right boundary cell:

$$(\phi_x)_E^- = \begin{cases} 0 & \text{if } \frac{\partial \phi}{\partial n} = 0 \text{ is the boundary conditions;} \\ -\frac{\phi_0}{\frac{1}{2}(\Delta X)_0} & \text{if } \phi = 0 \text{ is the boundary conditions.} \end{cases} \quad (237)$$

Left boundary cell:

$$(\phi_x)_W^+ = \begin{cases} 0 & \text{if } \frac{\partial \phi}{\partial n} = 0; \\ \frac{\phi_0}{\frac{1}{2}(\Delta X)_0} & \text{if } \phi = 0. \end{cases} \quad (238)$$

If the problem is two-dimensional, the gradients must be calculated for the z , y , or θ direction. This is done in exactly the same manner as the above calculation, except in the case of $R\theta$ geometry. For an interior cell,

$$\left. \begin{aligned} \text{a) } (\phi_\theta)_N^- &= \frac{D_N}{l_N D_0 + \delta_0 D_N} (\phi_N - \phi_0) \cos \left[\frac{(\Delta\theta)_N - (\Delta\theta)_0}{2} \right]; \\ \text{b) } (\phi_\theta)_S^+ &= \frac{D_S}{l_0 D_S + \delta_S D_0} (\phi_0 - \phi_S) \cos \left[\frac{(\Delta\theta)_0 - (\Delta\theta)_S}{2} \right]; \end{aligned} \right\} \quad (239)$$

where l_N , δ_0 , and l_0 are defined by

$$\left. \begin{aligned} \text{a) } l_N &= \frac{\delta_u \omega_u}{1 + \omega_u}, \\ \text{b) } \delta_0 &= \frac{\delta_u}{1 + \omega_u}, \\ \text{c) } l_0 &= \delta_0. \end{aligned} \right\} \quad (240)$$

and

Here δ_u and ω_u are defined by

$$\left. \begin{aligned} \text{a) } \delta_u &= (R_i + R_{i-1}) \sin \left[\frac{(\Delta\theta)_0 + (\Delta\theta)_N}{4} \right], \\ \text{b) } \omega_u &= \frac{\sin \frac{1}{2}(\Delta\theta)_N}{\sin \frac{1}{2}(\Delta\theta)_0} \end{aligned} \right\} \quad (241)$$

If the cell centered at O is a boundary cell, we handle it in the following manner:

Top boundary:

$$(\phi_\theta)_N^- \begin{cases} 0 & \text{if } \frac{\partial \phi}{\partial n} = 0; \\ -\frac{\phi_0}{\delta_0} & \text{if } \phi = 0. \end{cases} \quad (242)$$

Bottom boundary:

$$(\phi_\theta)_S^+ = \begin{cases} 0 & \text{if } \frac{\partial \phi}{\partial n} = 0; \\ \frac{\phi_0}{\delta_0} & \text{if } \phi = 0. \end{cases} \quad (243)$$

Having thus approximated the gradients in both dimensions and all geometries, we define the approximation to the leakage contribution in the following way:

$$A_1 = -\frac{1}{H} \sum_m \sum_g \sum_{r \in m} \delta D_{gm} \{W_m (\nabla \phi)_r \cdot (\nabla \phi^*)_{rg} + S_m \phi_{rq} \phi^*_{rg}\} \Delta V_r, \quad (244)$$

where the factor S_m arises from integration of transverse gradient terms, and where δD_{gm} denotes the change in the macroscopic diffusion constant in region m for energy group g . All macroscopic cross sections are constant within a given region.

(2) Removal. The removal contribution to the change in $1/k$ is defined by

$$A_2 = -\frac{1}{H} \sum_m W_m \sum_g \sum_{r \in m} (\delta \Sigma R)_{mg} \phi_{rg} \phi^*_{rg} \Delta V_r, \quad (245)$$

where $(\delta \Sigma_R)_{mg} = (\Sigma_R)_{mg} - (\hat{\Sigma}_R)_{mg}$ and the $\hat{}$ denotes the perturbed macroscopic removal cross section. The macroscopic removal cross sections is defined by

$$(\Sigma_R)_{mg} = (\Sigma_c)_{mg} + (\Sigma_f)_{mg} + \sum_{g' \neq g} \Sigma_m^{g \rightarrow g'}, \quad (246)$$

where Σ_c is the capture, Σ_f the fission, and $\Sigma^{g \rightarrow g'}$ the scattering cross section.

(3) Scattering. The scattering contribution is given by

$$A_3 = \frac{1}{H} \sum_m W_m \sum_g \sum_{r \in m} (\delta Q)_{rg} \phi_{rg}^* \Delta V_r, \quad (247)$$

where Q_{rg} is defined by

$$Q_{rg} = \sum_{g' \neq g} \Sigma_m^{g' \rightarrow g} \phi_{rg'}, \text{ for } r \in m, \quad (248)$$

and

$$\delta Q_{rg} = \hat{Q}_{rg} - Q_{rg}.$$

(4) Fission. The fission contribution is given by

$$A_4 = \frac{1}{kH} \sum_m W_m \sum_g \sum_{r \in m} \delta S_{rg} \phi_{rg}^* \Delta V_r, \quad (249)$$

where

$$\delta S_{rg} = \hat{S}_{rg} - S_{rg}.$$

Having thus defined the four contributing terms, we approximate the change in $1/k$ by

$$\delta \left(\frac{1}{k} \right) = -(A_1 + A_2 + A_3 + A_4) = A. \quad (250)$$

Thus,

$$\frac{\delta k}{k} = k(A_1 + A_2 + A_3 + A_4) = kA. \quad (251)$$

The inverse reactor period (regarding delayed neutrons) is defined by

$$\alpha = \frac{\langle F\phi, \phi^* \rangle}{\langle v^{-1}\phi, \phi^* \rangle} \cdot \frac{\delta k}{k^2}, \quad (252)$$

where

$$\langle v^{-1}\phi, \phi^* \rangle = \sum_m \hat{W}_m \sum_{g \in m} \sum_r \frac{1}{v_g} \phi_{rg} \phi_{rg}^* \Delta V_r$$

and v_g is the speed for the g th energy group.

The prompt-neutron lifetime is then defined by^{7†}

$$l_p = \frac{1}{\alpha} \frac{\delta k}{k^2}. \quad (253)$$

The delayed-neutron fraction for family i and isotope j is given by^{6,8}

$$\begin{aligned} \bar{\beta}_i^j = & \left(\sum_m \hat{W}_m \sum_{r \in m} \Delta V_r \sum_{g'} \phi_{rg'}^* \chi_i^{g'} \sum_g \left\{ a_{jy_j}^{ig} N_{j,m} (\sigma_f)_j^g \phi_{rg} \right\} \right) \\ & \div \left(\sum_m \hat{W}_m \sum_{r \in m} \Delta V_r \left[\sum_{g'} \phi_{rg'}^* \sum_g \chi_c^{g \rightarrow g'} (\nu_p \Sigma_f)_c^g \phi_{rg} \right. \right. \\ & \left. \left. + \sum_i \sum_{g'} \phi_{rg'}^* \chi_i^{g'} \sum_g \left\{ \chi_c^{gi} (\nu_p \Sigma_f)_c^g \phi_{rg} \right\} \right] \right). \end{aligned} \quad (254)$$

Thus, the delayed-neutron fraction for isotope j is

$$\bar{\beta}^j = \sum_i \bar{\beta}_i^j, \quad (255)$$

and the effective delayed-neutron fraction is

$$\beta_{\text{eff}} = \bar{\beta} = \sum_i \bar{\beta}^i \quad (256)$$

[†]For this and other references in this portion of Appendix B, see references listed on pp. 159-160.

The following additional calculations are performed for display purposes. The scattering contribution to the change in $1/k$ is rewritten as

$$\overline{A}_3 = \frac{1}{H} \sum_m W_m \sum_g \sum_{r \in m} (\delta \overline{Q})_{rg} \phi_{rg} \Delta V_r$$

where

$$\overline{Q}_{rg} = \sum_{g' \neq g} \Sigma_m^{g \rightarrow g'} \phi_{rg'}^*$$

and

$$(\delta \overline{Q})_{rg} = \hat{\overline{Q}}_{rg} - \overline{Q}_{rg}.$$

The scattering-out transfer contribution to the change in $1/k$ is given by

$$A_5 = -\frac{1}{H} \sum_m W_m \sum_g \sum_{r \in m} \left\{ \sum_{g' \neq g} (\delta \Sigma_m^{g' \rightarrow g}) \right\} \phi_{rg} \phi_{rg}^* \Delta V_r. \quad (257)$$

The difference in the scattering contribution and the scattering-out transfer contributions is

$$A_6 = \overline{A}_3 - A_5. \quad (258)$$

The absorption contribution $\left(\Sigma_a = \Sigma_c + \Sigma_f = \Sigma_R - \sum_{g' \neq g} \Sigma_m^{g \rightarrow g'} \right)$ is

$$A_7 = A_2 - A_5. \quad (259)$$

c. References

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4. G. K. Leaf and A. S. Kennedy, 1D-Diffusion NUC002, Section 16 of this appendix.

5. G. K. Leaf and A. S. Kennedy, 2D-Diffusion NUC004, Section 18 of this appendix.
6. D. A. Meneley, ANL internal memorandum (June 1966).
7. D. H. Shaftman, ANL internal memorandum (March 1965).
8. D. A. Sargis, Interface Variables for the One-dimensional Perturbation Module, ANL internal memorandum (Oct 1966).

d. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
PT.D1	Modified buckling, modified composition-to-region assignment.
GEOM	General descriptive data. Mesh structure. Region-to-mesh correspondence. Original composition-to-mesh assignment, original buckling, integration limits, and weights.
BC	External and internal boundary-condition definitions.
XS.C.MIN	Original composition cross sections Σ_{tr} , Σ_R , Σ_S , $\nu\Sigma_f$, χ , prompt $\nu\Sigma_f$, $\chi_{delayed}$.
XS.C.MM	Modified composition cross sections $\bar{\Sigma}_{tr}$, $\bar{\Sigma}_R$, $\bar{\Sigma}_S$, $\nu\bar{\Sigma}_f$, $\bar{\chi}$.
FR.D1 (or FR.D2)	Unperturbed value of eigenvalue (k_{eff}). Real one- (or two-) dimensional diffusion-theory flux.
FA.D1 (or FA.D2)	Adjoint one- (or two-) dimensional diffusion-theory flux.
DELAY	Delayed data. Delayed-neutron yield, fractions of yield appearing in each delayed family.
B.HOMOG	Atom density and volume fractions.
<u>Lower-interface Data Module</u>	<u>Quantities Produced</u>
PT.DOT	The normalization integral over the entire reactor, H . The inverse reactor period, α . The prompt-neutron lifetime, ℓ_p . The delayed-neutron fraction for family i and isotope j , $\bar{\beta}_i^j$. The delayed-neutron fraction for isotope j , $\bar{\beta}^j$. The effective

Lower-interface Data Module

PT.DOT (Contd.)

Quantities Produced

delayed-neutron fraction, β_{eff} . The following quantities by region and group, by region summed over group, by group summed over region, and summed over the entire reactor: A_1 , A_2 , $\bar{A}_3$, A_4 , A_5 , A_6 , and A_7 .

27. Transport Perturbation AJC003

Prepared by: G. J. Duffy

a. Nature of Physical Problem Solved

Given real and adjoint currents, scalar fluxes, and angular fluxes; volume elements, density factors, cross sections, fission fractions, weights, and direction cosines; this module computes the perturbation in the inverse period and in k_{eff} corresponding to various specified changes in cross sections at isotope and/or composition level. Anisotropic contributions are included. The calculations will be done for either a one- or a two-dimensional configuration.

b. Method of Solution

The following set of equations, defined by Kelber,^{6†} will be used initially. In what follows, we use the notation of Butler et al.⁵

For each reactor region, R, form

$$F_{j,j',0}^R = \frac{1}{2} \sum_{\ell \in R} \phi_{\ell,j} \phi_{\ell,j'}^+ V_{\ell} D F_{\ell},$$

$$G_j^R = \sum_{\ell \in R} \sum_m \phi_{m,\ell,j} \phi_{-m,\ell,j}^+ V_{\ell} W_m D F_{\ell},$$

$$H_j^R = \frac{1}{v_j} \sum_{\ell \in R} \sum_m \phi_{m,\ell,j} \phi_{-m,\ell,j}^+ V_{\ell},$$

and

$$\begin{aligned} F_{j,j',1}^R &= -\frac{3}{2} \sum_{\ell \in R} V_{\ell} D F_{\ell} \left(\sum_m W_m \mu_m \phi_{m,\ell,j} \right) \left(\sum_{m'} W_{m'} \mu_{m'} \phi_{m',\ell,j}^+ \right) \\ &= -\frac{3}{2} \sum_{\ell \in R} V_{\ell} D F_{\ell} J_{\ell,j} J_{\ell,j'}^+, \end{aligned}$$

where the reference to -m is the flux in the direction specified by $-\mu_m$, and the superscript + indicates adjoint.

[†]For this and other references in this portion of Appendix B, see references listed on page 164.

The perturbation equations are

1. For the perturbation, $\delta\alpha$, in the inverse period,

$$\Delta\alpha = \frac{\left\{ \left[\left(\sum_R \sum_{i=0}^1 \sum_j \sum_{j'} \delta M_{j,j',i}^R \right) F_{j,j',i}^R - \sum_j \delta\sigma_j^R G_j^R \right] \right\}}{\sum_R \sum_j H_j^R}.$$

2. For the perturbation in $1/k_{\text{eff}}$,

$$\Delta \frac{1}{k_{\text{eff}}} = \frac{\sum_R \left\{ \sum_j \left[\delta\sigma_j^R G_j^R - \sum_{i=0}^1 \sum_{j'} \delta M_{j,j',i}^R F_{j,j',i}^R + \left(1 - \frac{1}{k_{\text{eff}}} \right) \sum_{j'} \delta M_{j,j',F_{j,j',0}^R}^R \right] \right\}}{\sum_R \sum_j \sum_{j'} M_{j,j',F_{j,j',0}^R}^R}.$$

If $k_{\text{eff}} = 1$, the lifetime, ℓ , is equal to $\Delta k / \Delta\alpha$ or

$$\ell = \frac{\sum_R \sum_j H_j}{\sum_R \sum_j \sum_{j'} M_{j,j',F_{j,j',0}^R}^R}.$$

Other symbols are

$$M_{j,j',0}^R = \sigma^{R(0)}(j \rightarrow j') + \chi_R(j \rightarrow j') \nu \sigma_{f,j}^R,$$

$$M_{j,j'}^R = \chi_R(j \rightarrow j') \nu \sigma_{f,j}^R,$$

and

$$M_{j,j',1}^R = 3\sigma^{R(1)}(j \rightarrow j').$$

(We have assumed that fission is isotropic.)

The operator δ refers to an increment in the quantity operated on; thus $\delta\sigma_j$ is the increment in σ_j .

Clearly simplifications are possible; for example,

$$\sum_j \sum_j M F_{j,j'}^R F_{j,j',0}^R = \frac{1}{2} \sum_{j'} \sum_{\ell \in R} \phi_{\ell,j'}^+ F_{\ell,j'}^I.$$

The equations are in the same form as for diffusion theory with the terms in $G_j^{(R)}$ replacing the gradient terms. Thus we can specify at least the same output as the DEL code plus, at least, the perturbation arising from the change in any given isotope cross section. Thus, it will be convenient to break up $F_{\ell,j'}^I$ into components, prompt and delayed, for each fissionable species, i , and compute

$$\beta_{\text{eff}}^{m,i} = \frac{k \sum_j \sum_R \sum_{\ell \in R} \phi_{\ell,j'}^+ F_{\ell,j'}^{m,i}}{\sum_m \sum_{j'} \sum_R \sum_{\ell \in R} \phi_{\ell,j'}^+ F_{\ell,j'}^m},$$

where $\beta_{\text{eff}}^{m,i}$ is the effective fraction of the component m of fission neutrons coming from fission in isotope i . The matrix χ and yield per fission, $\nu\sigma_f$, are obviously m -dependent.

c. References

1. G. E. Hansen and C. Maier, Perturbation Theory of Reactivity Coefficients for Fast Neutron Critical Systems, Nucl. Sci. Eng. 8, 532-542 (1960).
2. W. Fader, TDP - A Two Dimensional Perturbation Calculation Code Based on TDC, for IBM-7090, DECK<B516, PWAC-446 (Nov. 20, 1964).
3. E. D. Pendlebury, The Mechanized Application of Perturbation Theory in Multigroup Neutron Transport Calculations, AWRE-0-32/64 (July 1964).
4. M. E. Gubbins, Reactor Perturbation Calculations by Monte Carlo Methods, AEEW-M 581 (Sept 1965).
5. M. K. Butler, G. Duffy, H. Greenspan, E. Mueller, S. Sparck, and J. Zapatka, ANL-CDC Reprogramming Series IV, SNARG 1D, TM 95 (July 1965).
6. C. Kelber, private communication.

d. Machine Requirements

Disk storage will be needed as temporary storage.

e. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
GEOM	Composition-mesh correspondence.
FR.D1 (or FR.D2)	One- (or two-) dimensional fluxes.
FA.D1 (or FA.D2)	One- (or two-) dimensional adjoint fluxes.
FR.D1A (or FR.D2A)	One- (or two-) dimensional angular fluxes.
FA.D1A (or FA.D2A)	One- (or two-) dimensional adjoint angular fluxes.
JR.D1 (or JR.D2)	One- (or two-) dimensional currents.
JA.D1 (or JA.D2)	One- (or two-) dimensional adjoint currents.
XS.C.MIN	Composition cross sections, Σ_a , Σ_{total} , $\Sigma_{removal}$, Σ_f , $\nu\Sigma_f$, x .
XS.C.AUX	Composition cross sections, Σ_{el} , Σ_{inel} , $\Sigma_{n,zn}$.
XS.ISO	Isotope cross section, σ_f , $\nu\sigma_f$, σ_{inel} , σ_{el} , $\sigma_{n,zn}$.
SP.NEUT1 (or SP.NEUT2)	Density factors, DF_ℓ . Weights and direction cosines.
PT.TIN	Increments for all cross sections.
<u>Lower-interface Data Modules</u>	<u>Quantities Produced</u>
PT.D1.TR (or PT.D2.TR)	Perturbation in inverse reactor period and in k_{eff} .

28. Fuel-cycle Specifications FCI001

Prepared by: P. L. Walker

a. Nature of Physical Problem Solved

This module reads the BCD card-image data set and produces binary data sets to be used in a fuel-cycle problem. The data considered are the fuel-cycle code-dependent data such as reaction-chain data, external fuel-cycle data, and guesses and error criteria for the searches. Input manipulation is done on the reactions that take place in the reactor and $\sigma_{n,\gamma}$, σ_f , $\sigma_{n,p}$, $\sigma_{n,2n}$, $\sigma_{n,\alpha}$ isotope cross sections and decay constants for β^- , β^+ , and α decays. Burnup matrices are constructed which will later incorporate the proper flux. The decay parts will also be used for real-time accounting.

b. Method of Solution

For each material the information given in data set A.BURN is considered for each isotope. The matrix is constructed with the isotopes in the same order as in the input. Each reaction for a given isotope is analyzed to see which isotope will be produced. A label is set corresponding to the column in the matrix of the isotope produced and the row of the given isotope. Corresponding cross sections or decay constants are stored, depending on the reaction.

The reactions allowed are n,γ ; f ; n,p ; $n,2n$; n,α ; and β^- , β^+ , and decays.

The structure produced here is used to simplify formation of the burnup matrices using the proper flux when they are needed in iterative procedures.

c. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
A.BURN	Material definitions.
	Stage and region correspondence.
	Densities.
	Guesses, maximum iteration counts, and convergence criteria.
	Option flags.
	Reaction-chain information.
	External cycle data.

Upper-interface Data Modules

XS.ISO2

Quantities Used

Isotope cross sections including $\sigma_{n,\gamma}$, σ_f ,
 $\sigma_{n,p}$, $\sigma_{n,zn}$, $\sigma_{n,\alpha}$.

Lower-interface Data Module

BRN

Quantities Produced

Number of materials.
 Number of active isotopes in materials.
 Number of stages.
 Stage and region correspondence.
 Isotope names in each material.
 Densities.
 Guesses, maximum iteration counts, and
 convergence criteria.
 Option flags.
 Number of feed lines.
 Number of reprocessing plants.
 Reprocessing fractions.
 Densities in feed lines.
 Densities in reprocessing lines (optional).
 Volume of each material.
 Supply table.
 Demand table.
 Class-separation factors.
 ρ constants.
 Reactions undergone by each isotope.
 Number and positions of nondecay
 reactions.
 Number and positions of decay reactions.
 Cross sections for nondecay reactions.
 Decay constants.

29. Fuel Cycle FCC001

Prepared by: G. K. Leaf, D. A. Meneley, and P. L. Walker

a. Nature of Physical Problem Solved

Given complete specifications of a reactor in zero-, one-, or two-space dimensions, including fluxes, microscopic cross sections, isotope-to-material assignments, material volumes and locations in spatial regions, internal fuel-handling schemes, charge/discharge criteria, and external cycle definitions, this module computes the long-time behavior of the system with reference to criticality, flux, and power changes, fuel burnup, breeding ratio, and external cycle.

The charge enrichment may be adjusted to achieve a desired unpoisoned k -effective at a given point during the at-power phase. Criticality may be adjusted by means of space-dependent fuel or poison control adjustment at a given number of time points during the burn step. Burn time may be adjusted to achieve desired burnup conditions in selected discharge batches.

The fuel-management scheme allows all the flexibility possible in a real reactor with solid-fuel elements, under the restrictions imposed by the spatial model of the core. The total in-pile history of a fuel material is divided into a number of "stages," defined by the points in time at which fuel management is carried out. The fresh charge is Stage 1 and is assigned to a particular spatial region. After one fuel-management operation, this charge is at Stage 2 and may or may not have been moved to another spatial region. At the same time a fresh charge of material replaces the original charge at Stage 1. After the final (k th) stage, the charge is removed from the reactor and placed in the cooling tanks. Thus at any time during operation there are k stages of the same material in the reactor, not necessarily in the same spatial region. Any number of different stages of the same material or of different materials may be assigned to the same spatial region. The total volume of all stages must be equal to the region volume. The enrichment, composition, and volume of a given stage of a material may be different than those of any other stage of the same material. The identification of a "material" is therefore only a bookkeeping convenience. It is used to describe a linear path of fuel movement in space and time from fuel loading to unloading.

A discharged fuel batch may be assigned to any one of multiple reprocessing plants, each of which may produce two effluents, designated as Class 1 (high reactivity) and Class 2 (low reactivity). Each class of effluent from the several plants may be used for refabrication of one or more fuel charges or sold off, according to a user-defined priority-ordering scheme. Makeup fuel may be taken from any number of predefined external

feed lines, also according to the given priority ordering. A number of charge batches having different composition and enrichment may be fabricated.

The isotopic chain matrix may contain β^- , β^+ , and α -decay terms as well as (n,γ) , (n,p) , (n,α) , $(n,2n)$, and (n,f) terms. Fission reactions may produce fractional yields of discrete as well as lumped fission products.

Real-time accounting is carried throughout the system. Reprocessing and fabrication are assumed to require a fixed time for completion; that is, the continuous nature of the real processes are ignored. Isotope decay chains are computed throughout the external cycle.

The entire system may be operated in nonequilibrium or equilibrium modes. In nonequilibrium operation the computation may be interrupted at the end of any burn phase. Special fuel-management operations may be carried out and system parameters redefined before the next burn step. Approach-to-equilibrium studies may be made using this option. In equilibrium-mode operation, the solution sought is the infinite-time operating condition of a completely specified system.

Microscopic group cross sections are currently assumed to be constant throughout the problem. This restriction will be removed later either by use of interpolation tables or by direct connection to the cross-section generating module. Fuel cycle economics computations also will be added at a later time.

b. Method of Solution

(1) Core Cycle. Two methods are available for starting a computation. In the first, the user guesses the contents of reprocessing storage pots and each fuel-charge enrichment. The core will be loaded initially by assigning the resultant fuel-charge atom densities to all stages of each material. The second method of starting is by specifying the atom-density vectors of each stage of each material. The calculation will then proceed differently depending on whether the problem being solved is in equilibrium or nonequilibrium mode.

Consider first the equilibrium problem. The case under discussion is a k irradiation stage model. In this model, the volume of each material (m) in the reactor is divided into K_m parts of equal volume. Each part may be called a "charge." The charges are distributed in the various regions of the reactor according to the user's specifications of material stages and spatial locations.

In this model all charges assigned to a given spatial region are assumed to be subjected to the region-averaged group flux. At the end of each burn step the charges of the materials that have been in the reactor for K_m burn steps are discharged from the reactor. The charges at Stage $K_m - 1$ then move to Stage K_m , and so on. A fresh charge of each material is then loaded at Stage 1. The fuel that is discharged after every step enters the external cycle, where it undergoes reprocessing and refabrication thus, producing new initial charges for loading into the reactor. The object of an equilibrium calculation is to find a charge density for each material and an operating time for any burn step such that the charges produced by the external cycle are the same for every burn step. This solution is subject to the following three constraints:

(a) Let M denote the total number of materials under consideration, and e_m , $m = 1, 2, \dots, M$, the enrichment associated with the charge density for each material m . Then the solution is sought by varying the enrichment vector $(e_1, e_2, \dots, e_M)$ along a specified straight line.

(b) The burnup of the system at the end of each burn step assumes a specified value. The burnup criterion for the system can be fixed by one of two options. The first is the average burnup over a specified set of materials. The second is the maximum burnup over a specified set of materials.

(c) The third constraint is that the unpoisoned k_{eff} of the reactor at a given fraction of the burn-step time takes on a specified value.

We shall now describe the methods used to solve the equilibrium problem beginning with the calculations that describe the burning of the reactor. Consider any region r of the reactor, and suppose that material m has at least one of its K_m stages in region r . In fact, suppose that $I_{m,r}$ stages of material m reside in region r . Let $n_{m,i}$ denote the density vectors of these stages. Then define the vector $n_{m,r}$ by

$$n_{m,r} = \frac{1}{I_{m,r}} \sum_i n_{m,i}, \quad (260)$$

where the sum is taken over those stages of m that are in region r . The dimension of $n_{m,r}$ is J , where J is the number of isotopes being considered. The following set of equations is then taken to govern the reactor as a function of time:

$$\frac{dn_m(t)}{dt} = A_r(\phi(t)) n_m(t), \quad (261)$$

where r ranges over the regions of the reactor, and m varies over the set $M(r)$ of materials having at least one stage in r . The burnup matrices $A_r(\phi(t))$ have the form

$$A_r(\phi(t)) = \Lambda + \hat{A}_r(\phi(t)), \quad (262)$$

where Λ is a constant matrix arising from radioactive decay, and the elements $a_{jk}(t)$ of $\hat{A}$ have the form

$$a_{jk}(t) = \sum_{g=1}^G \sigma_{jk}^g \phi_{gr}(t). \quad (263)$$

Here ϕ_{gr} is the average flux at time t over the region r , and σ_{jk}^g denotes the microscopic cross section for each isotope and type of reaction. The coupling between the isotope densities and the flux is governed by a fixed-power static-neutronics calculation with or without maintaining criticality, at the option of the user.

If a distribution of charge densities is given at $t = 0$, then the distribution at time t is found by numerically solving the coupled system consisting of the burnup Eq. 262 together with the static neutronics equations. The resulting densities can be represented in the form

$$n_{m,i}(t) = B_r(t; n(0)) n_{m,i}(0). \quad (264)$$

Here $B_r(t; n(0))$ is the $J \times J$ dimensional matrix resulting from solving the coupled system. Note that through the coupling of the region averaged flux, the matrix depends on the total initial-charge distribution of all the materials in the reactor. This dependence is indicated by the symbol $n(0)$.

We shall next consider the repetitive loading, burning, and discharging of the reactor. Let the burn time for each step be fixed, and let the charge density for each material loaded in at the beginning of each burn step be fixed. Consider any material m ; suppose that during its K_m stages it resides in regions $r_1, r_2, \dots, r_L$ such that it is in r_1 for the first i_1 stages, then r_2 for the next i_2 stages, and so on. Thus $i_1 + i_2 + \dots + i_L = K_m$; moreover, when it reaches the K_m th stage in region r_L , it is discharged. Let the charge density for material m which is introduced at the beginning of every burn step be denoted by $n_{m,1}$. Starting at the beginning of some burn step, let us follow this charge density through the K_m burn steps until it is discharged. After i_1 burn steps in region r_1 , the density is given by $B_{r_1}^{(i_1)} \dots B_{r_1}^{(1)} n_{m,1}$. The charge then moves to region r_2 for the next i_2 burn steps, and then on to the next region, until at the end of the K_m th burn step after it was introduced, it is discharged. This discharge density is given by

$$B_{r_L}^{(K_m)} \dots B_{r_2}^{(i_1+i_2)} \dots B_{r_1}^{(i_1)} \dots B_{r_1}^{(1)} n_{m,1}. \quad (265)$$

However, if we had followed the same charge density $n_{m,1}$ that was introduced one time step later than the preceding one, its value upon discharge would be given by

$$\bar{B}_{r_L}^{(K)} \dots \bar{B}_{r_1}^{(i_1)} \dots \bar{B}_{r_1}^{(1)} n_{m,1}. \quad (266)$$

Because the B operators depend on the densities of all the materials in the reactor, the operators that appear in Eq. 264 are different from those in Eq. 266. Thus the densities discharged after each time step are different even though the same charge is loaded at the beginning of each step. However, it would seem plausible that in the limit we would obtain the same discharge density after every burn step. In terms of the B operators, this would mean that we would move in limit operators $B_{r_1}, \dots, B_{r_L}$ such that the discharged density after every step is given by

$$B_{r_L}^{i_L} B_{r_{L-1}}^{i_{L-1}} \dots B_{r_1}^{i_1} n_{m,1}. \quad (267)$$

When the state is achieved where the discharge densities are the same after every burn step, the core is said to be in its cyclic mode. Note that this is achieved for a given set of charges and a given burn-step time.

Consider next the interaction between the external and internal paths. As noted earlier, the enrichments of the various materials are constrained by a linear relationship; thus for each material m the enrichment, e_m has the form $e_m(x) = e_m(0)(1 + x\delta_m)$. Hence when we speak of adjusting the enrichment, we are referring to the enrichment parameter. Starting with a given enrichment x and a discharge density distribution $\hat{n}^{(0)}$, form the charge distribution $n^{(0)}$ for loading by passing through the external path of reprocessing and refabrication with $\hat{n}^{(0)}$ and x , as described in the following section. Using this charge, find a burn-step time such that when the core is in its cyclic mode, the burnup achieves its desired value. Let the corresponding discharge density distribution be denoted by $\hat{n}^{(1)}$. Now $\hat{n}^{(1)}$ will not in general be equal to $\hat{n}^{(0)}$ since $n^{(0)}$ depends on $\hat{n}^{(0)}$ as well as the enrichment x ; i.e., the system is nonlinear. Thus holding x fixed, we can pass $\hat{n}^{(1)}$ through the external and internal paths as before, thereby generating $\hat{n}^{(2)}$. If this process is repeated indefinitely, we can assume that the sequence $\hat{n}^{(\ell)}$ will converge to some

charge distribution $\hat{n}(x)$. Then, by virtue of its definition, when we send $\hat{n}(x)$ through the external path to form $n(x)$ and then through the internal path where the desired burnup time $t(x)$ is found, the discharge distribution from the reactor is equal to $\hat{n}(x)$. When the system achieves this state, it is said to be in its equilibrium mode.

With these concepts defined, the basic approach used in solving the equilibrium problem can be described very simply. Starting with a guess $x^{(0)}$ for the proper enrichment, the system is put in its equilibrium mode. The unpoisoned k_{eff} at a specified fraction α of the burn-step time $(tx^{(0)})$ is then adjusted so that the unpoisoned k_{eff} achieves its desired value. This is the basic approach used in solving the equilibrium problem. Note that nonlinearities are present at every level of the problem. Because of these nonlinearities, the total calculation is laborious. However, certain modifications have been implemented at various levels to reduce the time needed for a complete calculation. These modifications have taken the form of partially linearizing the problem at a point where the nonlinearity is weak. For example, recall that the B matrices depend not only on the burn-step time, but also on the densities of all stages for all materials present in the reactor at the beginning of the burn step. Thus the achievement of the cyclic mode for the core is of necessity an iterative process involving the repetitive loading of fixed initial-charge distribution, burning for a fixed time, and then discharging the last stage charges. As noted earlier, the B operators differ from step to step because of their dependence on the total distribution of densities. To reach the limiting state (cyclic mode) more rapidly, the dependence of the B matrices on the total density distributions is ignored for K_m burn steps at the end of which the dependence is taken into account. A similar modification is used in the iterative process by which the equilibrium mode is reached. In this case we ignore the dependence of the desired burn-step time as well as the corresponding cyclic mode B matrix on the initial charge distribution from the external path. Thus for a given enrichment, we achieve an approximate equilibrium state or mode by cycling through the external and internal paths as before, but with the internal path held fixed.

The nonequilibrium problem may be viewed as the equilibrium problem without the cyclic mode for the core and a modified procedure in the external path. Again, each material in the reactor is divided into K stages called charges. The charges are then ordered according to the degree of burnup. The last K - 1 stages of each material are specified. The object of the calculation is to adjust the enrichment x of the first stage-charge distributions $n(x)$ and the operating time to such that the burnup of the reactor at the end of the burn step achieves its desired value. In addition, the unpoisoned k_{eff} at a specified fraction of this burn step achieves its desired value. Furthermore, the makeup of the loading charge in the external path differs from that of the equilibrium case in that the reprocessing components are held fixed.

The reason for this is that the contents of the reprocessing storage represent fuel discharged at an earlier time and hence are completely determined. In the equilibrium case, however, a change made in Stage 1 of the in-pile history eventually results in a change in reprocess plant output, so that it is valid to consider that the changes occur immediately. This treatment will accelerate the convergence of the equilibrium problem.

The solution to the nonequilibrium problem is found in the following way: Starting with a guess for the enrichment x , a loading charge is made up in the modified external path. With this charge distribution loaded in as a first stage, the operating time is adjusted so that the burnup requirements are met. For this operating time, the unpoisoned k_{eff} is found at the specified location of the burn time. The enrichment is then adjusted so that the unpoisoned k_{eff} achieves its desired value.

In this case, the charge that reaches its burnup limit first may be at other than the last stage, because of the nonequilibrium nature of the problem. Thus all stages of all materials must be scanned in fixing of the burn criterion. The occurrence of this condition indicates that a change in fuel-management policy is required. A restart dump will be formed and an edit given which shows the condition of the system; then the job will be terminated. The user may specify new fuel-management methods and other parameters when the problem is restarted.

(2) External Cycle. The components of the external cycle are assumed to be cooling, disposition of cooled fuel to reprocessing plants, direct sale, or recharge, reprocessing with or without admixture of externally specified material, separation into two effluents per plant, storage, selection of effluents along with one or more external feed .

materials for makeup of a fresh fuel charge, and refabricated fuel storage prior to loading. Reprocessing plant effluent remaining after fabrication may also be sold. Real time is accounted throughout the cycle. Figure 7 is a schematic diagram of the model.

Fig. 7. External Cycle Schematic Diagram

The user specifies a post-discharge cooling time for each discharge fuel batch. He also supplies destination information indicating what fraction of each batch is to be sold after cooling, recycled directly to recharge, and sent to each reprocessing plant.

For each reprocessing plant the user specifies the amount and isotopic distribution of admixture to be processed with each batch, the isotope-dependent recovery fractions and separation fractions, and the amount of each effluent to be removed from the cycle. (The admixture of plant feed material and removal of effluent simulates plant input batch mixture of fuel from the system under study with fuel from other reactor systems.) Reprocessing time is also given for each plant.

Effluent storage times are determined from the length of cooling, reprocessing, refabrication, finished-element storage, core shutdown, and burn phases of the cycle. Effluent batches are each assigned a time at which they are available for refabrication. In makeup of a charge, the time at which fabrication must start determines which effluents will be used. All effluent batches of one type from a single plant which are available at this time are mixed to form one component of the charge. Selloff is assumed to occur at the time of reprocess plant discharge.

Refabrication is carried out using a distribution priority scheme, specified for each class of plant effluents. The two classes are high-reactivity effluent and low-reactivity effluent, as determined by the separation fractions given for each plant. (This distribution is necessary to allow reactivity adjustments through charge-enrichment changes.) A number of external feed lines may also contribute to the charge. These are completely specified in quantity, isotopic distribution, and class separation.

The priority system allows the user to predetermine the distribution of each class of effluent from each plant in the makeup of the several charge materials. This distribution may be given as a combination of (1) a graded priority, in which fractions of total available effluent are assigned to each charge material, and (2) an absolute priority, in which the effluent is used to make up a given charge exclusively unless there is an excess. This excess will then be used for the next lower-priority charge material, and so on. Material volume is preserved with changes in enrichment and isotopic distribution.

Two selloff schemes are available. The first one is included in the priority system described above. This gives the user the capability of selling the excess of blanket-produced plutonium after requirements of the core charge are satisfied, as an example. The second type of selloff is of effluent remaining after fabrication is complete. Part of this remainder may also be retained in the effluent storage.

Finished-element storage times are indicated relative to the time of shutdown of the reactor at the end of the last burn phase. This time, along with the fabrication time, determines the time at which fabrication must start. Fuel-charge selection specifications are given in the case of

directly recycled fuel, that is, fuel that has been discharged, cooled, and is to be recharged without refabrication. (This mode of operation is only meaningful, of course, in nonequilibrium problems.)

All external cycle parameters may be changed periodically at the option of the user by means of the interrupt facility.

c. Related Programs

Many programs of varying levels of sophistication are available. The starting points of this development were the IBM-704 codes CYCLE1 and CYCLE2, both unpublished ANL work.

d. References

Reactor Development Program Progress Reports, ANL-7176, -7193, -7204, -7219, -7249, -7267 (1966).

e. Machine Requirements

The minimum configuration for running of practical one-dimensional problems is approximately 32K of core storage and a large quantity of peripheral storage. Efficiency should increase uniformly with available random access volume up to around 128K for one-dimensional problems, and to greater than the largest contemplated machine configuration for two-dimensional problems. Data-handling methods would have to vary with machine size in order to improve efficiency.

f. Upper- and Lower-interface Data Modules

Upper-interface Data Modules

BRN

Quantities Used

Number of materials.

Number of active isotopes in materials.

Number of stages.

Stage and region correspondence.

Isotope names in each material.

Densities.

Guesses, maximum iteration count, and convergence criteria.

Option flags:

Number of feed lines.

Upper-interface Data Modules

BRN (Contd.)

Quantities Used

Number of reprocessing plants.
 Reprocessing fractions.
 Densities in feed lines.
 Densities in reprocessing lines (optional).
 Reactions undergone by each isotope.
 Number and positions of nondecay reactions.
 Number and positions of decay reactions.
 Cross sections for nondecay reactions.
 Decay constants.

FR.PN

 k_{eff} , power-normalized regional fluxes.Lower-interface Data ModulesQuantities Produced

SP.CRIT

Criticality search information such as
 guesses and convergence criteria.

BRN.OUT

Unpoisoned k .

Burn time.

Material atom densities.

Burnups.

Quantities fed and sold in external cycle.

Convergence criteria.

HOMOB (same structure as
 B.HOMOG)

Material mixture tables.

Volume fractions.

30. Fuel-cycle Output Edit FCE001

Prepared by: P. L. Walker

a. Nature of Physical Problem Solved

This module reads all data sets created by the fuel-cycle modules, edits the data, and prints data in a form desired by the users. A complete edit of the input data is included.

b. Upper- and Lower-interface Data ModulesUpper-interface Data ModulesQuantities Used

BRN

Number of materials.
 Number of active isotopes in materials.
 Number of stages.
 Stage and region correspondence.
 Isotope names in each material.
 Densities.
 Guesses, maximum iteration counts, and convergence criteria.
 Option flags.
 Number of feed lines.
 Number of reprocessing plants.
 Reprocessing fractions.
 Densities in feed lines.
 Densities in reprocessing lines (optional).
 Volume of each material.
 Supply table.
 Demand table.
 Class-separation factors.
 ρ constants.
 Reactions undergone by each isotope.
 Number and positions of nondecay reactions.
 Number and positions of decay reactions.
 Cross sections for nondecay reactions.
 Decay constants.

BRN.OUT

Unpoisoned k.
 Burn time.
 Material atom densities.
 Burnups.
 Quantities fed and sold in external cycle.
 Convergence criteria.

Lower-interface Data ModulesQuantities Produced

Printer output

User output

31. Heat Transfer SAC003

Prepared by: C. K. Sanathanan, J. C. Carter, and N. A. McNeal

a. Nature of Physical Problem Solved

(1) Steady State. Given the dimensions, material composition, thermal properties of the materials, the steady volumetric heat-generation rate, coolant flow rate, and inlet coolant temperature of a fuel cell, this portion of the module computes the radial and axial temperature profiles, the unrestricted thermal expansion in the axial increments, the average temperature and the volume fraction of the various materials in the various axial regions,[†] the height of the interface between the various axial regions, the liquid-solid interface in each axial increment, and the percentage of the total fuel melted.

(2) Transient State. Given the dimensions of the fuel cell, its material composition and thermal properties at the end of k th time increment, the average volumetric heat-generation rate in $(k+1)$ th time interval, the two-dimensional temperature profile at the end of $(k-1)$ th and k th time intervals, and the axial coolant temperature profile at the end of $(k+1)$ th time interval, this part of the module computes the radial and axial temperature profiles, the unrestricted thermal expansion in each of the axial increments, the average temperature and volume fraction of the various materials in the various axial regions, the height of the interface between the various axial regions, the liquid-solid interface in each axial increment, and the percentage of the total fuel melted at the end of the $(k+1)$ th time interval, and projects the axial profile of the heat flux to the coolant during time interval $(k+2)$.

b. Method of Solution(1) Steady State

(a) Summary. A heat balance is applied to the various (non-uniform) radial increments. The resulting nonlinear algebraic equations^{††} for the fuel are solved simultaneously by the Gauss-Sidel iterative scheme.

If the bond consists of a gas, the temperature drop in the bond is usually large and the drop is strongly dependent upon the gap size. Consequently, an iteration is necessary to make compatible the radial temperature profile in an axial increment and the corresponding thermal expansion and bond-gap size.

[†] An axial region may contain several axial increments.

^{††} Nonlinear because the thermal properties are functions of temperature.

Axial conduction of heat is neglected. Therefore the axial increments are thermally coupled only by the coolant temperature. Hence a straightforward marching procedure (starting from the inlet segment) is adopted to determine the radial temperature profile in all the axial segments.

(b) Procedure. (The radial and axial segments of the fuel cell are shown in Fig. 8.)

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Fig. 8. Radial and Axial Segments of Fuel Pin

i. The heat-generation rate, $\bar{q}_j$, watts/cm at the j th axial node is given directly by the neutronics module (or it is obtained from $\bar{q}(z)$ specified at a different set of axial nodes by the neutronics module).

ii. Compute the heat-generation rate in the i th radial segment at the j th axial node, per cm height,

$$q_{i,j} = \bar{q}_j \frac{R_{i+1}^{(0)2} - R_i^{(0)2}}{R_{N+1}^{(0)2}},$$

where $R_i^{(0)}$ is the value of R_i at $T^{(0)}$, the design temperature.

iii. Define $\pi Q_{i,j}$ as the total heat up to and including the i th radial segment at the j th axial node. That is,

$$Q_{ij} = \frac{1}{\pi} \sum_{k=1}^i q_{k,j}$$

Note that $\pi Q_{N,j} = \bar{q}_j$.

iv. Compute coolant enthalpy at the j th axial increment,

$$H_j = H_{j-1} + \frac{\bar{q}_j \Delta z_j}{(\bar{R}_c^2 - \bar{R}_e^2) G_0}$$

where G_0 is the steady mass flow rate of coolant. Coolant temperature at j ,

$$T_{cj} = T_{cj-1} + \frac{H_j - H_{j-1}}{C(T_{cj-1})}$$

the following computations apply to any $j: j = 1, \dots, M$. Hence, the subscript j is omitted in temperatures and radii:

v.[†] Compute the cladding center temperature,

$$T_e = T_c + \frac{\bar{q}_j}{2R_e^{(0)}} \left[\frac{R_e^{(0)} - R_b^{(0)}}{2k_e} + \frac{1}{h_c \left[1 + \alpha_e (T_e - T_f^{(0)}) \right]} \right],$$

where

$$T_c = \frac{1}{2} (T_{c(j-1)} + T_{cj})$$

and α_e = coefficient of thermal expansion of cladding.

vi. Compute the cladding inner-boundary temperature,

$$T_e'' = T_e + \frac{\bar{q}_j}{2R_b^{(0)}} \cdot \frac{R_e^{(0)} - R_b^{(0)}}{2k_e}$$

vii.[†] Compute the temperature of the outer boundary of fuel,

$$T_N = T_e'' + \frac{1}{h_b} \left[\frac{\bar{Q}_N}{2R_{N+1}} - \delta (T_N^4 - T_e''^4) \right],$$

[†] Indicates that the equation is solved by iteration.

where h_b , the heat transfer coefficient of the bond, is

$$h_b = \frac{h_{b0}}{R_b - R_{N+1}},$$

where h_{b0} is a constant, and

$$\delta = (\text{Stefan-Boltzmann constant}) \times (\text{Emissivity}).$$

viii. Compute the radial node temperatures in the fuel;
 T_i , $i = 1, \dots, N - 1$ (Gauss-Seidel iteration),

$$T_1 = T_2 + \frac{Q_{1,j}(R_3 + R_2 - 2R_1)}{4k_2R_2},$$

$$T_i = T_{i+1} + \frac{Q_{i,j}(R_{i+2} - R_i)}{4R_{i+1}k_{i+1}}, \quad i = 2 \text{ to } N - 2,$$

$$T_{N-1} = T_N + Q_{N-1,j} \frac{(2R_{N+1} - R_N - R_{N-1})}{4R_Nk_N},$$

where

$$k_i \equiv k(T(R_i))$$

and

$$T(R_i) = \frac{T_i - T_{i-1}}{R_{i+1} - R_{i-1}} (R_i - R_{i-1}) + T_{i-1} \quad \text{for } i = 3, \dots, N - 1,$$

$$T(R_2) = T_1 + \frac{2(T_2 - T_1)(R_2 - R_1)}{R_3 + R_2 - 2R_1},$$

$$T(R_N) = T_N - \frac{2(T_N - T_{N-1})(R_{N+1} - R_N)}{2R_{N+1} - R_N - R_{N-1}}.$$

ix. Compute new radial mesh size and nodal radii inside fuel. If $T_i < T_{\text{melt}}$,

$$\Delta R_i = \Delta R_i^{(0)} \left[1 + \alpha_{fs} (T_i - T^{(0)}) \right].$$

If $T_i > T_{\text{melt}}$,

$$\begin{aligned} \Delta R_i &= \Delta R_i^{(0)} \left[1 + \alpha_{fs}(T_{\text{melt}} - T^{(0)}) \right] \\ &\cdot (1 + \alpha_{fmelt}) \\ &\cdot [1 + \alpha_{fl}(T_i - T_{\text{melt}})], \end{aligned}$$

$R_1 = 0$ (at the present stage of coding),

$$R_i = \sum_{p=1}^{i-1} \Delta R_p, \quad i = 2, \dots, N+1.$$

x. Compute new bond-gap size,

$$R_b = R_{N+1}.$$

Repeat steps vii-x until the bond-gap size and the temperature drop in the bond are compatible.

xi. Compute the volume-averaged temperature of the fuel in axial region ℓ ,

$$\bar{T}_{f\ell} = \frac{\sum_{j=M_{\ell-1}+1}^{M_\ell} R_{fj}^2 T_j}{\sum_{j=M_{\ell-1}+1}^{M_\ell} R_{fj}^2},$$

where

$$T_j = \frac{1}{R_{fj}^2} \sum_{i=1}^N T_{i,j} (R_{i,j}^2 - R_{i-1,j}^2),$$

$$R_{fj} \equiv R_{N+1,j},$$

and

$$M_\ell = \sum_{k=1, \ell} N_k,$$

where N_k is the number of heat transfer Δz in the k th axial region

$$M_0 \equiv 0.$$

xii. Compute the volume-averaged temperature for the cladding or coolant in axial region ℓ ,

$$\bar{T}_{x_\ell} = \frac{\sum_{j=M_{\ell-1}+1}^{M_\ell} T_{x,j}}{N_\ell}$$

where

$$x = e \text{ or } c.$$

xiii. Compute the volume fraction of the fuel in the ℓ th axial region,

$$V_{f_\ell} = \frac{V_{f_\ell}^{(0)}}{1 + \alpha_f (\bar{T}_{f_\ell} - T^{(0)})}$$

xiv. Compute the volume fraction of the cladding in the ℓ th axial region,

$$V_{e_\ell} = V_{e_\ell}^{(0)} \frac{1 + \alpha_f (\bar{T}_{f_\ell} - T^{(0)})}{1 + \alpha_e (\bar{T}_{e_\ell} - T^{(0)})}$$

xv. Compute the volume fraction of the coolant in the ℓ th axial region,

$$V_{c_\ell} = V_{c_\ell}^{(0)} \times \frac{\text{coolant area}}{(\text{coolant area})^{(0)}} \times \frac{\rho_{c_\ell}}{\rho_c^{(0)}}$$

xvi. Compute the length of axial region ℓ ,

$$\Delta z_\ell = \Delta z_\ell^{(0)} \left[1 + \alpha_f (\bar{T}_{f_\ell} - T^{(0)}) \right],$$

and the height of the axial region interface between the ℓ th and $(\ell + 1)$ th regions,

$$z_\ell = \sum_{p=1, \ell} \Delta z_p.$$

(2) Transient State

(a) Summary. A two-level implicit scheme (or Crank-Nicolson Scheme[†]) is used to compute the radial temperature profile (at any axial increment) at the end of $(k+1)$ th time increment from the knowledge of the various quantities at the end of k th increment.

The present scheme differs from the standard Crank-Nicolson Scheme in two major aspects:

i. Radial temperature profile is predicted (or extrapolated at the middle of the $(k+1)$ th time interval from the profiles at the end of $(k-1)$ th and k th time intervals. Thermal properties are evaluated for this predicted profile for use in the computation of temperatures at the end of $(k+1)$ th time interval. (See Ref. 1.) This approach is adequate to take into account the nonlinearity of the heat-conduction equations; the method does not suffer from any numerical-stability limitations.

ii. Radial increments are not made uniform. This is done primarily to consider the unequal thermal expansions in the radial increments.

The Gauss elimination procedure is used to solve the (tridiagonal) matrix equation resulting from the implicit scheme.

The method assumes the knowledge of the axial coolant temperature profile at the end of time increment $(k+1)$. This is obtained from two-phase flow module where the projected average heat flux for $(k+1)$ th interval is used to obtain the coolant temperature profile at the end of the $(k+1)$ th interval.

Thermal expansion is considered in an "open-loop" sense, in that the change in the dimensions is computed directly from the change in temperatures in any time interval. Thermal expansions may or may not be constrained. If the thermal expansions are constrained, the expansion module is used to obtain the expansions.

(b) Procedure. The coolant temperature T_c^{k+1} at the end of Δt^{k+1} and the average heat-generation rate per centimeter of axis $\bar{q}_j^{k+\frac{1}{2}}$ at the axial node j , and time interval Δt^{k+1} are assumed to be supplied by the two-phase flow and the neutronics modules.

i. Compute volumetric heat-generation rates in all radial nodes at axial node j .^{††} Subscript j is omitted in radii and temperatures.

[†]For this and other references listed in this portion of Appendix B, see references on page 187.

^{††}Interpolation might be necessary if $\bar{q}^{k+\frac{1}{2}}(z)$ is specified at a different set of axial nodes in the neutronics module.

$$q_{i,j}^{k+\frac{1}{2}} = \bar{q}_j^{k+\frac{1}{2}} \frac{(R_{i+1}^{(0)})^2 - (R_i^{(0)})^2}{(R_{N+1}^0)^2} \cdot \frac{1}{\pi(R_{i+1}^k)^2 - (R_i^k)^2}.$$

ii. Generate the following set of coupled equations for $T_{i,j}^{k+1}$ for $i = 2$ to $(N-1)$ for any $k \geq 1$:

$$\begin{aligned} \beta_{i-\frac{1}{2}}^{k+\frac{1}{2}} T_{i-1}^{k+1} + \left(\beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} + \frac{1}{\alpha_i^{k+1}} + \beta_{i-\frac{1}{2}}^{k+\frac{1}{2}} \right) T_i^{k+1} - \beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} T_{i+1}^{k+1} &= \beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} T_{i-1}^k \\ - \left(\beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} - \frac{1}{\alpha_i^{k+1}} + \beta_{i-\frac{1}{2}}^{k+\frac{1}{2}} \right) T_i^k + \beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} T_{i+1}^k + \frac{\Delta t^{k+1} q_{i,j}^{k+\frac{1}{2}}}{\alpha_i^{k+1} c \rho (T_i^{k+\frac{1}{2}})}, \end{aligned}$$

where

$$\alpha_i^{k+1} \equiv \frac{2\Delta t^{k+1}}{(r_{i+1}^k + r_i^k)(r_{i+1}^k - r_i^k) c \rho (T_i^{k+\frac{1}{2}})},$$

$$\beta_{i+\frac{1}{2}}^{k+\frac{1}{2}} \equiv \frac{K_{i+1,j}^{k+\frac{1}{2}} r_{i+1,j}^k}{r_{i+2}^k - r_i^k}, \quad k + \frac{1}{2} \text{ for } i = 2, N-2,$$

$$\beta_{1+\frac{1}{2}}^{k+\frac{1}{2}} \equiv \frac{K_{2,j}^{k+\frac{1}{2}} r_{2,j}^k}{r_3^k + r_2^k - 2r_1^k}, \quad \beta_{N-1+\frac{1}{2}}^{k+\frac{1}{2}} \equiv \frac{K_{N,j}^{k+\frac{1}{2}} r_{N,j}^k}{2R_{N+1}^k - R_N^k - R_{N-1}^k},$$

$K_i^{k+\frac{1}{2}} \equiv$ Conductivity evaluated at the temperature of the boundary between radial nodes i and $i+1$ (namely at R_{i+1}). The temperature for this calculation is obtained by extrapolating the temperatures evaluated at the end of $(k-1)$ th and k th time increments to the middle of the $(k+1)$ th time increment. The temperature at R_{i+1} is obtained by interpolating between T_i and T_{i+1} . The nonuniform aspect of the time and space increments are considered in the above extrapolation and interpolation, respectively. T_1^{k+1} is obtained separately:

$$T_1^{k+1} \equiv \frac{1}{1+C_1} \left[T_1^k (1-C_1) + \Delta t^{k+1} q_{1,j}^{k+\frac{1}{2}} + C_1 (T_2^k + T_2^{k+1}) \right],$$

where

$$C_1 \equiv \frac{2\Delta t^{k+1} K_2^{k+\frac{1}{2}} R_2^k}{c \rho (T_1^{k+\frac{1}{2}}) (R_2^k - R_1^k) (R_2^k + R_1^k) (R_2^k + R_3^k - 2R_1^k)}.$$

iii. Use the implicit method that involves a heat balance for the Nth radial segment, as suggested by Back in Ref. 2, to obtain an equation for T_N^{k+1} . This equation contains T_{N-1}^{k+1} and T_e^{k+1} .

iv. Use Back's method again to obtain an equation for T_e^{k+1} that contains T_N^{k+1} and T_c^{k+1} .

Since T_c^{k+1} is known, solve the system of equations for T_i^{k+1} for $i = 1, \dots, N$ and T_e^{k+1} by the Gauss elimination method.

v. Apply correction for melting in essentially the same way as in Ref. 3.

vi. Compute regional average temperatures, $\bar{T}_{x_\ell}$ for $x = f, e, \text{ or } c$; volume fractions V_{x_ℓ} , and free thermal expansions in essentially the same way as in parts ix-xv of the computational procedure for the steady state. For reasonably small time increments, an iteration is not considered necessary to achieve compatibility between bond-gap size and the temperature drop in the bond. A certain thermal resistance alone is used to compute the bond drop when the bond gap is essentially zero. When the gap is not zero, the contribution to the heat transfer through the bond by radiation is computed using T_N^k and T_e^k .

c. Related Programs

1. P. Greebler et al., FORE, A Computational Program for the Analysis of Fast Reactor Excursions, GEAP-4090 (Oct 1962), and Addenda No. EA-2 (Feb 1965).
2. D. F. Schoeberle, J. Heestand, and L. B. Miller, "A Method of Calculating Transient Temperatures in a Multiregion, Axisymmetric, Cylindrical Configuration." The ARGUS Program, 1089/RE248, Written in FORTRAN II, ANL-6654 (Nov 1963).

d. References

1. Milton Lees, "An Extrapolated Crank-Nicolson Difference Scheme for Quasi-Linear Parabolic Equations," Proceedings of the Symposium on Non-Linear Partial Differential Equations, Edited by W. F. Ames, Academic Press, pp. 162-176 (1966).
2. Lloyd H. Back, technical brief, p. 89, J. Heat Transfer Trans. ASME (Feb 1962).
3. P. Greebler et al., FORE, A Computational Program for the Analysis of Fast Reactor Excursions, GEAP-4090 (Oct 1962) and Addenda No. EA-2 (Feb 1965).

e. Machine Requirements

Approximately 120,000 bytes (1 byte = 8 bits in IBM 360) of direct-access memory are required. Running time for the steady-state case is approximately 2 sec per axial segment. Running time for the transient case is approximately $1/2$ sec per time step per axial segment.

The above estimates are given for 11 radial nodes in the fuel, three for the clad and one for the coolant.

f. Upper- and Lower-interface Data Modules

Upper-interface Modules

HT.DATA

Quantities Used

Number of radial nodes for fuel, N .
 Number of axial nodes for heat transfer, M .
 Number of axial regions for neutronics, ℓ .
 Number of heat transfer axial nodes in the k th neutronic axial region, N_k .
 Volume average temperature in the k th neutronic axial region for initial guess, $\bar{T}_k$.
 Reference design temperature, $T^{(0)}$.
 Radius $T^{(0)}$,
 $x = 1$ central hole
 $= f$ outer fuel surface
 $= b$ inner cladding surface
 $= c$ outer coolant boundary, $R_x^{(0)}$.
 Length of fuel cell at $T^{(0)}$, $L^{(0)}$.
 Density of fuel at $T^{(0)}$, $\rho^{(0)}$.
 Coefficient of linear expansion in the solid state of x , $x = f$ or e , α_{sx} .
 Coefficient of linear expansion in the liquid state of x , $x = f$ or e , α_{lx} .
 Fractional expansion of x during melting, $x = f$ or e , α_{x-melt} .
 Melting point of x , $x = f$ or e , T_{x-melt} .
 Latent heat of fusion of x , $x = f$ or e , U_x .
 Constant used to calculate the bond heat-transfer coefficient (see Item vii of procedure for steady state) h_{b0} .
 Maximum-bond heat-transfer coefficient, h_{b-max} .
 (Emissivity) $\times$ (Stefan-Boltzmann constant) at the bond gap, δ .

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
HT.DATA (Contd.)	Thermal conductivity of clad, K_e . Volumetric specific heat of clad, $c\rho_e$.
HT.DFRM1	Radii up to the i th radial node at the j th axial segment, $R_{i,j}$. Distance to the top surface of the j th axial segment measured from the lower end of the fuel cell, Z_j .
HT.NUT1	Heat-generation rate per centimeter length of fuel cell at the j th axial node, $\bar{q}_j$.
HT.COOL1	Coolant temperature at the j th axial node, T_{ej} . Film heat-transfer coefficient at the clad coolant interface at the j th axial segment, h_{cj} . Present time step, Δt . Void fraction of coolant at j th axial node, α_j .
HT.HT	Radii to the i th radial node at reference temperature, $R_i^{(0)}$. Radii to the i th radial node at the j th axial segment, $R_{i,j}$. Temperature profile two time steps previous, [†] $T_{1i,j}$. Temperature profile of previous time step, $T_{2i,j}$. Heat flux to the coolant at j th axial node of previous time step, [†] ϕ_j . Film heat-transfer coefficient at clad surface at j th axial node of previous time step, [†] h_{cj} . Latent heat profile for previous time step, [†] $U_{i,j}$. Radial mesh size at reference temperature, ΔR . Radial mesh size just before melting, ΔR_{melt}^- . Radial mesh size just after melting, ΔR_{melt}^+ . Total time up to the previous time step, t_p .

[†]Also used for steady state.

Upper-interface Data Modules

HT.HT (Contd.)

Quantities Used

Previous time step, Δt_p .
 Specific heat of fuel during melting,
 $C_{f,melt}$.

Lower-interface Data Modules

HT.DFRM2

Quantities Produced

Temperature profile of the present time
 step, $T_{i,j}$.
 Subscript of the liquid-solid interface at
 axial node j , I_{melt-j} .
 Fraction melted in the i th radial node at
 axial node j , $f_{i,j}$.

HT.NUT2

Volume fraction of x in k th neutron axial
 region, $V_{x,k}$, $x = f, e, \text{ or } c$.
 Volume average temperatures at the k th
 axial neutronic region, $\bar{T}_k$.
 Height of interface between neutronic
 axial regions, k and $k + 1$, Z_k .

HT.COOL2

Extrapolation coefficient for heat flux
 to coolant at the j th axial node, ϕ_{1j} .
 Heat flux to coolant at the j th axial node,
 ϕ_j .

HT.HT

Same as those in the HT.HT of the upper
 interface, except that the time step is
 advanced once.

HT.OUT

Suitable steady-state and transient quan-
 tities for printout or storage.

32. Two-phase Coolant Flow SAC004

Prepared by: D. MacFarlane

a. Nature of the Physical Problem Solved

The analysis is carried out for an infinite-slab reactor with upper and lower axial blankets and identical coolant channels. The heat-transfer and fluid-flow analysis model thus is reduced to the description of a single fuel rod and its associated coolant.

An annular flow model is used in the treatment of the two-phase fluid. This model assumes the vapor to be moving in a central core surrounded by an annulus of liquid in contact with the walls of the channel.

In addition, the following assumptions are made in the formulation of the problem:

(1) No subcooled boiling occurs, and vapor is formed only when the local bulk coolant temperature exceeds the local saturation temperature plus a specified liquid superheat.

(2) There is thermodynamic equilibrium between phases, and liquid and vapor temperatures are equal to the saturation temperature after boiling starts.

(3) The heat transfer in the boiling region is treated in a simple manner in which the heat-transfer coefficient is calculated by assuming the liquid film stays in contact with the channel wall up to a void fraction of 80 or 90%. No "burnout" heat-flux limit is imposed as is commonly done for boiling-water systems.

b. Method of Solution

(1) Hydrodynamics Equations for Two-phase Flow. The conservation equations used for the two-phase mixture are:

Continuity:

$$\frac{\partial}{\partial t} [\alpha \rho_g + (1 - \alpha) \rho_l] + \frac{\partial G}{\partial z} = 0, \quad (268)$$

Momentum:

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial z} \left[\alpha \frac{G_g^2}{\rho_g} + (1 - \alpha) \frac{G_l^2}{\rho_l} \right] + \frac{\partial p}{\partial z} + g[\alpha \rho_g + (1 - \alpha) \rho_l] + \frac{\partial \tau}{\partial z} = 0, \quad (269)$$

Energy:

$$\frac{\partial}{\partial t} [\alpha \rho_g H_g + (1 - \alpha) \rho_l H_l] + \frac{\partial}{\partial z} \{G[x H_g + (1 - x) H_l]\} = \gamma \phi(z, t), \quad (270)$$

where

α = volume fraction of vapor,

x = vapor quality = vapor flow rate/total flow rate,

ρ_g = vapor density,

ρ_l = liquid density,

$G = \alpha G_g + (1 - \alpha) G_l$ = total mass flow rate,

$\frac{\partial \tau}{\partial z}$ = frictional pressure gradient,

H_g = vapor enthalpy,

H_l = liquid enthalpy,

γ = ratio of channel perimeter to cross-sectional area,

p = pressure,

$\phi(z, t)$ = heat flux at channel wall,

and

g = acceleration of gravity.

The continuity and energy equations (Eqs. 268 and 270) are put in a more useful form for numerical solution by the following manipulations:

Performing the differentiation indicated in the first term of Eq. 268 yields

$$(\rho_g - \rho_l) \frac{\partial \alpha}{\partial t} + \frac{\partial G}{\partial z} = 0, \quad (271)$$

if the terms $\alpha(\partial \rho_g / \partial t)$ and $[(1 - \alpha)(\partial \rho_l / \partial t)]$ are neglected. This is permissible since these terms are small with respect to $[(\rho_g - \rho_l)(\partial \alpha / \partial t)]$ in a boiling-sodium system. Similarly, the energy equation can be written as

$$(\rho_g H_g - \rho_l H_l) \frac{\partial \alpha}{\partial t} + \frac{\partial G}{\partial z} (x \lambda + H_l) + G \lambda \frac{\partial x}{\partial z} = \gamma \phi(z, t), \quad (272)$$

where λ = heat of vaporization = $H_g - H_\ell$, if we assume that the terms

$$\alpha \frac{\partial}{\partial t} (\rho_g H_g)$$

and

$$(1 - \alpha) \frac{\partial}{\partial t} (\rho_\ell H_\ell),$$

can be neglected (also a reasonable assumption for a boiling-sodium system). Combining Eqs. 271 and 272 gives

$$(\lambda \rho_g + \lambda x \rho_\ell - \lambda x \rho_g) \frac{\partial \alpha}{\partial t} + G \lambda \frac{\partial x}{\partial z} = \gamma \phi(z, t).$$

Since $\rho_g \ll \rho_\ell$, this can be approximated as

$$(\rho_g + \rho_\ell x) \frac{\partial \alpha}{\partial t} + G \frac{\partial x}{\partial z} = \frac{\gamma \phi(z, t)}{\lambda}. \quad (273)$$

The momentum equation is rewritten in the following way:

The second term, representing the momentum pressure gradient, can be written in terms of the total flow rate as

$$\begin{aligned} \left[\frac{\partial p}{\partial z} \right]_{\text{mom}} &= \frac{\partial}{\partial z} \left[\alpha \frac{G^2}{\rho_g} + (1 - \alpha) \frac{G^2}{\rho_\ell} \right] \\ &= \frac{\partial}{\partial z} \left\{ \frac{G^2}{\rho_\ell} \left[\frac{\beta x^2}{\alpha} + \frac{(1 - x)^2}{1 - \alpha} \right] \right\} \end{aligned}$$

where

$$\beta = \frac{\rho_\ell}{\rho_g}.$$

Also, the static head term can be written in terms of β as

$$\left[\frac{\partial p}{\partial z} \right]_{\text{stat}} = g[\alpha \rho_g + (1 - \alpha) \rho_\ell] = g \rho_\ell \left(\frac{\alpha}{\beta} - \alpha + 1 \right).$$

Further, the friction gradient is

$$\left[\frac{\partial p}{\partial z} \right]_{fr} = \frac{\partial \tau}{\partial z} = \frac{f_{sp} G^2}{2 \rho_\ell D_h} (1-x)^{2-a} \phi_\ell^2,$$

where

$$\phi_\ell^2 = \text{two-phase friction multiplier} = f_1(X_{tt}),$$

$$X_{tt} = \text{Lockhart-Martinelli flow parameter (see Eq. 282),}$$

$$a = 0.2,$$

$$f_{sp} = \text{single-phase friction factor,}$$

and

$$D_h = \text{channel equivalent diameter.}$$

Thus, the momentum equation becomes

$$\begin{aligned} \frac{\partial G}{\partial t} + \frac{\partial}{\partial z} \left\{ \frac{G^2}{\rho_\ell} \left[\frac{\beta x^2}{\alpha} + \frac{(1-x)^2}{1-\alpha} \right] \right\} + g \rho_\ell \left(\frac{\alpha}{\beta} - \alpha + 1 \right) \\ + \frac{f_{sp} G^2}{2 \rho_\ell D_h} (1-x)^{2-a} \phi_\ell^2 + \frac{\partial p}{\partial z} = 0. \end{aligned} \quad (274)$$

Integrating Eq. 274 over the length of the channel gives

$$\begin{aligned} \int_0^L \frac{\partial G}{\partial t} dz + \frac{G^2}{\rho_\ell} v' \Big|_0^L + g \int_0^L \rho_\ell \left(\frac{\alpha}{\beta} - \alpha + 1 \right) dz \\ + \int_0^L \frac{f_{sp} G^2 (1-x)^{2-a}}{2 \rho_\ell D_h} \phi_\ell^2 dz + p \Big|_{P_0}^{P_{ex}} = 0, \end{aligned} \quad (275)$$

where

$$v' = \frac{\beta x^2}{\alpha} + \frac{(1-x)^2}{1-\alpha},$$

and

$$L = \text{channel length.}$$

In this form, the transfer of momentum across the control volume boundaries (ends of the reactor channels) is treated explicitly, while the details of momentum transfer within the channel are suppressed.

Equation 275 is then put in a form convenient for computations

$$\frac{\partial \hat{G}(t)}{\partial t} = \frac{1}{L} (\Delta p(t) - F), \quad (276)$$

where

$$\hat{G}(t) = \frac{1}{L} \int_0^L G(z, t) dz,$$

$$\Delta p(t) = P_0(t) - P_{ex},$$

and

$$F = \frac{G^2}{\rho_\ell} v' \Big|_0^L + g \int_0^L \rho_\ell \left(\frac{\alpha}{\beta} - \alpha + 1 \right) dz + \int_0^L \frac{f_{sp} G^2 (1-x)^{2-\alpha} \phi_\ell^2}{2\rho_\ell D_h} dz.$$

Thus, the time rate of change of average channel velocity, $\hat{G}(t)$, is given as the difference between the imposed channel pressure drop $\Delta p(t)$ and the three spatial integrals given by F .

(2) Equations for Single-phase Flow. The conservation equations for the single-phase fluid in the subcooled portion of the channel are readily obtained from the two-phase equations (Eqs. 268-270) by setting $\alpha = 0$. They are:

Continuity:

$$\frac{\partial \rho}{\partial t} + \frac{\partial G}{\partial z} = 0, \quad (277)$$

Momentum:

$$\frac{\partial G}{\partial t} + \frac{\partial}{\partial z} \left(\frac{G^2}{\rho} \right) + \frac{\partial p}{\partial z} + g\rho + \frac{\partial \tau}{\partial z} = 0, \quad (278)$$

Energy:

$$\frac{\partial}{\partial t} (\rho H) + \frac{\partial}{\partial z} (GH) = \gamma \phi(z, t), \quad (279)$$

Combining Eqs. 277 and 279 gives the energy equation in the form

$$\rho \frac{\partial H}{\partial t} + G \frac{\partial H}{\partial z} = \gamma \phi(z, t), \quad (280)$$

and since the liquid phase is incompressible; the continuity equation (Eq. 277) reduces to $\frac{\partial G}{\partial z} = 0$.

(3) Fuel Heat-transfer Equations. The details of the heat transfer within the fuel rod are treated in the Heat Transfer module (SAC003). The linkage between Two-phase Flow and Heat Transfer is via the heat flux at the fuel-rod surface, which is supplied in space and time to Two-phase Flow from Heat Transfer.

(4) Boundary Conditions and Equation of State for Two-phase Fluid. The boundary conditions required to complete the problem formulation are:

- i. Temperatures at $t = 0$ in the coolant are calculated from the steady-state form of Eq. 280.
- ii. Coolant temperature at the channel inlet as a function of time is assumed constant in calculations.
- iii. Channel outlet pressure as a function of time is assumed constant.
- iv. Channel inlet pressure as a function of time is constant or exponentially decreasing.

We need an expression giving the volume fraction of vapor, α , in a two-phase flow system. The experimental vapor void fraction is most frequently correlated by an expression of the form

$$\alpha = f_2(X_{tt}), \quad (281)$$

where

$$X_{tt} = \left(\frac{1-x}{x} \right)^{0.9} \left(\frac{\rho_g}{\rho_l} \right)^{0.5} \left(\frac{\mu_l}{\mu_g} \right)^{0.1}, \quad (282)$$

ρ_g = vapor density,

ρ_l = liquid density,

μ_g = vapor viscosity,

μ_l = liquid viscosity,

and the quantity X_{tt} is the Lockhart-Martinelli two-phase flow parameter.^{1†} The correlations represented by Eq. 281 include a vapor-liquid slip velocity since the slip ratio is implicit in it. Equation 281 and the assumption that the channel is completely filled with fluid either liquid or vapor, that is

$$\alpha_g + \alpha_l = 1.0,$$

fixes the fraction of the channel occupied by the liquid. Thus, Eq. 281 is used to relate the variable x and α in Eq. 273.

(5) Operation of the Computer Program. The single-phase equations are used to obtain space- and time-dependent coolant temperatures until boiling starts. The position of single-phase, two-phase interface is followed carefully after boiling starts. Each time a new coolant temperature is calculated it is compared with the saturation temperature plus a constant amount of liquid superheat (specified as program input) at that point. If the local saturation temperature plus superheat is exceeded, an interpolation is made to locate where boiling starts. A switch is then made to the two-phase equations, and the coolant temperatures are set equal to the local saturation temperature.

For the coupled two-phase continuity and energy difference equations to remain computationally stable, the interface must move through the mesh at the rate of one space node per time interval. Since the velocity of the interface is, in general, not constant, a variable time step is required. The interface velocity is determined by the relative axial gradients of the saturation and coolant temperatures at the interface. The velocity is highest when the gradients are most nearly equal, and lowest when they differ by the greatest amount. The computer program calculates these gradients at the interface, then sizes the time step so that the interface moves one space step toward the channel inlet. The saturation-temperature profile used is that for time zero and does not change during the calculation.

Equations for calculating the various temperature- and pressure-dependent coolant properties, obtained from the work of Tokar,² are built into the program.

c. Related Programs

1. R. C. Noyes et al., TRANS-FUGUE-1, A Digital Code for Transient Two-phase Flow and Heat Transfer, NAA-S12-11008 (July 25, 1965).
2. J. A. Redfield, CHIC-KIN, A FORTRAN Program for Intermediate and Fast Transients in a Water Moderated Reactor, WAPD-TM-479 (Jan 1965).

[†]For this and the other reference in this portion of Appendix B, see references listed on page 198.

d. References

1. R. W. Lockhart and R. C. Martinelli, Proposed Correlation of Data for Isothermal Two-phase, Two-component Flow in Pipes, Chemical Engineering Progress, Vol. 45, No. 1 (Jan 1949).
2. J. V. Tokar, unpublished work at Argonne National Laboratory.

e. Upper- and Lower-interface Data Modules

<u>Upper-interface Data Modules</u>	<u>Quantities Used</u>
HT.DATA	Number of axial nodes for heat transfer, N . Length of fuel cell at $T^{(0)}$, $L^{(0)}$. Radius $T^{(0)}$, $x = d$ outer cladding surface, $R_x^{(0)}$.
COOLDATA	Core coolant volume fraction, VFC . Coolant specific heat, CL . Convergence parameter for two-phase equations, $CONV$. Time step in single-phase part of calculation, $DELT$ (time step is under program control once boiling starts). Coolant flow decay parameter, $PDEC$ (for pump-coastdown cases). Coolant inlet temperature, $T0$. Channel exit pressure, PX . Coolant flow rate at time zero, $G0$. Parameters used in adjusting time-step size, $TM1$, $TM2$, $TM3$. Parameter that specifies fine space mesh overlay for two-phase flow. Calculation, $N8$. Constants in equation for calculating film heat-transfer coefficient, $C1$, $C2$, $C3$.
HT.COOL2	Heat flux to coolant at j th axial node, ϕ_j .
COOLCOOL	Coolant enthalpy profile for previous time step, $HL1_j$. Coolant average mass flow rate for previous time step, $GAV1$. Saturation temperature profile, TS_j . Two-phase vapor void fraction from previous time step, $A1_j$.

Upper-interface Data ModulesQuantities Used

COOLCOOL (Contd.)

Two-phase quality from previous time step, X_{1j} .Two-phase mass flow rate from previous time step, G_{1j} .Coolant density from previous time step, DL_{1j} .Coolant heat of vaporization from previous time step, HVA_{1j} .Pressure profile from previous time step, p_j .Lower-interface Data ModulesQuantities Produced

HT.COOL1

Coolant temperature at jth axial node, T_{ej} .Film heat-transfer coefficient at the clad coolant interface at the jth axial segment, h_{cj} .Present time step, Δt .Void fraction of coolant at jth axial node, A_{2j} .

COOL.OUT

Suitable steady-state and transient quantities for printout or storage.

33. Fuel-element Deformations . SAC007

Prepared by: C. K. Youngdahl

a. Nature of Physical Problem Solved

This module calculates the axial and radial deformations of a fuel element, given the time-dependent temperature distribution, the mechanical constraints, and the amount of fuel melted. A typical fuel element is made up initially of concentric layers, from the outside in, of cladding, bond gap, low-density fuel, full-density fuel, and central cavity. During a transient, some of the full-density fuel may melt and perhaps vaporize, while some of the low-density fuel may be compacted to full density. The elastic deformation of the full-density fuel and the elastic-plastic deformation of the cladding are calculated. Failure of the cladding as a consequence of plastic reduction in thickness is predicted. Pressure generation by vaporized fuel is introduced after other aspects of the module are functioning.

b. Method of Solution

References 1[†] and 2 contain details of the assumptions made, the mathematical analysis, and computer flow diagrams. Because of the number and complexity of the equations involved, only a verbal description is included here.

The full-density fuel and the cladding are treated as elastic solids with a switch to a plasticity analysis for the cladding when the stress level reaches the yield point. The low-density fuel is assumed to be mechanically equivalent to a compressible liquid since it can resist compression but very little tension or shear. The compressibility of melted fuel is taken into account. Temperature-dependent mechanical properties can be used whenever they are known. Rate-dependent effects are neglected, except in the criterion for cladding failure, as the solution is quasi-static.

The fuel element is divided axially into a number of segments so that only the axial average of the temperature field in each segment need be considered. Each radial layer of a segment, whether it be elastic solid, compressible liquid, or plastic solid, is essentially equivalent to a spring in that a (not necessarily linear) relationship between surface deformation and displacements can be determined. The free thermal expansion of a layer is resisted by the spring action of the other layers so deformations and stresses are balanced until equilibrium is attained. The shearing deformation induced by the relative radial expansion in adjacent segments of the full-density fuel and the cladding are accounted for by replacing the

[†]These references are listed on page 201.

shearing stress with equivalent radial boundary loads. The calculations are performed by first assuming values for these equivalent loads; new equivalent loads are computed from the resulting deformation pattern. This iteration process is repeated until it converges.

Various switchings of governing equations and boundary conditions are required in order to follow the course of the fuel deformation during a transient calculation: The initial bond gap may close, fuel may melt, low-density fuel may be compacted to become full-density fuel, and plastic yielding of the cladding may occur. The calculations for each time step are made by initially assuming the fuel is in the same condition as for the previous time interval. The testing of various inequalities determines whether this is the case; if not, the unsatisfied equations indicate which governing equations and boundary conditions are to be changed. For instance, if in the previous time step the cladding was still elastic, the calculations for the current interval are made on this basis. The circumferential stress in the cladding is then compared to the yield stress. If yielding has not occurred, the calculation stands; if it has occurred, the calculation is redone using the plasticity equations and appropriate boundary conditions to give the cladding behavior.

The plane strain elasticity solution for a tube, modified to allow for uniform axial expansion and axial constraints, is used for the elastic layers of the fuel element. The melted fuel is assumed to be linearly compressible; whatever compressive stress-deformation information is available for the low-density fuel will be incorporated in the solution. The cladding material is assumed for now to be elastic-perfectly-plastic, but strain hardening may be taken into account later. Variation of the circumferential stress across the cladding thickness is neglected. At the end of each step during which plastic flow of the cladding occurs, the deformations are partitioned into elastic and plastic components and the cladding dimensions are changed by the amount of the permanent deformation.

c. References

1. C. K. Youngdahl, Initial State Calculation for First Standard-path Fuel-element Deformation, ANL memorandum (1966).
2. C. K. Youngdahl, Analysis of Plastic Flow of Cladding for First Standard-path Fuel-element Deformation, ANL memorandum (1966).

d. Upper- and Lower-interface Data ModulesUpper-interface Data ModulesQuantities Used

DEF.DATA

Young's modulus for fuel and cladding.
 Coefficient of thermal expansion for fuel
 and cladding.
 Poisson's ratio for fuel and cladding.
 Cladding yield stress.
 Solid-fuel density.
 Liquid-fuel density.
 Liquid-fuel bulk modulus.
 Latent heat of melting for fuel.
 Cladding failure criterion.
 Fuel and cladding axial restraints.

DEF.SS

Initial radial and axial meshes.
 Initial temperature profile.

HT.DFRM2

Temperature profile in fuel pin.
 Subscript of liquid-solid interface at
 axial node j.
 Latent heat absorbed in radial node i
 at axial node j.

Lower-interface Data ModulesQuantities Produced

HT.DFRM1

Radii to the ith radial segment at the
 jth axial node.
 Distance to the top surface of the jth
 axial segment measured from the
 lower end of the fuel cell.

HT.OUT

Radial and axial deformation of fuel and
 cladding.
 Case number of axial segment j.
 Inner and outer fuel and cladding stresses.
 Permanent cladding deformation due to
 plastic flow.

APPENDIX C

ARC Data Module Glossary1. Introduction

The ARC data pool consists of a collection of structured data sets residing on any of the auxiliary storage devices attached to the computer. On the IBM System/360, each data set is a sequential file requiring full individual identification by both file and device reference number. Because closely related data are often more efficiently stored in more than one file, the phrase Data Module is used to indicate a group of one or more data sets that have the same ARC data-set name but different file numbers.

The ARC Glossary is organized by data-module names, which in general are composed of a category code followed by a delimiter. The various categories, such as Geometry, Real Flux, and External Source, are named and subdivided in the catalog of Table VIII.

TABLE VIII. Data Module Catalog

Name	Description	No. of Files	Created by	Read by
A	<u>Alphanumeric Specifications</u>			
A.BURN	Fuel cycle	1		FC1001
A.DIF1D	One-dimensional diffusion theory	1		NUC002
A.DIF2D	Two-dimensional diffusion theory	1		NUC004
A.DPLOAD	Datapool loader	1		DPLOAD
A.INPTR1	One-dimensional transport theory	1		NU1004
A.INPTR2	Two-dimensional transport theory	1		NU1005
A.NIP	General neutronics	1		NU1001, NU1002, NU1003
A.THIN	Thermal cross section	1		CSI002
A.XSSPC	Epithermal cross sections	1		CSI001
B	<u>Binary Specifications</u>			
B.HOMOG	Cross-section homogenization (Alias HOMOB)	1	NU1001 FC1001	NU1001, NUC001
B.XSSPC	Epithermal cross sections	1	CSI001	CSC001, CSC002, CSC004
BC	<u>Boundary Conditions</u>	1	NU1003	
BRN	<u>Burnup Fuel Cycle Data</u>	1	FC1001, FCC001	FCC001
ES	<u>External Source</u>			
ES.D1D	One-dimensional distributed	1	NU1003	NUC002, NUC003, NUE001, AJC001
ES.D1SH	One-dimensional shell	1	NU1003	NUC003
ES.D2D	Two-dimensional distributed	1	NU1003	NUC004, NUC005, NUE001, AJC001
ES.D2SH	Two-dimensional shell	1	NU1003	NUC005
FA	<u>Adjoint Flux</u>			
FA.D1	One-dimensional neutronics	1	NU1003, NUC002, NUC003, NUC006, NUC007	NUC002, NUC003, NUC006, NUC007, NUE001, AJC001, AJC002, AJC003
FA.D1A	One-dimensional angular	1	NU1003, NUC003	NUC003, NUE001
FA.D2	Two-dimensional neutronics	1	NU1003, NUC004, NUC005, NUC006, NUC007	NUC004, NUC005, NUC006, NUC007, NUE001, AJC001, AJC002, AJC003
FA.D2A	Two-dimensional angular	1	NU1003, NUC005	NUC005, NUE001
FR	<u>Real Flux</u>			
FR.D0	Fundamental mode--NIG ^a		CSC002	CSC004
FR.D1	One-dimensional neutronics	1	NU1003, NUC002, NUC003, NUC006, NUC007	NUC002, NUC003, NUC006, NUC007, NUE001, AJC001, AJC002, AJC003

TABLE VIII (Contd.)

Name	Description	No. of Files	Created by	Read by
FR (Contd.)	<u>Real Flux</u>			
FR.D1A	One-dimensional angular	1	NU1003, NUC003	NUC003, NUE001
FR.D2	Two-dimensional neutronics	1	NU1003, NUC004, NUC005, NUC006, NUC007	NUC004, NUC005, NUC006, NUC007, NUE001, AJC001, AJC002, AJC003
FR.D2A	Two-dimensional angular	1	NU1003, NUC005	NUC005, NUE001
FR.PN	Power-normalized regional	1	NUE001	FCC001
FSA	<u>Adjoint Fission Source</u>			
FSA.D1	One-dimensional	1	NU1003, NUC003	NUC003, NUE001, AJC001
FSA.D2	Two-dimensional	1	NU1003, NUC005	NUC005, NUE001, AJC001
FSR	<u>Real Fission Source</u>			
FSR.D1	One-dimensional	1	NU1003, NUC003	NUC003, NUE001, AJC001
FSR.D2	Two-dimensional	1	NU1003, NUC005	NUC005, NUE001, AJC001
GEOM	<u>Geometry Specifications</u>	1	NU1002, NUC003, NUC005, NUC006, NUC007, NUC008	NU1003, NU1004, NU1005, NUC002, NUC003, NUC004, NUC005, NUC006, NUC007, NUC008, NUE001, AJC001, AJC002, AJC003
HOMOB	Alias of B.HOMOG	1	FC1001	NU1001, NUC001
OUT	<u>Output</u>			
OUT.NI	Neutron inventory--NIG ^a		AJ1001, AJC001	AJC001
OUT.NM	Neutron manipulation specifications and data	3	NU1003, NUE001	NUE001
OUT.NMS	Special neutronics manipulations specifications	1	NU1003, FCC001	NUE001, FCC001
OUT.TR1	One-dimensional transport collected data	1	NUC003	
OUT.TR2	Two-dimensional transport collected data	1	NUC005	
PT	<u>Perturbation</u>			
PT.DIN	Diffusion-theory input--NIG ^a		AJ1002	AJC002
PT.DOUT	Diffusion-theory output--NIG ^a		AJC002	AJC002
PT.TIN	Transport-theory input--NIG ^a		AJ1003	AJC003
PT.D1.TR	One-dimensional transport output--NIG ^a		AJC003	
PT.D2.TR	Two-dimensional transport output--NIG ^a		AJC003	
SCR001	Scratch Data, Temporary Use--NIG ^a	1	NUC001	NUC001
SCR002		1	NUC001	NUC001
SP	<u>Specifications</u>			
SP.CICN	Code-independent constants	1	NU1003	NU1004, NU1005, NUC002, NUC003, NUC004, NUC005, NUE001, AJC001
SP.CRIT	Criticality search	1	NU1003	NUC003, NUC005, NUC008
SP.T1NEW	One-dimensional transport	2	NU1004	NUC003
SP.T1OLD	Alias of SP.T1NEW			NU1004
SP.T2NEW	Two-dimensional transport	2	NU1005	NUC005
SP.T2OLD	Alias of SP.T2NEW			NU1005
XS	<u>Cross Sections</u>			
XS.C.ANI	Anisotropic, composition level	2	NUC001	NU1005, NU1007, NUC001, NUC003, NUC005, NUE001
XS.C.AUX	Auxiliary (capture and scattering), composition level	2	NUC001	NUC001, AJC001, AJC003
XS.C.MIN	Minimal $(\chi, \Sigma_a, \Sigma_{tot}, \Sigma_{rem}, \Sigma_{tr}, \Sigma_f, \Sigma_{f \rightarrow k}, \Sigma_{scat})$, composition level	2	NUC001	NU1001, NU1005, NU1007, All NUC modules, NUE001
XS.C.RES	Resolved resonance, composition level	1	CSC001	CSC002
XS.C.SMT	Smooth, composition level--NIG ^a		CSC002	CSC004
XS.C.UFG	Ultrafine group, composition level--NIG ^a		CSC002	CSC004
XS.I.RES	Resolved resonance, isotope level	1	CSC001	CSC004
XS.I.UFG	Ultrafine group, isotope level--NIG ^a		CSC002	CSC004
XS.INSCT	Inelastic scattering--NIG ^a		CSC002	CSC004
XS.ISO	Isotope standard set	2	CSC004	NU1001
XS.ISO2	Alias of XS.ISO (a subset of required isotopes)	2	NU1001	NUC001
XS.M.ANI	Anisotropic, material level	1	NUC001	NU1005, NU1007, NUC001, NUC003, NUC005, NUE001, AJC001
XS.M.AUX	Auxiliary (capture and scattering), material level	1	NUC001	NUC001, AJC001, AJC003
XS.M.MIN	Minimal $(\chi, \Sigma_a, \Sigma_{tot}, \Sigma_{rem}, \Sigma_{tr}, \Sigma_f, \Sigma_{f \rightarrow k}, \Sigma_{scat})$, material level	1	NUC001	NU1005, NU1007
XS.SCRCH	Scratch data, temporary use--NIG ^a		CSC004	CSC004
XS.SCR1			CSC004	CSC004
XS.SCR2			CSC004	CSC004
XS.SCR3			CSC004	CSC004
XS.SHPE	Shape function--NIG ^a		CSC002	CSC004
XS.SORS	Source data--NIG ^a		CSC002	CSC004
XS.THERM	Thermal group	1	CS1002	CSC002
XS.UNRES	Unresolved resonance data	1	CSC001	CSC002

^aNIG: Not Included in Glossary.

Each data module listed in the catalog has one or more pages allotted to it in the glossary. On the page for a given module are its eight-character name, a concise description of its contents, a list of the modules that currently reference the given module, and notation of any deviations from the standards established for the ARC data-set organization. This is followed by a structured list of all the data in the set, normally one complete data array (or several arrays that are normally used together), along with the variables necessary to describe the array. The contents of the list are given record by record. Each piece of data has a descriptive FORTRAN name (which implies its data type) along with a definition. All exceptions to the assumptions about data organization and type are explicitly noted.

Figure 9 describes the general format for an entry in the data module glossary.

a. Data Module Name

Eight characters, including embedded periods. The names of BCD (card image) data modules must begin with the characters "A."

b. Description

A short title of several words.

c. Specifications

A data module is a specified collection of a fixed number of data sets, normally one. These standard specifications are assumed:

1. A data set is an ordered collection of records stored on a peripheral device as a single file or sequence.
2. Access to the records of a data set is sequential only, as opposed to random or direct access.
3. A data set exists in the same structure on all types of peripheral storage devices that are sequentially organizable, and can be freely moved or copied from one such device to another.
4. Only one generation of a data set exists at a given time.
5. Each data set is self-descriptive; i.e., the information in the data module glossary for each set alone enables a programmer to write a program to read the data set.
6. FORTRAN naming conventions are followed, but with both integers and floating-point variables assumed to be double-precision quantities (32 and 64 bits, respectively).

Additions to or deviations from these standard specifications are noted here.

Details of space and device requirements are noted whenever known.

d. Program Modules That Create (C) or Read (R) the Data Set

(C) (R) Program Module Name

e. Structure and Content

This is a list of record types comprising the data module and its structure in terms of these record types. In some of the more complex data sets, certain records are grouped together to form blocks and the module is described in terms of these blocks. For ease of notation, the record types are numbered and blocks, if used, are given names. Files are numbered and clearly delineated if used.

Each record of a data set corresponds to one READ statement; the list of contents of a record given here corresponds directly to the list in the program READ statement. If a record within a set is of variable length or appears only conditionally, its length and the quantities determining the conditions of its appearance are given in previous records of the module.

Fig. 9. Format for Data Module Glossary

The data-module names used in the glossary are linked by the operating system routine SNIFF to the reference numbers used in the read/write statements of program modules. Since different paths may use very different data module combinations, the linkage is uniquely a function of the path. When particular sets of data are cataloged on the S/360 at run time, they are given the prefix ARC and a suffix. The catalog reference to data module NAME is ARC.NAME.RII, where RII is a unique Run Identification Index. The actual stored data comprising the data module conform in format to the glossary specifications for data module NAME.

Alphanumeric data modules are special in that they exist initially as a deck of input cards. An ARC system utility program, BCDDS, reads these cards, performs some sorting and counting, and outputs an image of the data set on a direct access device. This data module is read by an ARC input module. Each alphanumeric data module has a name beginning with the character "A." and conforms to the following additional standards:

1. Columns 1-6 are reserved for ARC systematic counting and sorting.
2. Columns 73-80 are available for use by the user at his discretion.
3. Columns 7-72 contain module-determined input data.
 - a. All data fields terminate on columns that are multiples of 6.
 - i. Integer data is in I6 format.
 - ii. Floating-point data is in E12 format.
 - iii. Alphanumeric data will use spaces to force multiples of 6 boundaries but are not otherwise restricted.
 - b. Option choices are designated numerically, rather than by the marking of a specific column.
 - c. Columns 7-12 may or may not be used, depending upon the requirements of the module involved.

Portions of the glossary that are firmly established follow.

2. Data Module A.BURNa. Data Module Name

A.BURN.

b. Description

General input for fuel-cycle modules.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	FCI001 Fuel-cycle Specifications

e. Structure and Content

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below:

<u>Card Type</u>	<u>Description</u>
<u>01</u>	Title (I2,4X,11A6) As many Type <u>01</u> cards may be used as are necessary.
<u>02</u>	Input Processing Specifications (reserved for future definitions, to allow such nonstandard options as binary-BCD data merges, additional generations, requests to ignore certain input types, etc.)
<u>03</u>	Problem Definition Data (I2,10X,I6,3E12.5,2I6)
	Cols. 13-18 Type of problem.
	0 Equilibrium.
	1 Nonequilibrium.
	Cols. 19-24 Search procedure.
	0 Given burnup limit and unpoisoned k_{eff} at a specified fraction of the burn time. Find the burn time that satisfies the burnup limit as well as the reactor charge enrichment for which the specified k_{eff} is met.
	1 Given burn time and unpoisoned k_{eff} at a specified fraction of the burn time. Find the fuel charge enrichment for which the specified k_{eff} is met.

Card
Type

Description

03

(Contd.)

- 2 Given unpoisoned k_{eff} at the start and end of the burn time. Find the fuel-charge enrichment for which the initial k_{eff} is met and the burn time at which the final k_{eff} is reached.

Cols. 25-36 Burn-time guess (days) if the search procedure (Cols. 13-18) is 0 or 2. Specified burn time if search procedure is 1.

Cols. 37-48 Convergence criterion: relative error allowable in burnup (see Card Type 08).

Cols. 49-60 Total reactor power (watts).

Cols. 61-66 Number of subintervals into which the burn time is to be divided.

Cols. 67-72 Number of burn steps to be completed with the problem as defined (nonequilibrium case only). Problem will be edited and dumped before termination.

An equilibrium problem is defined as one in which the user wishes to find the operating conditions of the system after an infinite number of burn/discharge/fuel steps with the fixed reactor conditions as defined. A nonequilibrium problem is one in which the burn/refuel steps are computed successively with the given parameters and constraints. It may represent an approach to equilibrium with the conditions fixed as specified.

The total burn time of a single step is divided into a number of subintervals, as given in Cols. 61-66 of this card. Core flux distributions will be computed at the end of each interval, and if control-rod mockup materials are present, the appropriate control searches will be carried out to maintain $k_{eff} = 1.0$ at these end points. Burn-up matrix elements will be computed from linear averages of the start and end values over each subinterval. These averages will be used in computing the isotopic changes over the subinterval.

04

Charge Enrichment/Criticality Data (I2,10X,5E12.5)

Cols. 13-24 Desired unpoisoned k_{eff_0} .

Cols. 25-36 Allowable relative error in k_{eff_0} , ϵ_k , during charge-enrichment searches.

Card
Type

Description

04

(Contd.)

Cols. 37-48 Fraction of burn time at which k_{eff_0} is to be reached. This must be one of the end points of a subinterval of the burn step.

Cols. 49-60 Reactor charge-enrichment search parameter, X.

Cols. 61-72 Derivative of charge-enrichment search parameter with respect to k_{eff} . If no value is entered, 1.0 is assumed.

The enrichment of a batch of fresh fuel to be loaded in material m is adjusted according to the formula

$$e_m = e_m(0)(1 + X \delta_m),$$

where X is the charge-enrichment search parameter whose initial value is given in Cols. 49-60. The $e_m(0)$ and δ_m for each material are specified on Card Type 13.

In the following cards, a "label" will be identified from the card type (e.g., Card Type 24 indicates that external feed data are to follow). A label is defined as a six-character identifier that references the specific operations or data that follow. For example, a material-stage label identifies macroscopic cross sections made up of given atom densities of several isotopes as listed on the card.

The isotope labeling system allows different library labels (i.e., different microscopic cross sections) to be used in different fuel batches. The internal, or run-time, labels for "active" isotopes (those that are included in the transmutation matrix) are defined in the specification of the isotopic chain (Card Type 09). These run-time labels may coincide with the library labels for all materials, in which case no further input is required. The user may, however, specify (see Card Type 27) that a library isotope label (which defines appropriate cross sections for some fuel batch) is equivalent to one of those specified on Card Type 09. All library isotopes that are equivalenced to one of these run-time labels are considered identical in the external cycle. Appropriate microscopic cross sections for the fresh charge batches are selected through the Chemical Composition Data on Card Type 16. Active isotope labels appearing on card types other than 16 or 27 must be those that appear in Cols. 7-12 of the Type 09 cards.

Card Type	Description	
<u>05</u>	Burnup Test Specifications (I2,4X,11A6)	
Cols. 7-12	Label of burnup test group (repeated on additional cards).	
Cols. 13-18	}	Material label (see Card Type <u>13</u>) to be included in test group.
19-24		
25-30		
31-36		
37-42		
43-48		
49-54		
55-60		
61-66		
67-72		
<u>06</u>	Burnup Limits (I2,10X,3(A6,E12.5))	
Cols. 13-18	Test group or material label.	
Cols. 19-30	Burnup limit: ratio of total atoms destroyed in fission to total accountable atoms present initially. Unless specified otherwise (see Card Types <u>07</u> and <u>08</u>), the numerator includes all fission events, and the denominator includes all fissionable atoms present at the start of the burn.	
Cols. 31-36	Test group or material label.	
Cols. 37-48	Burnup limit.	
Cols. 49-54	Test group or material label.	
Cols. 55-66	Burnup limit.	
<u>07</u>	Burnup Numerator Definition (I2,4X,11A6)	
Cols. 7-12	Material label (repeated on additional cards).	
Cols. 13-18	}	Label of fissionable isotope to be included in numerator of burnup expression for the specified material. (Note: This is a label from Cols. 7-12 of the active chain specified on Card Type <u>09</u> .)
19-24		
25-30		

Card
Type

Description

07 (Contd.)

Cols. 31-36

37-42

43-48

49-54

55-60

61-66

67-72

Same as previous page in Cols. 13-30.

If this card is present, only fission reactions of isotopes appearing in this list contribute toward "burnup" of the material.

08 Burnup Denominator Definition (I2,4X,11A6)

Cols. 7-12 Material label (repeated on additional cards).

Cols. 13-18

19-24

25-30

31-36

37-42

43-48

49-54

55-60

61-66

67-72

Label of active isotope to be included in denominator of burnup expression for the specified material.

(Note: This is a label from Cols. 7-12 of the active chain specified on Card Type 09.)

For any atom vector at time t , the burnup is defined as the quotient of the sum over specified isotopes of the total fission reactions in each isotope from time zero to time t , divided by the sum over specified isotopes of the total atoms present at time zero. (Time zero in this context is the time at which the fuel charge was loaded into the core.) Unless Card Types 07 and/or 08 are present, these sums are taken over all isotopes undergoing fission.

Card
Type

Description

Atom vectors of several materials can be collected into a single test group (Card Type 05) for which an average burnup is computed. A burnup limit may be given on Card Type 06 for test groups specified on Card Type 05, on materials individually. If no burnup limit is given, no burnup test is made for that material or test group.

We define the relative burnup error as the value of the difference between allowable and achieved burnup relative to the allowable burnup for each material or test group. Then burn time will be adjusted until the smallest value of this difference becomes zero within the convergence limit on Card Type 03, Cols. 31-42.

$$\text{That is, } \min_m \left(\frac{\text{burnup allowed} - \text{burnup achieved}}{\text{burnup allowed}} \right)_m = 0 \pm \epsilon.$$

This will be the smallest time at which some material or test group has a burnup error of $\pm\epsilon$.

09 Isotopic Chain Data (I2,4X,A6,I6,3(A6,E12.5))

Cols. 7-12 Label of isotope undergoing reaction (repeated on all cards that specify other reactions for this isotope).

Cols. 13-18 Reaction type (repeated on additional cards).

0 No reaction.

1 (n, γ) reaction.

2 (n,f) reaction.

3 (n,p) reaction.

4 (n, α) reaction.

5 (n,2n) reaction.

6 β^- decay.

7 β^+ decay.

8 α decay.

Cols. 19-24 Label of product isotope from the reaction specified in Cols. 13-18.

Cols. 25-36 Yield fraction or isomeric state branching fraction to the isotope specified in Cols. 19-24.

Cols. 37-42 Label of product isotope from the reaction specified in Cols. 13-18.

Card Type	Description
<u>09</u> (Contd.)	
Cols. 43-54	Yield fraction or isomeric-state branching fraction to the isotope specified in Cols. 37-42.
Cols. 55-60	Label of product isotope from the reaction specified in Cols. 13-18.
Cols. 61-72	Yield fraction or isomeric-state branching fraction to the isotope specified in Cols. 37-42.
<p>All isotope labels appearing in Cols. 7-12 of one or more Type <u>09</u> cards are defined as "active"; that is, they are considered in burnup/decay calculations. All other isotopes are "inactive"; that is, they are assumed to undergo no reactions during the problem.</p> <p>If no Type <u>27</u> cards are given, the isotope labels on the Type <u>09</u> cards in Cols. 7-12 must be defined in the cross-section library. If any Type <u>27</u> cards are given, the labels on the <u>09</u> cards may be local; the Type <u>27</u> cards will relate the local labels to specific cross-section library labels. If the first product-isotope label (Cols. 19-24) is blank, it implies a yield or branching fraction of 1.0. This further implies that the product isotope is to be identified from the proton and mass numbers (Z,A) of the parent isotope (as given in the cross-section library), modified by the specified reaction. For fission reactions (n,f), at least one product-isotope label must be given (no linkage through A and Z is possible). If only one product isotope is named in Cols. 19-24 for any reaction, no yield fraction need be entered (1.0 is assumed). If more than one product isotope is listed, the yield fractions must be given for each.</p> <p>If the product-isotope label fields are nonblank, each label must be entered in Cols. 7-12 of one Type <u>09</u> card.</p> <p>All isotopes undergoing the (n,f) reaction are included in the calculation of burnup unless Type <u>07</u> or <u>08</u> cards are given. In that case, only the isotopes listed on <u>07</u> or <u>08</u> cards will be counted in the burnup calculation.</p>	
<u>10</u>	Mixture Data (I2,4X,A6,6X,3(A6,E12.5))
Cols. 7-12	Mixture label (repeated on additional cards).
Cols. 19-24	Isotope or mixture label.
Cols. 25-36	Atom density (atoms/cc $\times 10^{-24}$) or volume fraction.

Card Type	Description
<u>10</u> (Contd.)	
Cols. 37-42	Isotope or mixture label.
Cols. 43-54	Atom density or volume fraction.
Cols. 55-60	Isotope or mixture label.
Cols. 61-72	Atom density or volume fraction.
	A mixture (Cols. 7-12) may consist of any number of isotopes and/or other mixtures, defined on a Type <u>10</u> card. Inactive-isotope labels specified must correspond to labels contained in the cross-section library; active-isotope labels must correspond to those named on Card Type <u>09</u> . A mixture containing any isotope named on a Card Type <u>09</u> (the so-called active isotopes) is known as an active mixture.
<u>11</u>	Material-Stage Specifications (I2,4X,A6,2E12.5)
Cols. 7-12	Material-stage label.
Cols. 13-24	Volume of material-stage, cm ³ .
Cols. 25-36	Fraction of volume of material-stage which consists of active isotopes.
	A material-stage is defined as a batch of fuel that is charged into the reactor at a particular time. It may reside in the core over several burn steps, but cannot be subdivided during the time it remains in the core. It may be moved from one spatial region to another between burn steps, or may remain in the same region. The movements are specified on Card Type <u>14</u> .
<u>12</u>	Material-Stage Data (I2,4X,A6,6X,3(A6,E12.5))
Cols. 7-12	Material-stage label (repeated on additional cards).
Cols. 19-24	Mixture label.
Cols. 25-36	Volume fraction.
Cols. 37-42	Mixture label.
Cols. 43-54	Volume fraction.
Cols. 55-60	Mixture label.
Cols. 61-72	Volume fraction.

Card
Type

Description

If the mixture list for a material-stage contains a label that is undefined in the mixture list on Card Type 10, this label is assumed to appear in the reactor-charge list (on Card Type 15); in this case, it must be the only active mixture in the material-stage. Alternatively, a material-stage may be completely specified on Type 12 cards. It need not contain any active mixtures.

13 Material Specifications (I2,4X,3A6,2E12.5)

- Cols. 7-12 Material label.
- Cols. 13-18 Reactor-charge label. (See Card Type 15.)
- Cols. 19-24 Reactor-discharge label. (See Card Type 17.)
- Cols. 25-36 Initial reactor-charge enrichment, $e_m(0)$.
(See Card Type 04.)
- Cols. 37-48 Reactor-charge enrichment modification factor, δ_m ,
for charge enrichment searches. (See Card Type 04.)
(Default value 1.0.)

A material is defined as a collection of material-stages which follow the same path (Card Type 14) through the core. The charge label defines the origin and composition of fresh batches of fuel. The discharge label determines the place of disposal of the last material-stage of the path.

14 In-core Path Specifications (I2,4X,A6,3(A6,I6,A6))

- Cols. 7-12 Material label (repeated on additional cards).
- Cols. 13-18 Material-stage label.
- Cols. 19-24 Stage number.
- Cols. 25-30 Region label.
- Cols. 31-36 Material-stage label.
- Cols. 37-42 Stage number.
- Cols. 43-48 Region label.
- Cols. 49-54 Material-stage label.
- Cols. 55-60 Stage number.
- Cols. 61-66 Region label.

Card
Type

Description

A path defines the spatial positions and motions of fuel in the core. The fresh batch of fuel charged at a particular time is placed in the region specified as Stage 1 for that material. After one burn step (unless the management pattern is changed by an interrupt), this partially burned material-stage moves to the second specified region (which may or may not be the same as the first). The last material-stage is discharged to the destination specified on Card Type 13 (Cols. 19-24). Therefore, after one burn step, the material-stage label specified in the input as being at a particular stage number and region will be located in the region initially specified for the next-higher-numbered material-stage. For equilibrium problems, or non-equilibrium problems with uniform initial loadings, the material-stage label will be the same for the entire path.

The path definition must be such that the total volume of all material-stages that appear in a spatial region at any time equals the volume of the region.

15 Reactor-charge Specifications (I2,4X,2A6,2E12.5)

Cols. 7-12 Reactor-charge label.

Cols. 13-18 Chemical-composition label. (See Card Type 16.)

Cols. 19-30 Refabrication time, days.

Cols. 31-42 Storage time, days.

16 Chemical Composition Data (I2,4X,A6,6X,3(A6,E12.5))

Cols. 7-12 Chemical-composition label.

Cols. 19-24 Active-isotope label.

Cols. 25-36 Full atomic density (atoms/cc $\times 10^{-24}$).

Cols. 37-42 Active-isotope label.

Cols. 43-54 Full atomic density (atoms/cc $\times 10^{-24}$).

Cols. 55-60 Active-isotope label.

Cols. 61-72 Full atomic density (atoms/cc $\times 10^{-24}$).

Active isotopes specified here must appear in the library; they may or may not be named on a Type 09 card. Full atomic density means the number of atoms of the pure isotope per unit volume in the given chemical combination and state (e.g., oxide at some percentage of theoretical density).

Card Type	Description
<u>17</u>	Reactor-discharge Cooling Times (I2,4X,3(A6,E12.5))
	Cols. 7-12 Reactor-discharge label.
	Cols. 13-24 Cooling time, days.
	Cols. 25-30 Reactor-discharge label.
	Cols. 31-42 Cooling time, days.
	Cols. 43-48 Reactor-discharge label.
	Cols. 49-60 Cooling time, days.
<u>18</u>	Reactor-discharge Destination Data (I2,4X,A6,6X,3(A6,E12.5))
	Cols. 7-12 Reactor-discharge label (repeated on additional cards).
	Cols. 19-24 Reprocessing-plant label.
	Cols. 25-36 Fraction of discharge to be delivered to reprocessing plant.
	Cols. 37-42 Reprocessing-plant label.
	Cols. 43-54 Fraction of discharge to be delivered to reprocessing plant.
	Cols. 55-60 Reprocessing-plant label.
	Cols. 61-72 Fraction of discharge to be delivered to reprocessing plant.
	All reactor discharge not delivered to some reprocessing plant will be sold.
<u>19</u>	Reprocessing-plant Specifications (I2,4X,3A6,2E12.5)
	Cols. 7-12 Reprocessing-plant label.
	Cols. 13-18 Recovery-factor specification label.
	Cols. 19-24 Class-separation specification label.
	Cols. 25-36 Reprocessing time, days.
	Cols. 37-48 Volume of reprocessing plant output (cm ³).
	Cols. 37-48 are pertinent only if Card Type <u>26</u> is provided.
<u>20</u>	Recovery-factor Data (I2,4X,A6,6X,3(A6,E12.5))
	Cols. 7-12 Recovery-factor specification label (repeated on additional cards).

Card Type	Description
<u>20</u> (Contd.)	
Cols. 19-24	Active-isotope label.
Cols. 25-36	Recovery fraction.
Cols. 37-42	Active-isotope label.
Cols. 43-54	Recovery fraction.
Cols. 55-60	Active-isotope label.
Cols. 61-72	Recovery fraction.
	All isotope labels must be defined on Type <u>09</u> cards.
<u>21</u> Class-separation Data (I2,4X,A6,6X,3(A6,E12.5))	
Cols. 7-12	Class-separation specification label (repeated on additional cards).
Cols. 19-24	Active-isotope label.
Cols. 25-36	Fraction of isotope assigned to Class 1 fuel.
Cols. 37-42	Active-isotope label.
Cols. 43-54	Fraction of isotope assigned to Class 1 fuel.
Cols. 55-60	Active-isotope label.
Cols. 61-72	Fraction of isotope assigned to Class 1 fuel.
	All isotope labels must be defined on Type <u>09</u> cards.
	Class 1 fuel is normally considered to be fuel that adds greater reactivity to the reactor than does Class 2 fuel. The complements of the fractions given in Cols. 25-36, 43-54, and 61-72 are the fractions assigned to Class 2 fuel.
	Any active isotope specified on Card Type <u>09</u> that is not given on Card Type <u>21</u> will have a fraction 0 assigned to Class 1 fuel.
<u>22</u> Class 1 Fabrication Specifications (I2,4X,A6,6X,2(A6,I6,E12.5))	
Cols. 7-12	Reactor-charge label or sale label (repeated on additional cards).
Cols. 19-24	Reprocessing-plant label or external-feed label.
Cols. 25-30	Priority level.

Card Type	Description
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22 (Contd.)

- Cols. 31-42 Distribution fraction (default 1.0).
- Cols. 43-48 Reprocessing-plant label or external-feed label.
- Cols. 49-54 Priority level.
- Cols. 55-66 Distribution fraction (default 1.0).

The priority level establishes the order of preference for use of reprocessing-plant output or external-feed atoms in fabrication of the various batches of the reactor charge. The most straightforward system is one in which only one batch (specified by the charge label) requires atoms from a given plant or feed at each priority level. In this case all atoms required for the batch with priority 1 will be taken first, then those required for priority 2 (if any remain), and so on.

If two or more charges specify the same plant output or feed at the same priority level, the available atoms will first be distributed in proportion to the distribution fraction of each charge. If the requirements of some of these batches are satisfied while others are not, further proportional distributions are made to the remaining batches until either all requirements are satisfied or all available atoms are used.

23 Class 2 Fabrication Specifications (I2,4X,A6,6X,2(A6,I6,E12.5))

- Cols. 7-12 Reactor-charge label or sale label (repeated on additional cards).
- Cols. 19-24 Reprocessing-plant label or external-feed label.
- Cols. 25-30 Priority level.
- Cols. 31-42 Distribution fraction (default 1.0).
- Cols. 43-48 Reprocessing-plant label or external-feed label.
- Cols. 49-54 Priority level.
- Cols. 55-66 Distribution fraction (default 1.0).

The priority system is identical to that described above for Class 1 makeup.

Card Type	Description
<u>24</u>	External-feed Specifications (I2,4X,2A6,E12.5)
	Cols. 7-12 External-feed label.
	Cols. 13-18 Class-separation specification label.
	Cols. 19-30 Volume of feed (cm ³).
	The volume of one of the external feeds must be large to ensure that there will always be enough fuel to fabricate all charges. An infinite volume will be assigned to the feed if Cols. 19-30 are blank.
<u>25</u>	External-feed Composition (I2,4X,A6,6X,3(A6,E12.5))
	Cols. 7-12 External-feed label (repeated on additional cards).
	Cols. 19-24 Isotope label.
	Cols. 25-36 Atomic density (atoms/cc x 10 ⁻²⁴).
	Cols. 36-42 Isotope label.
	Cols. 43-54 Atomic density (atoms/cc x 10 ⁻²⁴).
	Cols. 55-60 Isotope label.
	Cols. 61-72 Atomic density (atoms/cc x 10 ⁻²⁴).
<u>26</u>	Reprocessing-plant Output Initial Composition (I2,4X,A6,3(A6,E12.5))
	Cols. 7-12 Reprocessing-plant label (repeated on additional cards).
	Cols. 19-24 Isotope label.
	Cols. 25-36 Atomic density (atoms/cc x 10 ⁻²⁴).
	Cols. 37-42 Isotope label.
	Cols. 43-54 Atomic density (atoms/cc x 10 ⁻²⁴).
	Cols. 55-60 Isotope label.
	Cols. 61-72 Atomic density (atoms/cc x 10 ⁻²⁴).

All isotope labels must be defined on Type 09 cards.

Card Type 26 is provided only if it is desired to specify the composition of the reprocessing-plant output storage at the start of the problem. If Card Type 26 is given, Cols. 37-48 on Card Type 19 must specify the volume of the processing-plant output.

Card Type	Description
<u>27</u>	Active Isotope-label Equivalence List (I2,4X,11A6)
Cols. 7-12	Local isotope label from Cols. 7-12 of Type <u>09</u> cards (repeated, if necessary, on additional cards).
Cols. 13-18	Library isotope label to be equivalenced to the local label in Cols. 7-12.
Cols. 19-24	
Cols. 25-30	
Cols. 31-36	
Cols. 37-42	
Cols. 43-48	
Cols. 49-54	
Cols. 55-60	
Cols. 61-66	
Cols. 67-72	

Card Type 27 is required only if different library isotope labels (i.e., different microscopic cross sections) are required for the same isotope in different materials. See discussion of Card Type 04.

3. Data Module A.DIF1Da. Data Module Name

A.DIF1D.

b. Description

Module-dependent input for 1D-Diffusion.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUC002 1D-Diffusion

e. Structure and Content

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below. All cards are required. Blank fields produce the default options noted in parentheses.

Card
Type

Description

01 (I2X,10A6) Problem Title Card01 (I2,10X,4I6)

Cols. 13-18 Kinetics options (0).

0 Not desired.

1 Use Option 1.

2 Use Option 2.

Cols. 19-24 Debugging print option (0).

0 No printout.

1 Standard full printout.

2 Debugging dumps printout.

3 Full debugging printout.

Card Type	Description
<u>01</u>	(Contd.)
Cols. 25-30	Maximum number of upscatter iterations (0).
Cols. 31-36	Output option.
0	No output edit.
1	Output edit.
<u>02</u>	(I2,10X,2E12.5)
Cols. 13-24	Convergence criterion for upscatter iterations (0).
Cols. 25-36	Flux normalization factor for burnup.
<u>03</u>	(I2,10X,6I6)
Cols. 13-18	Maximum number of outer iterations (10000).
Cols. 19-24	Extrapolation option (1).
0	No extrapolation.
1	Chebyshev extrapolation.
2	Overrelaxation (source calculations only).
Cols. 25-30	Number of unextrapolated outer iterations before extrapolating (5).
Cols. 31-36	Number of extrapolated outer iterations before testing for extrapolation payoff (3).
Cols. 37-42	Maximum number of extrapolated outer iterations in an extrapolated sequence (8).
Cols. 43-48	Number of unextrapolated outer iterations between extrapolation sequences (3).
<u>04</u>	(I2,10X,4E12.5)
Cols. 13-24	Outer-iteration convergence criterion on the sum of the absolute value of flux differences (10^{-5}).
Cols. 25-36	Outer-iteration convergence criterion on the difference of the flux bounds (10^{-5}).
Cols. 37-48	Outer-iteration convergence criterion on the difference in k_{eff} (10^{-5}).
Cols. 49-60	Interval shift factor when applying Chebyshev extrapolation to outer iterations (0).

4. Data Module A.DIF2Da. Data Module Name

A.DIF2D.

b. Description

Module-dependent input for 2D-Diffusion.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUC004 2D-Diffusion

e. Structure and Content

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below. All cards are required. Blank fields produce the default values noted in parentheses.

Card
Type

Description

01 (I2X,10A6) Problem Title Card01 (I2,10X,4I6)

Cols. 13-18 Kinetics option (0).

0 Not desired.

1 Use Option 1.

2 Use Option 2.

Cols. 19-24 Debugging print option (0).

0 No printout.

1 Standard full printout.

2 Debugging dumps printout.

3 Fuel debugging printout.

Card Type	Description
<u>01</u> (Contd.)	
Cols. 25-30	Maximum number of upscatter iterations (0).
Cols. 31-36	Output option.
0	No output edit.
1	Output edit.
<u>02</u> (I2,10X,2E12.5)	
Cols. 13-24	Convergence criterion for upscatter iterations (0).
Cols. 25-36	Flux normalization factor for burnup.
<u>03</u> (I2,10X,6I6)	
Cols. 13-18	Maximum number of outer iterations (10000).
Cols. 19-24	Extrapolation option (0).
0	No extrapolation.
1	Chebyshev extrapolation.
2	Overrelaxation (source calculation only).
Cols. 25-30	Number of unextrapolated outer iterations before extrapolation (5).
Cols. 31-36	Number of extrapolated outer iterations before testing for extrapolation payoff (3).
Cols. 37-42	Maximum number of extrapolated outer iterations in an extrapolation sequence (8).
Cols. 43-48	Number of unextrapolated outer iterations between extrapolation sequences (3).
<u>04</u> (I2,10X,4E12.5)	
Cols. 13-24	Outer-iteration convergence criterion on the sum of the absolute value of flux differences (10^{-5}).
Cols. 25-36	Outer-iteration convergence criterion on the difference of the flux bounds (10^{-5}).
Cols. 37-48	Outer-iteration convergence criterion on the difference in k_{eff} (10^{-5}).
Cols. 49-60	Interval shift factor when applying Chebyshev extrapolation to outer iterations (0).

Card
Type

Description

05

(I2,10X,6I6)

Cols. 13-18 Maximum number of inner iterations per outer iteration (0).

Cols. 19-24 Inner-iteration extrapolation option (0).

0 No extrapolation.

1 Chebyshev extrapolation.

2 Successive overrelaxation.

Cols. 25-30 Number of unextrapolated inner iterations before extrapolating (2).

Cols. 31-36 Number of extrapolated inner iterations before testing for extrapolation payoff (3).

Cols. 37-42 Maximum number of extrapolated inner iterations in an extrapolated sequence (8).

Cols. 43-48 Number of unextrapolated inner iterations between extrapolation sequences (3).

06

(I2,10X,3E12.5)

Cols. 13-24 Inner-iteration convergence criterion on the sum of the absolute value of flux differences (10^{-4}).

Cols. 25-36 Interval shift factor when applying Chebyshev extrapolation to inner iterations (0.0).

Cols. 37-48 Initial estimate of convergence rate of inner iterations (0).

5. Data Module A.INPTR1a. Data Module Name

A.INPTR1.

b. Description

Module-dependent input for 1D-Transport Specifications.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUI004 1D-Transport Specifications

e. Structure and Content

Cards are in standard ARC format, listed by card type (as appears in Cols. 1 and 2) below.

Card Type	Description
<u>01</u>	(I2,10X,4I6,3D12.11)
Cols. 13-18	ISN, the S_n order desired. ($ISN < 0$ if S_n constants are to be taken from stored data rather than from Type <u>03</u> cards. In this case, the order is $ ISN $).
Cols. 19-24	MAXII, the maximum number of inner iterations for all groups. If Cols. 19-24 are blank, MAXII is set to 25.
Cols. 25-30	MAXOI, the maximum number of outer iterations for the problem. If Cols. 25-30 are blank, MAXOI is set to 50.
Cols. 31-36	For future use.
Cols. 37-48	EPS, convergence criterion constant for inhomogeneous solutions or k_{eff} calculations; leave blank for criticality searches.

Card Type	Description
<u>01</u> (Contd.)	
Cols. 49-60	PAROD, the parameter oscillation damper for criticality searches only. If Cols. 49-60 are blank, 1.0 is used for a geometry search, 0.75 for a time absorption calculation, and 0.50 for a concentration search.
Cols. 61-72	CONNF, the normalization factor. (0.0 means no normalization; "blank" means CONNF = 1.0.)
<u>02</u>	For future use.
<u>03</u>	NUMDIR cards (I2,I0X,2D12.11), where NUMDIR = ISN + 1 for plane or sphere; = ISN * (ISN + 4)/4 for cylinder. Cols. 13-24 DIRWGT weight used for integration. Cols. 25-36 DIRMU direction cosine. If ISN < 0 (Type <u>01</u> cards), the Type <u>03</u> cards are irrelevant.
<u>04</u>	For future use. When input data saved in the data pool from a former ARC run are used, it is possible to delete that portion of the input on the Type <u>05</u> , <u>06</u> , <u>07</u> , or <u>08</u> cards. This is achieved by entering the word "DELETE" as data in Cols. 13-18 of the card type to be deleted.
<u>05</u>	ℓ Number Specification (I2,4X,A6,I6) Cols. 7-12 NAMANS, composition label for which ℓ number is to be specified. Cols. 13-18 LNOANS, ℓ number to be defined for this composition. $\ell = 0$ for isotropic only, = 1 for linear anisotropic scattering, > 1 for higher-order scattering. The absence of this information for a composition indicates that all scattering information available will be used for that composition.

Card Type	Description
<u>06</u>	Density-factor Specification (I2,4X,A6,5D12.11)
	For density factor specified by region:
Cols. 7-12	REGLBL, region label. (1.0 is assumed for DENSFC for those regions not specified.)
Cols. 13-24	DENSFC, density factor for this region.
	For density factor specified by interval (Cols. 7-12 blank):
Cols. 13-24	CSCFAC(I), density factors by interval. First blank field specifies end of string. All elements not specified are set to 1.0.
Cols. 25-36	
Cols. 37-48	
Cols. 49-60	
Cols. 61-72	
<u>07</u>	Diffusion-theory Option Specification (I2,10X,10I6)
Cols. 13-18	Groups for which diffusion-theory approximation will be used.
Cols. 19-24	
Cols. 25-30	
Cols. 31-36	
Cols. 37-42	
Cols. 43-48	
Cols. 49-54	
Cols. 55-60	
Cols. 61-66	
Cols. 67-72	
<u>08</u>	Group-skipping Option (I2,10X,10I6)
Cols. 13-18	Groups to be skipped.
Cols. 19-24	
Cols. 25-30	
Cols. 31-36	

Card Type	Description
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<u>08</u>	(Contd.)
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Cols. 37-42	} Groups to be skipped.
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Cols. 43-48	} Groups to be skipped.
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Cols. 49-54	} Groups to be skipped.
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Cols. 55-60	} Groups to be skipped.
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Cols. 61-66	} Groups to be skipped.
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Cols. 67-72	} Groups to be skipped.
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6. Data Module A.INPTR2a. Data Module Name

A.INPTR2.

b. Description

Module-dependent input for 2D-Transport Specifications..

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUI005 2D-Transport Specifications

e. Structure and Content

Cards are in standard ARC format, listed by card type (as appears in Cols. 1 and 2) below.

<u>Card Type</u>	<u>Description</u>
<u>01</u> (I2,10X,4I6,3D12.11)	
Cols. 13-18	ISN, the S_n order desired. ($ISN < 0$ if S_n constants are to be taken from stored data rather than from Type 03 cards. In this case, the order is $ ISN $.)
19-24	MAXII, the maximum number of inner iterations for the problem. If Cols. 19-24 are blank, MAXII is set equal to 25.
25-30	MAXOI, the maximum number of outer iterations for the problem. If Cols. 25-30 are blank, MAXOI is set equal to 50.
31-36	For future use.
37-48	EPS, convergence-criterion constant for inhomogeneous solutions or k_{eff} calculations; leave blank for criticality searches.

Card Type	Description
<u>01</u>	(Contd.)
Cols. 49-60	PAROD, the parameter oscillation damper, for criticality searches only. If Cols. 49-60 are blank, 1.0 is used for a geometry search, 0.75 for a time-absorption calculation, and 0.50 for a concentration search.
61-72	CONNF, the normalization factor. (0.0 means no normalization; "blank" means CONNF = 1.0.)
<u>02</u>	For future use.
<u>03</u>	(I2,10X,3D12.11)
Cols. 13-24	DIRWGT, weight used for integration.
25-26	DIRETA, direction cosine.
37-48	DIRMU, direction cosine.
If $ISN < 0$ (Type <u>01</u> cards), the Type <u>03</u> cards are irrelevant.	
If $ISN > 0$, the number of Type <u>03</u> cards required is $ISN \cdot (ISN + 4)/2$.	
<u>04</u>	For future use.
When using input data saved in the data pool from a former ARC run, it is possible to delete that portion of the input on the Type <u>05</u> , <u>06</u> , <u>07</u> , or <u>08</u> cards. This is achieved by entering the word "DELETE" as data in Cols. 13-18 of the card type to be deleted.	
<u>05</u>	ℓ Number Specification (I2,4X,A6,I6)
Cols. 7-12	NAMANS, composition label for which ℓ number is to be specified.
13-18	LNOANS, ℓ number to be defined for this composition.
	$\ell = 0$ for isotropic only,
	$= 1$ for linear anisotropic scattering,
	> 1 for higher-order scattering.
NOTE: The absence of this information for a composition indicates that all scattering information available will be used for that composition.	

Card Type	Description
<u>06</u>	Density-factor Specification (I2,4X,A6,5D12.11)
	For density factor specified by region:
Cols. 7-12	REGLBL, region label (1.0 is assumed for DENSFC for those regions not specified).
13-24	DENSFC, density factor for this region.
	For density factors specified by interval (Cols. 7-12 blank):
Cols. 13-24	} CSCFAC(I), density factors by interval. First blank field specifies end of string. All elements not specified are set to 1.0. The ordering of the intervals is from left to right along each x or r axis, proceeding in the direction of increasing y, θ , or z.
25-36	
37-48	
49-60	
61-72	
<u>07</u>	Diffusion-theory Option Specification (I2,10X,10I6)
Cols. 13-18	} Groups for which diffusion-theory approximation will be used.
19-24	
25-30	
31-36	
37-42	
43-48	
49-54	
55-60	
61-66	
67-72	
<u>08</u>	Group-skipping Option (I2,10X,10I6)
Cols. 13-18	} Groups to be skipped.
19-24	
25-30	
31-36	

Card
TypeDescription08

(Contd.)

Cols. 37-42

43-48

49-54

55-60

61-66

67-72

Groups to be skipped.

7. Data Module A.NIPa. Data Module Name

A.NIP

b. Description

General input for neutronics calculations.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUI001 Cross-section Homogenization Specifications
	X	NUI002 Geometry Specifications
	X	NUI003 Neutronics Specifications

e. Structure and Contents

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below.

<u>Card Type</u>	<u>Description</u>
<u>01</u>	Title (I2,4X,11A6). As many Type <u>01</u> cards as necessary may be used.
<u>02</u>	Input Processing Specification (reserved for future definitions, to allow such nonstandard options as binary-BCD data merges, additional generations, requests to ignore certain input types, etc.).
<u>03</u>	Basic Problem Identification (I2,10X,3I6,18X,2E12.5)
	Cols. 13-18 Geometry type.
	10 Slab, infinite.
	11 Slab, cylindrical.
	12 Slab, finite in one transverse direction.
	13 Slab, finite in both transverse directions.

Card
Type

Description

03

(Contd.)

20	Cylinder, infinite.
21	Cylinder, finite.
30	Sphere.
40	x-y, infinite.
41	x-y, finite.
42	x-y, 45° symmetry, infinite.
43	x-y, 45° symmetry, finite.
50	r-z.
51	z-r.
60	r- θ , infinite.
61	r- θ , finite.
Cols. 19-24	Problem type.
0	Real.
1	Adjoint.
2	Both real and adjoint (may be selected only if Cols. 25-30 below are zero or blank).
Cols. 25-30	Calculation type.
0	Homogeneous.
1	Inhomogeneous.
Cols. 49-60	Fixed k_{eff} for the problem.
61-72	Initial α , for an α -criticality search problem, or fixed α for the problem.

04

External Boundary Conditions (I2,10X,4I6)

Cols. 13-18	Boundary condition at lower "x" boundary of reactor.
19-24	Boundary condition at upper "x" boundary of reactor.
25-30	Boundary condition at lower "y" boundary of reactor.

Card
Type

Description

04

(Contd.)

Cols. 31-36 Boundary condition at upper "y" boundary of reactor.

1 $\phi = a.$

2 $\phi = 0.$

3 $\phi' = 0.$

4 $\phi' + \frac{a}{D} \phi = 0.$

5 $\phi' + a\phi = 0.$

6 Periodic ($r-\theta$).

7 $a\phi' + b\phi = 1.$

8 $a\phi' + \frac{b}{D} \phi = 1.$

9 Incoming angular flux zero.

10 Reflective.

11 Periodic.

12 White.

ϕ' is the derivative of the flux in the direction of the reactor outward normal. D is the diffusion coefficient in the mesh interval immediately inside the reactor boundary.

Conditions 1-8 apply to diffusion-theory problems, and 9-12 apply to transport-theory problems.

05

External Boundary Condition Constants (I2,8X,A2,2E12.5,2I6,2E12.5)

Cols. 11-12 Boundary designator.

XL: "x" lower.

XU: "x" upper.

YL: "y" lower.

YU: "y" upper.

Cols. 13-24 Value of constant a referred to on Card Type 04.

25-36 Value of constant b referred to on Card Type 04.

Card Type	Description
<u>05</u>	(Contd.)
Cols. 37-42	Higher-energy group number for which constants apply.
43-48	Lower-energy group number for which constants apply.
49-60	Lower coordinate on boundary for which constants apply.
61-72	Upper coordinate on boundary for which constants apply.

If Cols. 37-42 are blank, constants given apply to all energy groups. If Cols. 43-48 are blank, constants given apply to group specified in Cols. 37-42. If Cols. 49-72 are blank, constants given apply to the entire external boundary concerned. Lower and upper coordinates must coincide with mesh lines, which bound mesh intervals.

06 Region Boundary Coordinates and Constant Mesh Structure
(I2,4X,A6,2E12.5,2I6,2E12.5)

Cols. 7-12	Region label (repeated on additional cards).
13-24	"x"-direction lower-boundary coordinate.
25-36	"x"-direction upper-boundary coordinate.
37-42	Number of intervals in "x" direction.
43-48	Number of intervals in "y" direction.
49-60	"y"-direction lower-boundary coordinate.
61-72	"y"-direction upper-boundary coordinate.
	"x" represents x, r, or z for z-r geometry.
	"y" represents y, z, θ , or r for z-r geometry.

Regions may be defined using the overlay procedure with the latest region assignment overlaying the previous configuration. Region labels must be nonblank. The mesh for a direction must be completely specified either on the Type 06 or 09 cards. If mesh data are supplied on both Type 06 and 09 cards, the Type 09 data will be used. For one-dimensional problems, only the "x"-direction upper boundaries need be given for regions after the first.

Card Type	Description
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07 Area Specifications (I2,4X,11A6)

Cols. 7-12 Area label (repeated on additional cards).

13-18	} Labels of regions comprising area.
19-24	
25-30	
31-36	
37-42	
43-48	
49-54	
55-60	
61-66	
67-72	

Area labels must be nonblank.

08 Zone Specifications (I2,4X,A6,4E12.5)

Cols. 7-12 Zone label (repeated on additional cards).

13-24 Lower "x" boundary of section.

25-36 Upper "x" boundary of section.

37-48 Lower "y" boundary of section.

49-60 Upper "y" boundary of section.

As many sections may be specified as necessary to define the zone. Each zone boundary must coincide with some mesh line. Zone labels must be nonblank.

09 Variable-mesh Structure (I2,9X,A1,3(I6,E12.5))

Col. 12 Coordinate direction.

X "x" coordinate direction.

Y "y" coordinate direction.

Cols. 13-18 Number of intervals.

19-30 Upper coordinate.

Card Type	Description
<u>09</u>	(Contd.)
Cols. 31-36	Number of intervals.
37-48	Upper coordinate.
49-54	Number of intervals.
55-66	Upper coordinate.
<p>"x" represents x, r, or z in z-r geometry; "y" represents y, z, θ, or r in z-r geometry. Each number pair is of the form (n_i, x_i). There are n_i intervals between x_{i-1} and x_i, where x_0 is the lower reactor boundary in this direction. Number pairs must be given in order of increasing mesh. All region boundaries must coincide with the mesh lines that bound mesh intervals.</p>	
<u>10</u>	Internal Boundary or Interface Conditions (I2,4X,A6,5X,A1,I6,3E12.5)
Cols. 7-12	Internal interface label.
Col. 18	Coordinate direction of internal boundary or interface.
X	"x"-coordinate direction.
Y	"y"-coordinate direction.
Cols. 19-24	Internal condition
0	$\phi' + (a/D) \phi = b.$
1	$\phi' + a\phi = b.$
2	$\phi_{i+1} = a\phi_i + b\phi'_i;$
	$\phi'_{i+1} = c\phi_i + d\phi'_i.$
Cols. 25-36	"y" coordinate along which "x"-direction interface lies, or "x" coordinate along which "y"-direction interface lies.
37-48	Coordinate of lower end of interface.
49-60	Coordinate of upper end of interface.

Each Type 10 card above must be followed by one or more Type 11 cards which contain the necessary constants for the spatial interval defined above. The internal interface label is used on the Type 11 cards to designate the interface defined on the Type 10 card with the same label.

Card
Type

Description

11 Internal-boundary or Interface-condition Constants
(I2,4X,A6,4E12.5,2I6)

Cols. 7-12 Internal-interface label.

13-24 }
25-36 } Constants defined below.
37-48 }
49-60 }

61-66 Higher-energy group number for which constants apply.

67-72 Lower-energy group number for which constants apply.

If Cols. 61-66 are blank, constants apply to all energy groups. If Cols. 67-72 are blank, constants apply to group specified in Cols. 61-66.

For the logarithmic boundary conditions, options 0 and 1: $\phi' + (a/D)\phi = b$, and $\phi' + a\phi = b$, respectively, one pair of constants, a and b , are given for each side of the boundary. The constants a and b given in Cols. 13-24 and 25-36, respectively, will be applied at the side of the boundary encountered first as the mesh is swept, and the constants a and b in Cols. 37-48 and 49-60 will be applied at the other side of the boundary line. The mesh is swept in the direction of increasing dimension. D is the diffusion coefficient in the corresponding region; ϕ' is the derivative of the flux in the direction of the outward normal to the boundary. For the general interface condition, option 2,

$$\phi_{i+1} = a\phi_i + b\phi_i',$$

$$\phi_{i+1}' = c\phi_i + d\phi_i',$$

the constants a , b , c , and d are given in Cols. 13-24, 25-36, 37-48, and 49-60, respectively. The indices i and $i+1$ refer to mesh intervals on either side of the interface, i being encountered before $i+1$ as the mesh is swept; ϕ' is the derivative of the flux in the direction of the mesh sweep.

Card Type	Description
<u>12</u>	Finite-geometry Transverse Distances (I2,4X,A6,4E12.5)
	Cols. 7-12 Region label. 13-24 Actual transverse half-distance. 25-36 Transverse extrapolation distance. 37-48 Actual transverse half-distance in the second direction, for a finite slab. 49-60 Transverse extrapolation distance in the second direction, for a finite slab.
	If Cols. 7-12 are blank, the data in Cols. 13-60 apply to all regions of the reactor. If Cols. 13-24 and/or 37-48 are blank, the reactor is assumed to be infinite in the corresponding transverse direction.
<u>13</u>	Material Specifications (I2,10X,A6,3(A6,E12.5))
	Cols. 13-18 Material label (repeated on additional cards). 19-24 Isotope label. 25-36 Isotope atom density (atoms/cc x 10^{-24}). 37-42 Isotope label. 43-54 Isotope atom density (atoms/cc x 10^{-24}). 55-60 Isotope label. 61-72 Isotope atom density (atoms/cc x 10^{-24}). Material labels must be nonblank.
<u>14</u>	Composition Specifications (I2,10X,A6,3(A6,E12.5))
	Cols. 13-18 Composition label (repeated on additional cards). 19-24 Material label. 25-36 Material volume fraction. 37-42 Material label. 43-54 Material volume fraction. 55-60 Material label. 61-72 Material volume fraction. Composition labels must be nonblank.

Card Type	Description																				
<u>14</u>	(Contd.)																				
	If Card Type <u>13</u> is not given, "material" on Card Type <u>14</u> corresponds to isotope, and "volume fraction" corresponds to atom density.																				
<u>15</u>	Composition and Region Assignments (I2,4X,11A6)																				
	<table> <tr> <td>Cols. 7-12</td><td>Composition label (repeated on additional cards).</td></tr> <tr> <td>13-18</td><td rowspan="10">} Region label of region containing specified composition.</td></tr> <tr> <td>19-24</td></tr> <tr> <td>25-30</td></tr> <tr> <td>31-36</td></tr> <tr> <td>37-42</td></tr> <tr> <td>43-48</td></tr> <tr> <td>49-54</td></tr> <tr> <td>55-60</td></tr> <tr> <td>61-66</td></tr> <tr> <td>67-72</td></tr> </table>	Cols. 7-12	Composition label (repeated on additional cards).	13-18	} Region label of region containing specified composition.	19-24	25-30	31-36	37-42	43-48	49-54	55-60	61-66	67-72							
Cols. 7-12	Composition label (repeated on additional cards).																				
13-18	} Region label of region containing specified composition.																				
19-24																					
25-30																					
31-36																					
37-42																					
43-48																					
49-54																					
55-60																					
61-66																					
67-72																					
<u>16</u>	Initial Fission Source or Flux Specifications (I2,10X,2I6,E12.5,2I6,E12.5)																				
	<table> <tr> <td>Cols. 13-18</td><td>Quantity-type being specified for real problem.</td></tr> <tr> <td>0</td><td>Fission source.</td></tr> <tr> <td>1</td><td>Flux.</td></tr> <tr> <td>Cols. 19-24</td><td>Spectrum distribution for real problem.</td></tr> <tr> <td>0</td><td>Use specified quantities as given.</td></tr> <tr> <td>1</td><td>Distribute specified quantities into the energy groups using fission-spectrum weighting at each mesh interval.</td></tr> <tr> <td>Cols. 25-36</td><td>Base value for real problem.</td></tr> <tr> <td>37-42</td><td>Quantity-type being specified for adjoint problem.</td></tr> <tr> <td>0</td><td>Fission source.</td></tr> <tr> <td>1</td><td>Flux.</td></tr> </table>	Cols. 13-18	Quantity-type being specified for real problem.	0	Fission source.	1	Flux.	Cols. 19-24	Spectrum distribution for real problem.	0	Use specified quantities as given.	1	Distribute specified quantities into the energy groups using fission-spectrum weighting at each mesh interval.	Cols. 25-36	Base value for real problem.	37-42	Quantity-type being specified for adjoint problem.	0	Fission source.	1	Flux.
Cols. 13-18	Quantity-type being specified for real problem.																				
0	Fission source.																				
1	Flux.																				
Cols. 19-24	Spectrum distribution for real problem.																				
0	Use specified quantities as given.																				
1	Distribute specified quantities into the energy groups using fission-spectrum weighting at each mesh interval.																				
Cols. 25-36	Base value for real problem.																				
37-42	Quantity-type being specified for adjoint problem.																				
0	Fission source.																				
1	Flux.																				

Card Type	Description
<u>16</u>	(Contd.)
Cols. 43-48	Spectrum distribution for adjoint problem.
0	Use specified quantities as given.
1	Distribute specified quantities into energy groups j using $(\nu\Sigma_f)_j / \sum_j (\nu\Sigma_f)_j$ for weighting at each mesh interval.
Cols. 49-60	Base value for adjoint problem.
<p>If no Card Type <u>16</u> is given, initial real and/or adjoint flux values of 1.0 will be assumed for all energy groups and for all mesh intervals according to the problem type given in Cols. 19-24 on Card Type <u>03</u>.</p> <p>Card Type <u>16</u> must be used if Card Types <u>17</u> and/or <u>18</u> are used. The base values given in Cols. 25-36 and 49-60 will be modified according to Cols. 19-24 and 43-48 and assigned to each mesh interval in the problem. Quantities given on Card Types <u>17</u> and/or <u>18</u> will override this original array. Columns 19-24 and 43-48 also influence the data from Card Types <u>17</u> and <u>18</u> except for the data on Card Types <u>17</u> or <u>18</u> that are given specifically as a function of energy groups.</p>	
<u>17</u>	Distributed Initial Fission Source or Flux Data (I2,AX,I6,A6,I6,E12.5,2I6,E12.5,2I6)
Cols. 7-12	
0	Cols. 13-18 contain a region label.
1	Cols. 13-18 contain an area label.
2	Cols. 13-18 contain a zone label.
Cols. 13-18	Label of region, area, or zone (repeated on additional cards as necessary).
19-24	
0	Quantities specified apply to both real and adjoint problems.
1	Quantities specified apply to real problems only.
2	Quantities specified apply to adjoint problems only.
Cols. 25-36	Quantity being specified.
37-42	Higher-energy group number to which quantity specified in Cols. 25-36 applies.

Card Type	Description
<u>17</u>	(Contd.)
Cols. 43-48	Lower-energy group number to which quantity specified in Cols. 25-36 applies.
49-60	Quantity being specified.
61-66	Higher-energy group number to which quantity specified in Cols. 49-60 applies.
67-72	Lower-energy group number to which quantity specified in Cols. 49-60 applies.
Columns 19-24 are ignored unless Cols. 19-24 of Card Type 03 specify both real and adjoint problems.	
The quantity specified is assigned to each mesh interval of the region, area, or zone indicated. If Cols. 13-18 are blank, the data on this card are applied to the entire reactor. If Cols. 37-42 are blank, the quantity in Cols. 25-36 is modified according to Cols. 19-24 or Cols. 43-48 on Card Type 16, and the remainder of the card is ignored.	
If Cols. 43-48 and/or 67-72 are blank, the quantity specified in Cols. 25-36 and/or 49-60 applies to the energy group in Cols. 37-42 and/or 61-66.	
<u>18</u>	Mesh-distributed Initial Fission Source or Flux Data (I2,4X,3I6,4E12.5)
Cols. 7-12	
0	Quantities specified apply to both real and adjoint problems.
1	Quantities specified apply to real problems only.
2	Quantities specified apply to adjoint problems only.
Cols. 13-18	Energy group number to which quantities specified apply (repeated on additional cards).
19-24	Card number.
25-36	} Initial fission source or flux data by mesh intervals, in order of increasing "x" direction.
37-48	
49-60	
61-72	

Card Type	Description
<u>18</u>	(Contd.)
	Columns 7-12 are ignored unless Cols. 19-24 of Card Type <u>03</u> specify both real and adjoint problems.
	If Cols. 13-18 are blank, the data are assigned to all energy groups, as modified by Cols. 19-24 or 43-48 on Card Type <u>16</u> .
	The data on Card Type <u>18</u> override initial data on Card Types <u>16</u> and/or <u>17</u> . For each energy group of data being given on Card Type <u>18</u> , the entire space mesh must be covered. The space mesh is covered by a sweep in the direction of increasing "x" values. Columns 19-24 of the first card for each energy group must be 1 to indicate the beginning of the sweep. For two-dimensional geometries, the sweep proceeds across the first row, then begins on a new card, proceeding in the direction of increasing "x" values again, for each new row. Card numbers, in Cols. 19-24, increase consecutively until the mesh sweep is completed.
<u>19</u>	Distributed Isotropic Inhomogeneous Source Data (I2,4X,I6,A6,3I6,3E12.5)
	Cols. 7-12
	0 Cols. 13-18 contain a region label.
	1 Cols. 13-18 contain an area label.
	2 Cols. 13-18 contain a zone label.
	Cols. 13-18 Label of region, area or zone (blank if data are given by mesh intervals).
	19-24 Spectrum distribution for data not given by specific group numbers.
	0 Use specified source as given.
	1 Distribute specified source into the energy groups using fission spectrum weighting at each mesh point for a real problem, or
	$(\nu\Sigma_f)_j / \sum_j (\nu\Sigma_f)_j$
	weighting for group j in an adjoint problem.
	Cols. 25-30 Higher-energy group number.

Card Type	Description
<u>19</u>	(Contd.)
Cols. 31-36	Lower-energy group number.
37-48	Isotropic source value in the specified mesh interval for this energy range.
49-60	Lower "x"-direction coordinate of mesh interval containing this source.
61-72	Lower "y"-direction coordinate of mesh interval containing this source.
<p>If Cols. 13-18 are blank, the data in Cols. 37-48 are placed in the one-mesh interval referenced by Cols. 49-60 and 61-72. If Cols. 13-18 are nonblank, Cols. 49-72 are ignored, and the value given in Cols. 37-48 is used everywhere in the region, area, or zone named in Cols. 13-18.</p> <p>If Cols. 25-30 are blank, the source value applies to all energy groups. If Cols. 31-36 are blank, the source value applies to the group specified in Cols. 25-30.</p>	
<u>20</u>	Anisotropic Inhomogeneous Source Data (I2,4X,I6,A6,3I6,3E12.5)
Cols. 7-12	
0	Cols. 13-18 contain a region label.
1	Cols. 13-18 contain an area label.
2	Cols. 13-18 contain a zone label.
Cols. 13-18	Label of region, area or zone.
19-24	Portion of region, area, or zone in which source occurs.
0	Source occurs in the single-mesh interval with highest "x" dimension (one-dimensional geometry) or with highest "x" and "y" dimensions (two-dimensional geometry).
1	Source occurs down the mesh channel of highest "x" dimension for the region, area, or zone specified.
2	Source occurs across the mesh row of highest "y" dimension for the region, area, or zone specified.

Card
Type

Description

20

(Contd.)

- Cols. 25-30 Higher-energy group number for which source applies.
- 31-36 Lower-energy group number for which source applies.
- 37-48 Isotropic component of source.
- 49-60 Anisotropic "x" direction component of source.
- 61-72 Anisotropic "y" direction component of source.

If Cols. 25-30 are blank, the source values apply to all energy groups. If Cols. 31-36 are blank, the source values apply to the group specified in Cols. 25-30.

The source is assumed to occupy a one-mesh-interval-thick column or row segment.

21

Search Specifications (I2,10X,2I6,2E12.5)

Cols. 13-18

- 0 Search to obtain a prescribed k_{eff} .
- 1 Search to obtain a prescribed α .
- Cols. 19-24 Maximum number of search passes.
- 25-36 Prescribed k_{eff} , (k_{eff}_0) or α , (α_0) .
- 37-48 Convergence criterion, ϵ , for current value of k_{eff} or α :

$$\frac{k_{eff} - k_{eff_0}}{k_{eff_0}} \leq \epsilon \quad \text{or} \quad \left| \frac{\alpha - \alpha_0}{\alpha_0} \right| \leq \epsilon.$$

If Cols. 13-18 are 0, a blank in Cols. 25-36 implies 1.0 for the prescribed k_{eff} .

22

Search Parameters (I2,10X,4E12.5)

General search expression:

$$P(x) = P(0) + x \cdot M,$$

Card Type	Description
<u>22</u>	(Contd.)
	where P is the quantity being varied, x is the search parameter, and M is the quantity modifier obtained from information contained on Card Type <u>23</u> , <u>24</u> , <u>25</u> or <u>26</u> .
Cols. 13-24	Initial value of x .
25-36	Second value of x (ignored if Cols. 61-72 are nonzero).
37-48	Lower bound for x .
49-60	Upper bound for x .
61-72	Derivative of k_{eff} with respect to x (or α with respect to x).
<u>23</u>	Composition Modifier: Composition Assignments for Criticality Search (I2,4X,11A6)
Cols. 7-12	Composition label of composition (from Card Type <u>14</u>) to be used as the modifier M in the search formula.
13-18	Composition labels of compositions (from Card Type <u>14</u>) with which modifier composition is to be used.
19-24	
25-30	
31-36	
37-42	
43-48	
49-54	
55-60	
61-66	Composition labels of compositions (from Card Type <u>14</u>) with which modifier composition is to be used.
67-72	

In the search formula $P(x) = P(0) + x \cdot M$, $P(x)$, $P(0)$, and M are macroscopic cross sections. $P(0)$ and M are obtained from the data on Card Type 14, with Card Type 23 selecting those compositions on Card Type 14 to be used in producing the M .

Card
Type

Description

24 Mesh Modifiers for Criticality Search (I2,9X,A1,3E12.5)

Col. 12 Coordinate direction.

X "x" coordinate direction.

Y "y" coordinate direction.

Cols. 13-24 Lower coordinate.

25-36 Upper coordinate.

37-48 Dimensionless mesh modifier, m , for each mesh interval between the above coordinates.

In the search formula, $P(x) = P(0) + x \cdot M$, M will be evaluated as $m \cdot P(0)$. The $P(x)$, $P(0)$, and M are mesh intervals.

25 Buckling Modifiers for Criticality Search (I2,4X,A6,2E12.5)

Cols. 7-12 Region label.

13-24 Buckling modifier, M , in first transverse direction.25-36 Buckling modifier, M , in second transverse direction.

In the search formula, $P(x) = P(0) + x \cdot M$, $P(x)$, $P(0)$, and M are bucklings. $P(0)$ will be evaluated from the transverse heights given on Card Type 12.

If Cols. 7-12 are blank, the data in Cols. 13-36 apply to all regions of the reactor.

26 Alpha Modifier for Criticality Search (I2,10X,E12.5)Cols. 13-24 Alpha modifier, M .

In the search formula, $P(x) = P(0) + x \cdot M$, $P(x)$, $P(0)$, and M are alphas. $P(0)$ is obtained from Cols. 60-72 of Card Type 03.

8. Data Module A.THINa. Data Module Name

A.THIN.

b. Description

General input for thermal cross-section calculations.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	CSI002 Thermal Cross-section Specifications

e. Structure and Contents

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below.

<u>Card Type</u>	<u>Description</u>
<u>01</u>	Title (I2,4X,11A6)
<u>02</u>	Input Processing Specifications (reserved for future definitions).
<u>03</u>	General Problem Specifications (I2,10X,I6,4A6,2I6,E12.5)
	Cols. 13-18 Bypass option.
	0 Standard.
	1 Cross sections used in a preceding problem will be used again.
	-1 Spectrum from a preceding problem will be used with new parameters.
	Cols. 19-24 Region label of innermost region of cell used for spatial averaging of cross sections.
	25-30 Region label of outermost region of cell used for spatial averaging of cross sections.

Card
Type

Description

03

(Contd.)

Cols. 31-36 Region label of innermost region of problem used for spatial-flux averaging. If blank, no spatial-flux averaging is done.

37-42 Region label of outermost region of problem used in spatial-flux averaging.

43-48 Geometry type.

0 Cylinder with reflecting boundary conditions.

1 Slab with reflecting boundary conditions.

2 Cylinder with vacuum boundary conditions.

3 Half slab with symmetry and vacuum boundary conditions.

4 Full slab with vacuum boundary conditions.

Cols. 49-54 Coarse-group elastic scattering transfer cross-section option.

0 Transfer cross sections not generated.

1 Transfer cross sections generated.

Cols. 55-60 Consistent P1-B1 Option.

0 No consistent calculations performed.

1 Consistent P1 cross sections calculated.

2 Consistent B1 cross sections calculated.

Cols. 61-72 Lowest neutron speed for the problem. Columns 61-72 are irrelevant unless Card Type 12 is provided.

If Cols. 13-18 are 1, Card Types 04, 06-08, 11, and 22-29 are required and Cols. 49-72 on Card Type 03 are irrelevant. If Cols. 13-18 are -1, Card Types 06 and 11 are required and only Cols. 19-30 on Card Type 03 are relevant.

04

Region Specifications (I2,I0X,A6,2E12.5,I6)

Cols. 13-18 Region label.

19-30 Region lower coordinate.

Card Type	Description
<u>04</u>	(Contd.)
	Cols. 31-42 Region upper coordinate.
	43-48 Number of space points in the region.
	The space points are implicitly numbered, with point 1 nearest the lowest coordinate of the problem.
<u>05</u>	Mixture Specifications (I2,I0X,3(A6,2I6))
	Cols. 13-18 Mixture label.
	19-24 Number of lowest space point to which mixture is assigned.
	25-30 Number of highest space point to which mixture is assigned.
	31-36 Mixture label.
	37-42 Number of lowest space point to which mixture is assigned.
	43-48 Number of highest space point to which mixture is assigned.
	49-54 Mixture label.
	55-60 Number of lowest space point to which mixture is assigned.
	61-66 Number of highest space point to which mixture is assigned.
<u>06</u>	Coarse-group Cross-section Specifications (I2,I0X,I0I6)
	Cols. 13-18 Number of lower-speed fine group to be used in coarse-group cross-section generation.
	19-24 Number of upper-speed fine group to be used in coarse-group cross-section generation.
	25-30 Number of lower-speed fine group to be used.
	31-36 Number of upper-speed fine group to be used.
	37-42 Number of lower-speed fine group to be used.
	43-48 Number of upper-speed fine group to be used.

Card Type	Description
<u>06</u>	(Contd.)
Cols. 49-54	Number of lower-speed fine group to be used.
55-60	Number of upper-speed fine group to be used.
61-66	Number of lower-speed fine group to be used.
67-72	Number of upper-speed fine group to be used.
<p>If Card Type <u>06</u> is omitted, coarse-group cross sections will be generated for all fine groups. Card Type <u>06</u> is irrelevant if pseudo cross sections are to be generated as indicated by the presence of Card Type <u>11</u>.</p>	
<u>07</u>	Floating-point Iteration Parameters (I2,10X,5E12.5)
Cols. 13-24	Neutron-density convergence criterion (default 10^{-5}).
25-36	Initial over-relaxation factor (default 1.2).
37-48	Extrapolation criterion (default 0.05).
49-60	Maximum extrapolation factor (default 100.0).
61-72	Under extrapolation factor (default 1.0).
<u>08</u>	Integer Iteration Parameters (I2,10X,5I6)
Cols. 13-18	Minimum iterations before extrapolation (default 5).
19-24	Number of over-relaxation factors tested (default 5).
25-30	Minimum delay between extrapolations (default 5).
31-36	Maximum number of iterations allowed (default 100).
37-42	Iteration printout flag.
0	Print is omitted.
1	Record of each iteration is printed.
<u>09</u>	Spatial Distribution for Slowing-down Source (I2,10X,3(I6,E12.5))
Cols. 13-18	Number of space point.
19-30	Spatial slowing-down source at this point.
31-36	Number of space point.

Card Type	Description
<u>09</u>	(Contd.)
Cols. 37-48	Spatial slowing-down source at this point.
49-54	Number of space point.
55-66	Spatial slowing-down source at this point.
If Card Type <u>09</u> is omitted, a spatially flat slowing-down source is assumed.	
<u>10</u>	Slowing-down Source Parameters (I2,10X,A6,4E12.5)
Cols. 13-18	Mixture label in which this source is used.
19-30	Mass used in calculation of this source.
31-42	Microscopic high-energy scattering cross section for this source (barns).
43-54	Concentration of isotope (atoms/cc $\times 10^{-24}$).
55-66	Effective temperature of protons for use in error-function correction (in units of 293.6°K). If error-function correction is not to be used, this field is blank.
<u>11</u>	Pseudo-material Generation Specifications (I2,10X,A6,3(A6,E12.5))
Cols. 13-18	Pseudo-material label (repeated on additional cards).
19-24	Label of region included in spatial averaging for pseudo-material generation.
25-36	Volume of region (cm ³).
37-42	Label of region included in spatial averaging for pseudo-material generation.
43-54	Volume of region (cm ³).
55-60	Label of region included in spatial averaging for pseudo-material generation.
61-72	Volume of region (cm ³).

If Cols. 25-36, 43-54, or 61-72 are blanks, the regional volumes will be determined from the specifications given on Card Types 03 and 04.

Card
Type

Description

12 Speed Mesh (I2,10X,3(I6,E12.5))

Cols. 13-18	Neutron-speed group number.
19-30	Neutron speed at upper energy interface of group.
31-36	Neutron-speed group number.
37-48	Neutron speed at upper energy interface of group.
49-54	Neutron-speed group number.
55-66	Neutron speed at upper energy interface of group.

Columns 61-72 on Card Type 03 must be used to specify the lowest neutron speed for the problem if Card Type 12 is provided. Group 1 is the group of lowest neutron speed. Card Type 12 is required only if neither Card Type 13 nor 22 is supplied.

13 Mixture Compositions Determined from Library Isotopes (I2,10X,A6,3(A6,E12.5))

Cols. 13-18	Mixture label (repeated on additional cards).
19-24	Library isotope label.
25-36	Atom density (atoms/cc x 10^{-24}).
37-42	Library isotope label.
43-54	Atom density (atoms/cc x 10^{-24}).
55-60	Library isotope label.
61-72	Atom density (atoms/cc x 10^{-24}).

14 Mixture Compositions Determined from User-supplied Isotopes (I2,10X,A6,3(A6,E12.5))

Cols. 13-18	Mixture label (repeated on additional cards).
19-24	User-supplied isotope label.
25-36	Atom density (atoms/cc x 10^{-24}).
37-42	User-supplied isotope label.
43-54	Atom density (atoms/cc x 10^{-24}).
55-60	User-supplied isotope label.
61-72	Atom density (atoms/cc x 10^{-24}).

Card
Type

Description

14 (Contd.)

User-supplied isotope labels specified in Cols. 19-24, 37-42, and 55-60 must correspond to labels given on Card Types 16-21.

15 Mixture Compositions Determined from Pseudo Materials (I2,10X,A6,3(A6,E12.5))

Cols. 13-18 Mixture label (repeated on additional cards).

19-24 Pseudo-material label.

25-36 Atom density (atoms/cc x 10^{-24}).

37-42 Pseudo-material label.

43-54 Atom density (atoms/cc x 10^{-24}).

55-60 Pseudo-material label.

61-72 Atom density (atoms/cc x 10^{-24}).

Pseudo-material labels specified in Cols. 19-24, 37-42, and 55-60 must correspond to a label of a previously generated pseudo material as specified on Card Type 11.

16 User-supplied Isotope Specifications for Mixture (I2,4X,A6,5E12.5)

Cols. 7-12 Isotope label.

13-24 Absorption cross section σ_a^0 , where $\sigma_a(v_i) = \sigma_a^0/v_i$ and v_i is the group i velocity.

25-36 Average cosine of scattering angle, $\bar{\mu}$.

37-48 Temperature for scattering kernel (in units of 293.6°K).

49-60 Fission cross section σ_f^0 , where $\sigma_f(v_i) = \sigma_f^0/v_i$.

61-72 Average number of neutrons per fission, ν .

If speed-dependent values for σ_a , $\bar{\mu}$, σ_f , and ν are required, these are given on Card Types 18, 19, 20, and 21, respectively. Values on Card Types 18, 19, 20, and 21 will override the values implied from Cols. 13-24, 25-36, 49-60, and 61-72, respectively, on Card Type 16.

Card Type	Description
<u>17</u>	User-supplied Scattering-kernel Data for Mixture (I2,10X,A6,3E12.5)
Cols. 13-18	Isotope label (repeated on additional cards).
19-30	Cross section σ_n used in nth term of isotope-scattering kernel.
31-42	Mass used in nth term of isotope-scattering kernel.
43-54	Value κ_n used in nth term of isotope-scattering kernel.
<u>18</u>	User-supplied Isotope Speed-dependent Absorption Cross Sections for Mixture (I2,10X,A6,3(I6,E12.5))
Cols. 13-18	Isotope label (repeated on additional cards).
19-24	Speed group number.
25-36	Absorption cross section for this group.
37-42	Speed group number.
43-54	Absorption cross section for this group.
55-60	Speed group number.
61-72	Absorption cross section for this group.
<u>19</u>	User-supplied Isotope Speed-dependent Average Cosines of Scattering Angle for Mixture (I2,10X,A6,3(I6,E12.5))
Cols. 13-18	Isotope label (repeated on additional cards).
19-24	Speed group number.
25-36	$\bar{\mu}$ for this group.
37-42	Speed group number.
43-54	$\bar{\mu}$ for this group.
55-60	Speed group number.
61-72	$\bar{\mu}$ for this group.
<u>20</u>	User-supplied Isotope Speed-dependent Fission Cross Sections for Mixture (I2,10X,A6,3(I6,E12.5))
Cols. 13-18	Isotope label (repeated on additional cards).
19-24	Speed group number.

Card Type	Description
<u>20</u>	(Contd.)
	Cols. 25-36 Fission cross section for this group.
	37-42 Speed group number.
	43-54 Fission cross section for this group.
	55-60 Speed group number.
	61-72 Fission cross section for this group.
<u>21</u>	User-supplied Speed-dependent Number of Neutrons per Fission for Mixture (I2,I0X,A6,3(I6,E12.5))
	Cols. 13-18 Isotope label (repeated on additional cards).
	19-24 Speed group number.
	25-36 ν for this group.
	37-42 Speed group number.
	43-54 ν for this group.
	55-60 Speed group number.
	61-72 ν for this group.
<u>22</u>	Library Isotope Edit Specifications (I2,I0X,3(A6,E12.5))
	Cols. 13-18 Library isotope label.
	19-30 Library isotope atom density (atoms/cc x 10^{-24}).
	31-36 Library isotope label.
	37-48 Library isotope atom density (atoms/cc x 10^{-24}).
	49-54 Library isotope label.
	55-66 Library isotope atom density (atoms/cc x 10^{-24}).
<u>23</u>	User-supplied Isotope Edit Specifications (I2,I0X,3(A6,E12.5))
	Cols. 13-18 User-supplied isotope label (repeated on additional cards).
	19-30 User-supplied isotope atom density (atoms/cc x 10^{-24}).
	31-36 User-supplied isotope label.
	37-48 User-supplied isotope atom density (atoms/cc x 10^{-24}).

Card Type	Description
<u>23</u>	(Contd.)
Cols. 49-54	User-supplied isotope label.
55-66	User-supplied isotope atom density (atoms/cc $\times 10^{-24}$).
<u>24</u>	User-supplied Isotope Specifications for Edit (I2,4X,A6,5E12.5)
Cols. 7-12	Isotope label.
13-24	Absorption cross section σ_a^0 , where $\sigma_a(v_i) = \sigma_a^0/v_i$ and v_i is the group i velocity.
25-36	Average cosine of scattering angle, $\bar{\mu}$.
37-48	Temperature for scattering kernel (in units of 293.6°K).
49-60	Fission cross section σ_f^0 , where $\sigma_f(v_i) = \sigma_f^0/v_i$.
61-72	Average number of neutrons per fission, ν .
<p>If speed-dependent values for σ_a, $\bar{\mu}$, σ_f, and ν are required, these are given on Card Types <u>26</u>, <u>27</u>, <u>28</u>, and <u>29</u>, respectively. Values on Card Types <u>26</u>, <u>27</u>, <u>28</u>, and <u>29</u> will override the values implied from Cols. 13-24, 25-36, 49-60, and 61-72, respectively, on Card Type <u>24</u>.</p>	
<u>25</u>	User-supplied Scattering Kernel Data for Edit (I2,10X,A6,3E12.5)
Cols. 13-18	Isotope label (repeated on additional cards).
19-30	Cross section σ_n used in n th term of isotope scattering kernel.
31-42	Mass used in n th term of isotope scattering kernel.
43-54	Value κ_n used in n th term of isotope scattering kernel.
<u>26</u>	User-supplied Isotope Speed-dependent Absorption Cross Section for Edit (I2,10X,A6,3(I6,E12.5))
Cols. 13-18	Isotope label (repeated on additional cards).
19-24	Speed group number.
25-36	Absorption cross section for this group.
37-42	Speed group number.
43-54	Absorption cross section for this group.

Card Type	Description
<u>26</u>	(Contd.)
	Cols. 55-60 Speed group number.
	61-72 Absorption cross section for this group.
<u>27</u>	User-supplied Isotope Speed-dependent Average Cosines of Scattering Angle for Edit (I2,10X,A6,3(I6,E12.5))
	Cols. 13-18 Isotope label (repeated on additional cards).
	19-24 Speed group number.
	25-36 $\bar{\mu}$ for this group.
	37-42 Speed group number.
	43-54 $\bar{\mu}$ for this group.
	55-60 Speed group number.
	61-72 $\bar{\mu}$ for this group.
<u>28</u>	User-supplied Isotope Speed-dependent Fission Cross Sections for Edit (I2,10X,A6,3(I6,E12.5))
	Cols. 13-18 Isotope label (repeated on additional cards).
	19-24 Speed group number.
	25-36 Fission cross section for this group.
	37-42 Speed group number.
	43-54 Fission cross section for this group.
	55-60 Speed group number.
	61-72 Fission cross section for this group.
<u>29</u>	User-supplied Speed-dependent Number of Neutrons per Fission for Edit (I2,10X,A6,3(I6,E12.5))
	Cols. 13-18 Isotope label (repeated on additional cards).
	19-24 Speed group number.
	25-36 ν for this group.
	37-42 Speed group number.
	43-54 ν for this group.
	55-60 Speed group number.
	61-72 ν for this group.

9. Data Module A.XSSPCa. Data Module Name

A.XSSPC.

b. Description

General input for epithermal cross-section calculations.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	CSI001 Epithermal Cross-section Specifications

e. Structure and Contents

Cards are in standard ARC input format, listed by card type (as appears in Cols. 1 and 2) below.

Card
Type

Description

<u>01</u>	Title (I2,4X,11A6).
<u>02</u>	Input Processing Specifications (reserved for future definitions).
<u>03</u>	General Problem Specifications (I2,10X,8I6,E12,5).
Cols. 13-18	Fundamental-mode type.
1	P1.
2	Consistent B1 for isotropic neutronics.
3	Consistent P1 for isotropic neutronics.
4	Consistent B1 for anisotropic neutronics.
5	Consistent P1 for anisotropic neutronics.
Cols. 19-24	Fuel-pin geometry.
1	Slab.
2	Cylinder.

Card Type	Description
<u>03</u>	(Contd.)
Cols. 25-30	Thermal-group option.
0	No thermal-group cross sections used.
1	Problem uses thermal-group cross sections obtained from Type <u>08</u> and <u>09</u> cards or from the datapool.
Cols. 31-36	Library identification number for fission source.
37-42	Weighting spectrum obtained from Type <u>10</u> cards or from the datapool.
43-48	Broad-group cross-section calculation specification.
0	Calculate broad-group cross sections.
1	Broad-group cross sections not calculated.
Cols. 49-54	Fine-group detail.
0	All-fine-group problem.
1	Ultrafine-group problem.
Cols. 55-60	Fine-group weighting option.
1	1/E weighting spectrum.
2	Constant weighting spectrum.
3	E weighting spectrum.
Cols. 61-72	Fine-group lethargy width (typically 0.25).
<u>04</u>	Broad-group Specifications (I2,I0X,3(I6,E12.5))
Cols. 13-18	Broad-group number.
19-30	Upper energy of group, eV.
31-36	Broad-group number.
37-48	Upper energy of group, eV.
49-54	Broad-group number.
55-66	Upper energy of group, eV.

Group 1 is the group of highest energy. The thermal group having the largest group number has as upper energy the interface between the thermal and epithermal groups.

Card Type	Description
<u>05</u>	Fuel-pin Specifications (I2,10X,2E12.5)
Cols. 13-24	Radius of fuel pin if Cols. 19-24 on Card Type <u>03</u> equal 2; half thickness of fuel slab if Cols. 19-24 on Card Type <u>03</u> equal 1.
25-36	Radius of outer cladding-coolant region if Cols. 19-24 on Card Type <u>03</u> equal 2, outer bound of cladding-coolant region relative to center of fuel slab if Cols. 19-24 on Card Type <u>03</u> equal 1.
Card Type <u>05</u> is pertinent only for a heterogeneous problem.	
<u>06</u>	Problem Composition Specifications (I2,10X,A6,I6,4E12.5)
Cols. 13-18	Nuclide identification label on library.
19-24	Legendre treatment specifications.
0	Non-Legendre treatment of elastic scattering.
1	Elastic scattering for nuclide uses the Legendre treatment.
Cols. 25-36	Nuclide atomic concentration used to compute homogenized macroscopic cross sections for use in the fundamental-mode calculation (atoms/cc x 10^{-24}).
37-48	Nuclide temperature ($^{\circ}$ K).
49-60	Nuclide concentrations in the fuel pin (atoms/cc x 10^{-24}). If blank, the values given in Cols. 25-36 will be used.
61-72	Nuclide concentrations in the fuel-coolant outer region (atoms/cc x 10^{-24}). Ignored if Card Type <u>05</u> is not supplied.
<u>07</u>	Fundamental Mode Iteration Specifications (I2,10X,3E12.5)
Cols. 13-24	First guess for buckling.
25-36	Second guess for buckling.
37-48	Convergence criterion, ϵ , for k_{eff} :
	$ k_{\text{eff}} - 1 \leq \epsilon.$

Card Type	Description
<u>08</u>	Thermal Cross-section Data (I2,10X,A6,6X,4E12.5)
	Cols. 13-18 Nuclide identification label.
	25-36 Microscopic thermal-group capture cross section (barns).
	37-48 Microscopic thermal-group fission cross section (barns).
	49-60 Number of neutrons emitted per fission in the thermal group.
	61-72 Microscopic thermal-group transport cross section (barns).
<u>09</u>	Thermal Cross-section Data (I2,10X,A6,6X,2E12.5)
	Cols. 13-18 Nuclide identification label.
	25-36 Microscopic thermal n- α cross section (barns).
	37-48 Microscopic thermal n-p cross section (barns).
<u>10</u>	Weighting Spectrum Data (I2,10X,3(I6,E12.5))
	Cols. 13-18 Fine-group number.
	19-30 Fine-group weighting spectrum.
	31-36 Fine-group number.
	37-48 Fine-group weighting spectrum.
	49-54 Fine-group number.
	55-66 Fine-group weighting spectrum.
<u>11</u>	Print Selection Options (I2,10X,6I6)
	Cols. 7-12 If nonzero, edit average microscopic-group cross sections summed over all contributing resonances in the resolved resonance region. Also edit point values of microscopic cross sections averaged over Porter-Thomas distributions in the unresolved region.
	13-18 If nonzero, edit average microscopic-group cross sections for each resonance in the resolved resonance region.

Card
Type

Description

11

(Contd.)

Cols. 19-24	If nonzero, edit microscopic average fine-group cross sections computed from linear-segment data.
25-30	If nonzero, edit homogenized macroscopic fine-group and ultrafine-group cross sections. Also edit fission spectrum.
31-36	If nonzero, edit fine- and ultrafine-group fluxes for each buckling iteration.
37-42	If nonzero, edit ultrafine-group material macroscopic elastic removal cross sections, elastic transport cross sections, and elastic transfer cross sections.

10. Data Module B.HOMOGa. Data Module Name

B.HOMOG.

b. Description

Binary version of homogenization input.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X	X	NUI001	Cross-section Homogenization Specifications
	X	NUC001	Cross-section Homogenization
X		FCI001	Fuel-cycle Specifications

e. Structure and Content

Record Types 1 and 2 to specify material mixtures followed by Record Types 3 and 4 to specify composition structures. Record Types 1 and 3 as well as 2 and 4 are identical in structure.

Record Type 1

<u>Variable Name</u>	<u>Description</u>
MSLTH	Length of material mix table in Record Type 2.
NMAT	Number of materials.
NIS02	Number of isotopes in list in Record Type 2.

Record Type 2

<u>Variable Name</u>	<u>Description</u>
DIMIX(I), I = 1, MSLTH	Mix table. [†]
ATMDEN(I), I = 1, MSLTH	Atomic density table. [†]

[†]Use of tables DIMIX and ATMDEN, DMMIX and VOLFRG.

<u>Variable Name</u>	<u>Description</u>
MSPEC(J), J = 1, NMAT	Number of isotopes comprising each material. [†]
DITBL(K), K = 1, NIS02	List of all isotopes used in this module, with each isotope label appearing once.
DMTBL(J), J = 1, NMAT	Labels of materials.

Record Type 3

<u>Variable Name</u>	<u>Description</u>
MCSLTH	Length of composition mix table in Record Type 4.
NCMP	Number of compositions.
NMAT	Number of materials.

Record Type 4

<u>Variable Name</u>	<u>Description</u>
DMMIX(I), I = 1, MCSLTH	Mix table. [†]
VOLFRC(I), I = 1, MCSLTH	Volume fraction table. [†]
MCSPEC(J), J = 1, NCMP	Number of materials comprising each composition. [†]
DMTBL(K), K = 1, NMAT	List of all materials used in this module with each material label appearing once. Same as DMTBL in Record Type 2.
DCTBL(J), J = 1, NCMP	Labels of compositions.

The material labelled DMTBL(J) in Record Type 2 is made up from MSPEC(J) isotopes, which are named in order in DIMIX and used with corresponding atomic densities in ATMDEN. The index of the first element in DIMIX and ATMDEN for material J is L(J), where

$$L(J) = 1 + \sum_{j=1}^{J-1} \text{MSPEC}_j.$$

Composition tables DMMIX and VOLFRC are used in the same manner with MCSPEC(J) to define composition DCTBL(J).

[†]Use of tables DIMIX and ATMDEN, DMMIX and VOLFRC.

11. Data Module BCa. Data Module Name

BC.

b. Description

Boundary-condition specifications.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
	X	NUC002 1D-Diffusion
	X	NUC003 1D-Transport
	X	NUC004 2D-Diffusion
	X	NUC005 2D-Transport
	X	NUE001 Neutronics Output Manipulation
	X	AJC001 Neutron Inventory
	X	AJC002 Diffusion Perturbation
	X	AJC003 Transport Perturbation

e. Structure and Content

(1) Structure. One descriptive Record Type 1, followed by NVB and then NHB records of Type 2.

(2) Record Type 1. For one-dimensional geometry, words 4-6 are 0.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NBCL	Boundary-condition type number, left side (I = 1).
2	NBCR	Boundary-condition type number, right side (I = NPTI).

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
3	NVB	Number of vertical faces for which boundary or interface conditions are given.
4	NBCB	Boundary-condition type number, bottom of reactor ($J = 1$).
5	NBCT	Boundary-condition type number, top of reactor ($J = \text{NPTJ}$).
6	NHB	Number of horizontal faces for which boundary or interface conditions are given.

(3) Record Type 2. One record given for each side of each face for which a boundary or interface condition is given. Each record always contains 10 words.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	MFACE	Mesh point number and side indicator for which this record refers. Sign of MFACE tells side of face reference. Example: for left reactor boundary $\text{MFACE} = +1$. ($1 \leq \text{MFACE} \leq \text{NPTI}$ for vertical interfaces: $1 \leq \text{MFACE} \leq \text{NPTJ}$ for horizontal interfaces.)
2	M1	Point number defining beginning of interval along this face.
3	M2	Point number defining end of interval along this face. $M1 < M2$.
4	NBIT	Type number of boundary or interface condition. (See boundary and interface conditions below.)
5	JI	Initial higher-energy group number to which this set of constants apply.
6	JF	Final lower-energy group number to which this set of constants apply.
7-10	C1, C2, C3, C4	Constants used in formulas for Types 1, 2 or 3. Unused constants are 0.

Boundary and Interface Conditions

<u>Type</u>	<u>Description and Formula</u>
1	General boundary: $C1 \cdot \phi' + C2 \cdot \phi = C3$
2	General boundary: $C1 \cdot D \cdot \phi' + C2 \cdot \phi = C3$, where D is energy-dependent diffusion coefficient.
3	General interface: $\phi_{i+1} = C1 \cdot \phi_i + C2 \cdot \phi_i'$ $\phi_{i+1}' = C3 \cdot \phi_i + C4 \cdot \phi_i'$
7	Incoming flux = 0
8	Reflective
9	Periodic
10	White

Types 1-3 and 9 are used in diffusion theory, Types 7-10 in transport theory.

Since boundary and interface conditions are given in records of Type 2 for each side of every face, $NVB = 2 + 2 \cdot NVI$ and $NHB = 2 + 2 \cdot NHI$, where NVI and NHI are the number of horizontal and vertical interfaces, respectively. When constants are given by energy range as well as by position, NVB and NHB are the actual numbers of records applied to give all constants used. The constants, C1, C2, C3, and C4, are always given with respect to the side of the face being referenced; if C1 is positive on the left side of a face, where $MFACE < 0$ and $NBIT = 1$ or 2, then C1 is negative on the right side, where $MFACE > 0$ and NBIT is the same. For $NBIT = 3$, the adjoint of the matrix

$$\begin{pmatrix} C1 & C2 \\ C3 & C4 \end{pmatrix}$$

is given on the second side of the face.

The only difference between Types 1 and 2 is that the program module inserts D in Type 2, using the diffusion coefficient of the composition on the side of the mesh line determined by the sign of MFACE.

12. Data Module BRNa. Data Module Name

BRN.

b. Description

A dump of all variables used in the fuel cycle Module FCC001 and tables to describe the structure.

c. Specifications

Reference: A. S. Kennedy, POINTR, A Dynamic Storage Allocation Program, ANL-AMD, Tech. Memo. No. 98 (February 28, 1967).

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		FCI001 Fuel-cycle Specifications
X	X	FCC001 Fuel Cycle

e. Structure and Content

Four records

(1) Logical Record 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	KFLAG	Flag to determine program flow: 0 First entry into FCC001. 1 A neutronics calculation has just been done.
2	NAME (Real *8)	Variable in common block NAMBLK.
3	NPERR	Number of errors encountered in POINTR.
4	LSTBLK	Last location used by POINTR.
5	MAXBLK	Array size for POINTR.
6	IPRINT	Print flag for POINTR.

(2) Logical Record 2

<u>Variable Name</u>	<u>Description</u>
NAMLST(I), I = 1, 401 (Real *8)	Common block TABLES used by POINTR.

(3) Logical Record 3

<u>Variable Name</u>	<u>Description</u>
ARRAY(I), I = 1, LSTBLK	Array of variables (common block BLK).

(4) Logical Record 4

<u>Variable Name</u>	<u>Description</u>
NOUT(I), I = 1, 250	Single variables used by FCC001 and pointers for arrays (common block SING).

13. Data Module B.XSSPCa. Data Module Name

B.XSSPC.

b. Description

Binary representation of EBCDIC input data.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		CSI001 Epithermal Cross-section Specifications
	X	CSC001 Resonance Cross Sections
	X	CSC002 Nonresonant Cross Sections and Fundamental-mode Spectrum
	X	CSC004 Broad-group Cross Sections and Fundamental-mode Spectrum

e. Structure and Content

Two records: .Record Type 1, followed by Record Type 2 if
IYOS $\neq$ 0; or by Record Type 3 if IYOS = 0.

(1) Record Type 1

NOI,NOBG,NOBGB,(DENT(I),I=1,10),(NUCID(I),ADEN(I),CCONC(I),FCONC(I),
NELMO(I),TEMP(I),I=1,NOI)(CGB(I),LGBN(I),I=1,NOBGB),DELU,DELUN,
EMAX,EMIN,EPSABS,EPSINT,EPSTOT,FACA,IA,IOPT,IYOS,KT1,KT2,KT3,
KT4,KT5,KT6,KT7,KTFLUX,MTOT,NDELU,NGEOM,NINT,NINTC,NJINT,
NMIC,NSORS,NTHRM,RADC,RADP

<u>Variable Name</u>	<u>Description</u>
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NOI	Number of materials in this problem.
NOBG	Number of broad groups.
NOBGB	NOBG + 1.
DENT	Problem identification.

<u>Variable Name</u>	<u>Description</u>
NUCID(I)	Nuclide identification on library tape. Real *8.
ADEN(I)	Atomic concentrations used to compute homogenized macroscopic cross sections for use in fundamental-mode calculations (atoms/cc x 10^{-24}).
CCONC(I)	Nuclide concentrations in outer region (atoms/cc x 10^{-24}).
FCONC(I)	Nuclide concentrations in fuel pin (atoms/cc x 10^{-24}).
NELMO(I)	>0, Legendre treatment used for elastic scattering for material NUCID(I). (NELMO should be 0 for hydrogen.)
TEMP(I)	Nuclide temperature ($^{\circ}$ K).
CGB(I)	Broad-group upper-boundary energy.
LGBN(I)	Lethargy-group boundary.
DELU	Ultrafine-group lethargy width.
DELUN	Fine-group lethargy width.
EMAX	Upper energy limit of highest-energy group (EV).
EMIN	Energy interface between thermal and epithermal group.
EPSABS	Resolved resonances that produce a $\sigma < \text{EPSABS}$ at the energy limits of an ultrafine group and do not lie within the group are not included in the effective ultrafine-group cross sections for that group. EPSABS is typically 0.001 barn.
EPSINT	Relative convergence criterion for integration to generate ultrafine-group cross sections in the resolved resonant region. EPSINT is typically 0.0005.
EPSTOT	Resolved resonances that produce an average $\sigma_t < \text{EPSTOT}$ at the energy limits of an ultrafine group and do not lie within the group are treated as having a constant average value over the group.
FACA	The constant a , used to improve the rational approximation to the escape probability. FACA is typically 1.35.
IA	>0, edit ultrafine-group material macroscopic elastic removal cross sections, elastic transport cross sections, and elastic transfer materials. = 0, no edit of ultrafine-group elastic cross sections.
IOPT	= 1, P1 fundamental-mode calculation. = 2, consistent B1 fundamental-mode calculations for isotropic neutronics.

<u>Variable Name</u>	<u>Description</u>
IOPT (Contd.)	<p>= 3, consistent P1 fundamental-mode calculation for isotropic neutronics.</p> <p>= 4, consistent B1 fundamental-mode calculation for anisotropic neutronics.</p> <p>= 5, consistent P1 fundamental-mode calculation for anisotropic neutronics.</p>
IYOS	>0, input weighting spectrum appears with problem data, and fundamental-mode spectrum is not generated.
KT1	>0, edit ultrafine-group average microscopic cross sections summed over all contributing resonances in the resolved resonance region. Also edit point values of microscopic cross sections averaged over Porter-Thomas distributions in the unresolved resonance region.
KT2	>0, edit ultrafine-group average microscopic cross sections for each resonance in the resolved resonance region.
KT3	>0, edit microscopic fine-group average cross sections computed from nonresonant linear segment data.
KT4	>0, edit homogenized macroscopic fine-group and ultrafine-group average cross sections. Also edit fission spectrum for fine groups.
KT5	>0, edit for code-debugging purposes.
KT6	>0, edit fine- and ultrafine-group fluxes for each buckling iteration.
KT7	Hydrogen flag, set by program.
KTFLUX	<p>= 1, $1/E$ weighting spectrum used for fine-group cross sections.</p> <p>= 2, constant weighting spectrum used for fine-group cross sections.</p> <p>= 3, E weighting spectrum used for fine-group cross sections.</p>
MTOT	Number of materials for which NELMO(I) > 0.
NDELU	<p>= 1, all-fine-group problem.</p> <p>= 2, ultrafine-group problem.</p>
NGEOM	Fuel pin geometry, 1 = slab, 2 = cylinder.

<u>Variable Name</u>	<u>Description</u>
NINT	Number of ultrafine groups in problem.
NINTC	Number of fine groups in problem.
NJINT	>0, flux-correction factor in unresolved resonance calculation set to unity.
NMIC	= 0, calculate microscopic and macroscopic broad group cross sections. >0, broad-group cross sections not calculated.
NSORS	Library identification number for fission source.
NTHRM	>0, read in thermal-group cross sections with problem data. = 0, code sets thermal fluxes and cross sections to zero.
RADC	Radius of outer cladding-coolant region i if NGEOM = 2; outer bound of cladding-coolant region relative to center of fuel slab if NGEOM = 1; in cm.
RADP	Radius of fuel pin if NGEOM = 2; half-thickness of fuel slab if NGEOM = 1; in cm.

(2) Record Type 2 (Present if IYOS $\neq$ 0)

NINTC,(PHIC(I),I=1,NINTC)

<u>Variable Name</u>	<u>Description</u>
NINTC	Number of fine groups.
PHIC(I)	Fine-group weighting spectrum.

(3) Record Type 3 (Present if IYOS = 0)

IBSQ,BSQ,BSQ2,EPS

<u>Variable Name</u>	<u>Description</u>
IBSQ	>0, iterate on buckling to critical.
BSQ	First guess for buckling.
BSQ2	Second guess for buckling.
EPS	Convergence criterion on $ k_{\text{eff}} - 1 $.

14. Data Module ES.D1Da. Data Module Name

ES.D1D.

b. Description

One-dimensional distributed external source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
	X	NUC002	1D-Diffusion
	X	NUC003	1D-Transport
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory

e. Structure and Content

Two records.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals.
2	NGROUP	Number of energy groups.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FSEXT(I,J), I=1, NINTI), J=1, NGROUP))	Fixed source at interval I, energy group J.

15. Data Module ES.D2Da. Data Module Name

ES.D2D.

b. Description

Two-dimensional distributed external source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
	X	NUC004	2D-Diffusion
	X	NUC005	2D-Transport
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory

e. Structure and Content

Record Type 1 followed by NGROUP records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NGROUP	Number of energy groups.

(2) Record Type 2

NGROUP records.

<u>Variable Name</u>	<u>Description</u>
((FSEXT(I,J), I=1, NINTI), J=1, NINTJ)	Fixed source at interval (I,J).

16. Data Module ES.D1SHa. Data Module Name

ES.D1SH.

b. Description

One-dimensional shell source.

c. Specifications

Standard.

d. Program Modules That Create (C) or READ (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
	X	NUC003 1-D-Transport

e. Structure and Content

One Record Type 1 followed by NSPEC records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NORDER	Number of highest anisotropy (NORDER = 0 when none present).
2	NGROUP	Number of energy groups.
3	NSPEC	Number of sources specified.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
INT	I-direction interval number.
(SHELL(I), I=1, NGROUP)	Isotropic component of shell source.
((SHELLI(I,N), I=1, NGROUP), N=1, NORDER)	Anisotropic component of shell source (SHELLI not present for NORDER = 0).

17. Data Module ES.D2SHa. Data Module Name

ES.D2SH.

b. Description

Two-dimensional shell source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutrons Specifications
	X	NUC005 2D-Transport

e. Structure and Content

One Record Type 1 followed by NSPEC records of Type 2, one for each shell source. Each shell source runs across in the mesh interval at $J = J2$ from interval $I = I1$ through $I = I2$, and then "down" in $I = I2$ from $J = J2$ through $J = J1$.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NORDER	Number of highest anisotropy (NORDER = 0 when none present).
2	NGROUP	Number of energy groups.
3	NSPEC	Number of sources specified.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
I1	I-direction interval number of "left" end of shell source.
I2	I-direction interval number of "right" end.

Variable NameDescription

J1

J-direction interval number of "lower" end.

J2

J-direction interval number of "top" end.

(SHELL(I,N), I=1, NGROUP)

Isotropic component of shell source.

((SHELLI(I,N), I=1, NGROUP),
N=1, NORDER)I-direction component of anisotropic
shell source (SHELLI not present when
NORDER = 0).((SHELLJ(I,N), I=1, NGROUP),
N=1, NORDER)J-direction component of anisotropic
shell source (SHELLJ not present when
NORDER = 0).

18. Data Module FA.D1a. Data Module Name

FA.D1.

b. Description

One-dimensional adjoint flux.

c. Specifications

More than one generation may exist.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC002	1D-Diffusion
X	X	NUC003	1D-Transport
X	X	NUC006	Diffusion-mesh Refinement
X	X	NUC007	Transport-mesh Refinement
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory
	X	AJC002	Diffusion Perturbation
	X	AJC003	Transport Perturbation

e. Structure and Content

Two records.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NGROUP	Number of energy groups.
3	EVALUE	Eigenvalue that corresponds to this set of fluxes.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
4	KIND	-1 for input guess values. +1 for guess taken from real flux diffusion-theory problem. +2 for guess taken from real flux transport-theory problem. +3 for adjoint diffusion-theory flux. +4 for adjoint transport-theory flux.
5	ITER	Iteration (or generation) number of this set: ITER = 0 if KIND < 0; ITER is meaningless if KIND = 1 or 2.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FANI(I,J), I=1, NINTI), J=1, NGROUP)	Adjoint flux by interval and energy group.

19. Data Module FA.D2a. Data Module Name

FA.D2.

b. Description

Two-dimensional adjoint flux.

c. Specifications

More than one generation may exist.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
	X	NUC004	2D-Diffusion
	X	NUC005	2D-Transport
	X	NUC006	Diffusion-mesh Refinement
	X	NUC007	Transport-mesh Refinement
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory
	X	AJC002	Diffusion Perturbation
	X	AJC003	Transport Perturbation

e. Structure and Content

Record Type 1 followed by NGROUP records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NGROUP	Number of energy groups.
4	EVALUE	Eigenvalue which corresponds to this set of fluxes.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
5	KIND	-1 for input guess values. +1 for guess taken from real flux diffusion theory problems. +2 for guess taken from real flux transport theory problems. +3 for adjoint diffusion theory flux. +4 for adjoint transport theory flux.
6	ITER	Iteration (or generation) number of this set: ITER = 0 if KIND < 0. ITER is meaningless if KIND = 1 or 2.

(2) Record Type 2

NGROUP Records

<u>Variable Name</u>	<u>Description</u>
((FAN2(I,J), I=1, NINTI), J=1, NINTJ)	Adjoint flux by interval and energy group.

20. Data Module FA.D1Aa. Data Module Name

FA.D1A.

b. Description

One-dimensional adjoint angular flux.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
X	X	NUC003 1D-Transport
	X	NUE001 Neutronics Output Manipulation

e. Structure and Content

One descriptive record and a block of NGROUP records of angular flux.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals.
2	NUMDIR	Number of directions.
3	NGROUP	Number of energy groups.
4	KIND	Source of flux: KIND = -1 for input from cards, +2 for output from a real transport calculation, +4 for output from an adjoint transport calculation.
5	ITER	Iteration (or generation) number of this set (ITER = 0 when KIND < 0).

(2) Record Type 2

One for each energy group.

<u>Variable Name</u>	<u>Description</u>
((FLXA(I,J), I=1, NINTI), J=1, NUMDIR)	Angular flux for interval I, at direction J.

21. Data Module FA.D2Aa. Data Module Name

FA.D2A.

b. Description

Two-dimensional adjoint angular flux.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC005	2D-Transport
	X	NUE001	Neutronics Output Manipulation

e. Structure and Content

One descriptive record followed by NGROUP blocks, each composed of NUMDIR records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NUMDIR	Number of directions.
4	NGROUP	Number of energy groups.
5	KIND	Source of flux: KIND = -1 for input from cards, +2 for output from a real transport calculation, +4 for output from an adjoint transport calculation.
6	ITER	Iteration (or generation) number of this set (ITER = 0 when KIND $\leq$ 0).

(2) Record Type 2

One for each energy group at each direction.

<u>Variable Name</u>	<u>Description</u>
((FLXA(I,J), I=1, NINTI, J=1, NINTJ)	Angular flux for interval (I,J).

22. Data Module FR.D1a. Data Module Name

FR.D1.

b. Description

One-dimensional real flux.

c. Specifications

More than one generation may exist.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC002	1D-Diffusion
X	X	NUC003	1D-Transport
X	X	NUC006	Diffusion-mesh Refinement
X	X	NUC007	Transport-mesh Refinement
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory
	X	AJC002	Diffusion Perturbation
	X	AJC003	Transport Perturbation

e. Structure and Content

Two records.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NGROUP	Number of energy groups.
3	EVALUE	Eigenvalue that corresponds to this set of fluxes.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
4	KIND	-1 for input guess values. +1 for real diffusion-theory fluxes. +2 for real transport-theory fluxes. +3 for guess from adjoint diffusion theory. +4 for guess from adjoint transport theory.
5	ITER	Iteration (or generation) number of this set: ITER = 0 if KIND < 0. ITER is meaningless if KIND = 3 or 4.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FRN1(I,J), I=1, NINT1), J=1, NGROUP)	Real flux by interval and energy group.

23. Data Module FR.D2a. Data Module Name

FR.D2

b. Description

Two-dimensional real flux.

c. Specifications

More than one generation may exist.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC004	2D-Diffusion
X	X	NUC005	2D-Transport
X	X	NUC006	Diffusion-mesh Refinement
X	X	NUC007	Transport-mesh Refinement
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory
	X	AJC002	Diffusion Perturbation
	X	AJC003	Transport Perturbation

e. Structure and Content

Record Type 1 followed by NGRQUP records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NGROUP	Number of energy groups.
4	EVALUE	Eigenvalue which corresponds to this set of fluxes.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
5	KIND	-1 for input guess values. +1 for real diffusion theory fluxes. +2 for real transport theory fluxes. +3 for guess from adjoint diffusion theory. +4 for guess from adjoint transport theory.
6	ITER	Iteration (or generation) number of this set: ITER = 0 if KIND < 0. ITER is meaningless if KIND = 3 or 4.

(2) Record Type 2

NGROUP Records.

<u>Variable Name</u>	<u>Description</u>
((FRN2(I,J), I=1, NINTI), J=1, NINTJ)	Real flux by interval and energy group.

24. Data Module: FR.D1A

a. Data Module Name

FR.D1A.

b. Description

One-dimensional real angular flux.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
X	X	NUC003 1D-Transport
	X	NUE001 Neutronics Output Manipulation

e. Structure and Content

One descriptive record followed by NGROUP records of angular flux.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals.
2	NUMDIR	Number of directions.
3	NGROUP	Number of energy groups.
4	KIND	Source of flux: KIND = -1 for input from cards, +2 for output from a transport calculation.
5	ITER	Iteration (or generation) number of this set (ITER = 0 when KIND < 0).

(2) Record Type 2

One for each energy group.

<u>Variable Name</u>	<u>Description</u>
((FLXA(I,J), I=1, NINTI), J=1, NUMDIR)	Angular flux for interval I, at direction J.

25. Data Module FR.D2Aa. Data Module Name

FR.D2A.

b. Description

Two-dimensional angular flux.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC005	2D-Transport
	X	NUE001	Neutronics Output Manipulation

e. Structure and Content

One descriptive record followed by NGROUP blocks, each composed of NUMDIR records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NUMDIR	Number of directions.
4	NGROUP	Number of energy groups.
5	KIND	Source of flux: KIND = -1 for input from cards, +2 for output from a real transport calculation, +4 for output from an adjoint transport calculation..
6	ITER	Iteration (or generation) number of this set (ITER = 0 when KIND < 0).

(2) Record Type 2

One for each energy group at each direction.

<u>Variable Name</u>	<u>Description</u>
((FLXA(I,J), I=1, NINTI), J=1, NINTJ)	Angular flux for interval (I,J).

26. Data Module FR.PNa. Data Module Name

FR.PN.

b. Description

Power-normalized real flux.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUE001 Neutronics Output Manipulation
	X	FCC001 Fuel Cycle

e. Structure and Content

Two records.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NREG	Number of regions.
2	NGROUP	Number of energy groups.
3	EVALUE	Eigenvalue corresponding to the point-group flux matrix given in FR.D1.
4	KIND	Kind of flux, as in FR.D1.
5	ITER	Iteration number of set, as in FR.D1.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FP(I,J), I=1, NGROUP), J=1, NREG)	Power-normalized flux for each group I and region J.

27. Data Module FSA.D1a. Data Module Name

FSA.D1.

b. Description

One-dimensional adjoint fission source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
X		NUC003 1D-Transport
	X	NUE001 Neutronics Output Manipulation
	X	AJC001 Neutron Inventory

e. Structure and Content

One Record Type 1 and one Record Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NORONE	Number of energy groups, NGROUP, if source is group-dependent. Otherwise 1.
3	KIND	-1 for initial. +1 for real diffusion theory. +2 for real transport theory. +3 for adjoint diffusion theory. +4 for adjoint transport theory.
4	ITER	Iteration number.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FS(I,J), I=1, NINTI), J=1, NORONE)	Fission source from group J.

28. Data Module FSA.D2a. Data Module Name

FSA.D2.

b. Description

Two-dimensional adjoint fission source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
X	X	NUC005 2D-Transport
	X	NUE001 Neutronics Output Manipulation
	X	AJC001 Neutron Inventory

e. Structure and Content

One Record Type 1 followed by 1 or NGROUP records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NORONE	Number of energy groups, NGROUP, if source is group-dependent. Otherwise 1.
4	KIND	-1 for initial. +1 for real diffusion theory. +2 for real transport theory. +3 for adjoint diffusion theory. +4 for adjoint transport theory.
5	ITER	Iteration number.

(2) Record Type 2

NORONE records.

<u>Variable Name</u>	<u>Description</u>
((FS(I,J), I=1, NINTI), J=1, NINTJ)	Fission source for group J.

29. Data Module FSR.D1a. Data Module Name

FSR.D1.

b. Description

One-dimensional real fission source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUI003 Neutronics Specifications
X	X	NUC003 1D-Transport
	X	NUE001 Neutronics Output Manipulation
	X	AJC001 Neutron Inventory

e. Structure and Content

One Record Type 1 and one Record Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NORONE	Number of energy groups, NGROUP, if source is group-dependent. Otherwise 1.
3	KIND	-1 for initial. +1 for real diffusion theory. +2 for real transport theory. +3 for adjoint diffusion theory. +4 for adjoint transport theory.
4	ITER	Iteration number.

(2) Record Type 2

<u>Variable Name</u>	<u>Description</u>
((FS(I,J), I=1, NINTI), J=1, NORONE)	Fission source from group J.

30. Data Module FSR.D2a. Data Module Name

FSR.D2.

b. Description

Two-dimensional real fission source.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
X	X	NUC005	2D-Transport
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory

e. Structure and Content

— One Record Type 1 followed by NORONE records of Type 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NINTI	Number of intervals, I-direction.
2	NINTJ	Number of intervals, J-direction.
3	NORONE	Number of energy groups, NGROUP, if source is group-dependent. Otherwise 1.
4	KIND	-1 for initial. +1 for real diffusion theory. +2 for real transport theory. +3 for adjoint diffusion theory. +4 for adjoint transport theory.
5	ITER	Iteration number.

(2) Record Type 2

NORONE records.

<u>Variable Name</u>	<u>Description</u>
((FS(I,J), I=1, NINTI), J=1, NINTJ)	Fission source from group J.

31. Data Module GEOMa. Data Module Name

GEOM.

b. Description

Geometry data.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI002	Geometry Specifications
	X	NUI003	Neutronics Specifications
	X	NUI004	1D-Transport Specifications
	X	NUI005	2D-Transport Specifications
	X	NUC002	1D-Diffusion
	X	NUC004	2D-Diffusion
X	X	NUC003	1D-Transport
X	X	NUC005	2D-Transport
X	X	NUC006	Diffusion-mesh Refinement
X	X	NUC007	Transport-mesh Refinement
X	X	NUC008	Criticality Search
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory
	X	AJC002	Diffusion Perturbation
	X	AJC003	Transport Perturbation

e. Structure and Content

Record Types 1-5 and Record Type 9 are always present (with default options inserted by NUI002). Record Types 6, 7, and/or 8 are present on option.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Default</u>	<u>Description</u>
1	NDIM		Number of dimensions given in geometry, NDIM = 1, 2, or 3.
2	NGEOM		Type of geometry: 1 for slab 2 for cylinder 3 for sphere 4 for x-y 5 for r-z 6 for r- θ 7 for x-y with 45° symmetry 8 for r-z inverted.
3	NPTI		Number of points, I-direction.
4	NPTJ	(1)	Number of points, J-direction.
5	NINTI	(1)	Number of intervals, I-direction, NINTI = NPTI - 1.
6	NINTJ	(1)	Number of intervals, J-direction, NINTJ = NPTJ - 1.
7	NREG	(1)	Number of regions.
8	NCMP	(1)	Number of compositions.
9	NAREA	(1)	Number of areas.
10	LAREA	(0)	Length of Record Type 6.
11	NZONE	(1)	Number of zones.
12	LZONE	(0)	Length of Record Type 7.
13	NFIN	(0)	Number of finite geometry type from table below. (NFIN = 0 if geometry is infinite; Card Types 10, 20, 30, 40, 50, 60.)
14	NIL	(0)	Number of finite directions (and integration limits) per region, for this type NFIN.

Finite Geometry Options

<u>Card Input Type in A.NIP</u>	<u>NGEOM</u>	<u>NFIN</u>	<u>NIL</u>	<u>Type Geometry</u>
11	1	1	1	Cylindrical slab.
12	1	2	1	Slab finite in y direction.
13	1	3	2	Slab finite in both y and z directions.
21	2	4	1	Finite cylinder.
41,43	4,7	5	1	x-y finite in z direction.
61	6	6	1	r- θ finite in z direction.

(2) Record Type 2

Mesh structure.

<u>Variable Name</u>	<u>Description</u>
XMESH (I), I=1, NPTI	I-direction abscissas.
YMESH (J), J=1, NPTJ	J-direction ordinates (default 0.0).

(3) Record Type 3

Region-mesh correspondence.

((MR(I,J), I=1, NINTI), J=1, NINTJ)	Region index. (If MR(I,J) = N, then REG(N) is the region label in this mesh space.)
--	---

(4) Record Type 4

Composition-mesh correspondence.

((MC(I,J), I=1, NINTI), J=1, NINTJ)	Composition index. (If MC(I,J) = N, then CNAME(N) is the composition label in this mesh space.)
--	---

(5) Record Type 5

Composition-region correspondence.

NC(I), I=1, NREG	Composition index. (If NC(I) = N, the CNAME(N) is the composition label in this region.)
------------------	--

(6) Record Type 6

Area definitions; record present only when LAREA > 0.

Variable NameDescription

NREGA(I), I=1, NAREA

Number of regions in each area I.

LREGA

Length of vector NRA:

$$LREGA = \sum_{I=1}^{NAREA} NREGA(I).$$

NRA(I), I=1, LREGA

List of region indices. (If NRA(I) = N, then REG(N) is the region label for this portion of an area.)

(7) Record Type 7

Zone definitions; record present only when LZONE > 0.

NSECTZ(I), I=1, NZONE

Number of sections in each zone I.

LSECT

Length of vector NSB:

$$LSECT = 2 \text{NDIM} \sum_{I=1}^{NZONE} NSECTZ(I).$$

NSB(I), I=1, LSECT

List of section boundaries for each of the NSECTZ sections of each of the NZONE zones. Each section is defined by the first and second I-direction point numbers (followed by first and second J-direction point numbers for 2D geometry).

(8) Record Type 8. (Present only when NIL > 0)

((BSQ(I,J), I=1, NREG), J=1, NIL)

Buckling, by regions.

((H(I,J), I=1, NREG), J=1, NIL)

Actual half-heights for each region, in each finite direction.

((X(I,J), I=1, NREG), J=1, NIL)

Extrapolated half-heights for each region, in each finite direction
(X = H + extrapolated distance).

(9) Record Type 9 (Always present)

<u>Variable Name</u>	<u>Description</u>
(REG(I), I=1, NREG)	Region labels.
(CNAME(I), I=1, NCMP)	Composition labels.
(AREA(I), I=1, NAREA)	Area labels.
(ZONE(I), I=1, NZONE)	Zone labels.

Default values are blanks.

32. Data Module OUT.NMa. Data Module Name

OUT.NM.

b. Description

Neutronics output manipulations.

c. Specifications

Three files.

File 1 is a specification file that functions first as an input request list, later as a tabulation of the contents of the set.

File 2, always generated by the output manipulations module, contains basic quantities as volume elements, normalized real and adjoint fluxes, and interval integrated fluxes. It may be extended at a later time with additional input requests.

File 3 is not usually kept in binary form. It contains the specific nonbasic quantities to be edited in a specific run. It may be used as an overflow, temporary, intermediate storage area during module execution.

d. Program Modules That Create (C) or Read (R) Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI008	Neutronics Output Manipulation Specifications
X	X	NUE001	Neutronics Output Manipulation

e. Structure and Contents

(1) File 1. General specifications for program module, contents list of this data module. DNAME list is a table at end of this document.

(a) Record Type 1

<u>Variable Name</u>	<u>Description</u>
----------------------	--------------------

INFORM	Normalization to be applied to fluxes:
--------	--

	INFORM = 1 for no normalization.
--	----------------------------------

	2 for normalization to unit fission height.
--	---

	3 for power normalization using POWER.
--	--

<u>Variable Name</u>	<u>Description</u>
POWER	Power to which fluxes are normalized.
NGROUP	Number of energy groups.
NINTI	Number of intervals, I-direction.
NINTJ	Number of intervals, J-direction.
NREG	Number of regions.
NAREAO	Number of areas listed in this data module, Record Type 5. NAREAO = 0 signals that all areas defined in GEOM are to be used.
NZONEO	Number of zones listed in this data module, Record Type 6. NZONEO = 0 signals that all zones defined in GEOM are to be used.
LF2	Number of records expected in File 2.
MLF2	Maximum length of File 2, in records.
LC3	Number of Level 3 computations to be done.
LF3	Number of records expected in File 3, $LF3 \leq LC3$.
MLF3	Maximum length of File 3.
(INF2(J), J=1, MLF2)	INF2(J) is the index in the DNAME list of the Jth record in File 2. (The first LF2 values of INF2, only, are nonzero.)
(b) <u>Record Type 2</u>	
(INF3(J), J=1, LF3)	INF3(J) is the index in the DNAME list assigned as the Jth record in File 3.
(c) <u>Record Type 3</u> (Present only when $LF2 > 0$)	
(ISTAT2(I), I=1, MLF2)	Computational status of each element in the DNAME list for File 2. ISTAT 2 $\leq$ 0 if computation is to be performed. = 1 if no interest. > 0 if completed.

<u>Variable Name</u>	<u>Description</u>
(LOC2(I), I=1, MLF2)	Absolute value of LOC2(I) is the binary record number assigned the Ith element in the DNAME list; LOC2(I) < 0 if record has not yet been written. (Maximum value of LOC2(I) is LF2.)

(d) Record Type 4 (Present only when LC3 > 0)

(ISTAT3(I), I=1, MLF2)	Computational status of each element in the DNAME list for File 3 ISTAT 3 < 0 if computation is to be performed. = 0 if no interest. > 0 if present.
(LOC3(I), I=1, MLF3)	Absolute value of LOC3(I) is the binary record number assigned the Ith element in the DNAME list for File 3; LOC3(I) < 0 if record has not been written yet. (Maximum value of LOC3(I) is LF3.)

(e) Record Type 5 (Present only when NAREAO > 0)

(AR(I), I=1, NAREAO)	Area labels, as defined in Data Module GEOM.
----------------------	--

(f) Record Type 6 (Present only when NZONEO > 0)

(ZN(I), I=1, NZONEO)	Zone labels, as defined in Data Module GEOM
----------------------	---

(2) Files 2 and 3. Files 2 and 3 are made up of records chosen from the following types, according to the array structure necessary for the data they represent. The first two words of each always contain the data type number (index in DNAME list) and the record type number, from table below.

<u>Record Type No.</u>	<u>Structure</u>
1	One-dimensional arrays plus one sum quantity.
2	Two-dimensional arrays plus one sum quantity.
3	Three-dimensional arrays plus one sum quantity.

(a) Record Type 1Variable NameDescription

IDNAME

Index in DNAME list.

IRT

Record type = 1.

IMAX

Length of data, IMAX is number areas, regions, points, etc., as implicitly defined by data type.

SUM

$$\sum_{I=1}^{IMAX} DATA(I)$$

(DATA(I), I=1, IMAX)

(b) Record Type 2

IDNAME

IRT

Record type = 2.

IMAX

JMAX

$$SUM = \sum_I \sum_J DATA(I,J)$$

((DATA(I,J), I=1, IMAX), J=1, JMAX)

(c) Record Type 3

IDNAME

IRT

IMAX

JMAX

KMAX

$$SUM = \sum_I \sum_J \sum_K DATA(I,J,K)$$

((DATA(I,J,K), I=1, IMAX), J=1, JMAX), K=1, KMAX)

33. Data Module OUT.NMSa. Data Module Name

OUT.NMS.

b. Description

Special output manipulations specifications required to produce the Output Data Module FR.PN.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Modules

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X	X	NUI003 Neutronics Specifications
	X	NUE001 Neutronics Output Manipulation
X	X	FCC001 Fuel Cycle

e. Structure and Content

One four-word record.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	IDO	Control parameter: 0 to do nothing. 1 to do only those calculations required to generate FR.PN. 2 to follow instructions in OUT.NM but with current flux and power from this data set. Produce FR.PN.
2	ICREFV	Cross-reference volume-elements Flag: 0 to generate volume elements as needed without reference to OUT.NM. 1 to use volume elements in OUT.NM if they are present; if not present there, generate them and insert them into OUT.NM.
3	ICREFF	Flux cross reference: 1 to put these fluxes into File 2 of OUT.NM when full normalization complete.
4	POWER	Power for normalization, watts.

34. Data Module OUT.TR1a. Data Module Name

OUT.TR1.

b. Description

Binary data; convergence and error statistics.

c. Specifications

None.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		NUC003 1D-Transport

e. Structure and Content

Logical Record 1 (NGROUP = number of groups).

<u>Variable Name</u>	<u>Description</u>
(IXXII(I), I=1, NGROUP)	Number of outer iterations for which the inner-iteration maximum has been exceeded for group I (i.e., for which inner loop convergence has not been reached).
(IIXXNB(I), I=1, NGROUP)	Number of outer iterations for which the neutron balance error limit has been exceeded for group I.
EV_p	Current parameter being searched for, or the current value of k_{eff} .
λ_p	Fission source ratio.
LC	Angular flux pass count.

35. Data Module OUT.TR2a. Data Module Name

OUT.TR2.

b. Description

Binary data; convergence and error statistics.

c. Specifications

None.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	Program Module Name
X		NUC005 2D-Transport

e. Structure and Content

Logical Record 1 (NGROUP = number of groups)

Variable NameDescription

(IXXII(I), I=1, NGROUP)

IXXII(I) is the number of outer iterations for which the inner-iteration maximum has been exceeded for group I (i.e., for which inner loop convergence has not been reached).

(IIXXNB(I), I=1, NGROUP)

IIXXNB(I) is the number of outer iterations for which the neutron balance error limit has been exceeded for group I.

EV_p

The current parameter being searched for, or the current value of k_{eff} .

 λ_p

Fission-source ratio.

LC

Angular-flux pass count.

36. Data Module SP.CICNa. Data Module Name

SP.CICN.

b. Description

Code-independent constants specifications.

c. Specifications

Standard.

d. Program Modules Which Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
	X	NUI004	1D-Transport Specifications
	X	NUI005	2D-Transport Specifications
	X	NUC002	1D-Diffusion
	X	NUC003	1D-Transport
	X	NUC004	2D-Diffusion
	X	NUC005	2D-Transport
	X	NUE001	Neutronics Output Manipulation
	X	AJC001	Neutron Inventory

e. Structure and Content

One record, with general information agreeing with that in the data modules named in parentheses.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	MKRTHY	0 for real solution. 1 for adjoint solution. 2 for both real and adjoint solutions.
2	NGEOM	Geometry type number (GEOM).
3	NDIM	Number of dimensions (GEOM).
4	NINTI	Number of intervals, I-direction (GEOM).

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
5	NINTJ	Number of intervals, J-direction (GEOM).
6	NGROUP	Number of energy groups (XS.C.MIN).
7	IPOB	Type of problem (not consistent with SP.CRIT). 1 for inhomogeneous. 2 for k_{eff} convergence. 3 for concentration search. 4 for buckling search. 5 for α search. 6 for dimension search.
8	CONVCR	Standard convergence criterion for search. (A.NIP card 21, Cols. 37-48); (SP.CRIT).
9	X(1)	Initial search parameter. (A.NIP card 22, Cols. 13-24); SP.CRIT.
10	X(2)	Second search parameter. (A.NIP card 22, Cols. 25-36); (SP.CRIT).
11	ALPHA	α_0 or 0.0. (A.NIP card 3, Cols. 61-72).
12	FIXEDK	Fixed k_{eff} or 1.0 (A.NIP card 3, Cols. 49-60).

37. Data Module SP.CRITa. Data Module Name

SP.CRIT..

b. Description

Criticality search specifications.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		NUI003	Neutronics Specifications
	X	NUC003	1D-Transport
	X	NUC005	2D-Transport
	X	NUC008	Criticality Search

e. Structure and Content

One specification Record Type 1 and one modifier description record of Types 2, 3, or 4, if required. The general formula to obtain P, the parameter(s) being varied, for the ith iteration is

$$P_N^i = P_N^{i-1} + X^i \cdot \text{DMOD}_N,$$

where P_N is the preceding value of the same parameter(s), DMOD_N is the user's change quantities, given in this data set, X^i is a function, computed by the program module, of the pairs (X^{i-1}, k_{i-1}) and (X^{i-2}, k_{i-2}) and the desired value of the criticality parameter k or α (DSKEFF), and N is a vector or array index. The exact form of this formula and the definitions of X and DMOD depend also on the particular parameter or family of parameters. For those quantities related to A.NIP, the card number and pertinent columns are given in parentheses under Description: as (card, columns).

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	KSRCH	1 for concentration search. 2 for I-direction. 3 for J-direction. 4 for buckling. 5 for α . 6 for both I- and J-direction search (other values may be defined).
2	ICONV	0 when convergence is not yet attained.
3	LORP	1 for linear interpolation on X. 0 or 2 for parabolic interpolation on X.
4	NPMAX	Maximum number of passes (21, 19-24).
5	NPASS	Pass number (0, initially).
6	LSPR	Length of specification record (see record 2, 3, or 4 for value).
7	CONVCR	Convergence criterion (21, 37-48).
8	XL	Lower limit on the range of X_i (22, 37-48).
9	XU	Upper limit on the range of X_i (22, 49-60).
10	DSKEFF	Desired k_{eff} or desired α (if KFLAG=1); (21, 25-36).
11-13	(X(I), I=1,3)	X_i ; (22, 13-24, 25-36).
14	DKDX	Slope used to compute initial X(2) if X(2) has been given as 0. (22, 61-72).
15	DMOD	Change quantity when only one is necessary (otherwise 0). (26, 13-24).
16	KFLAG	0 to search to fixed k_{eff} , 1 to search to fixed α (21, 13-18).

(2) Record Type 2. For concentration searches. P_N is the set of volume fractions of materials comprising compositions in the XS.C Data Modules. $DMOD_N$ is the set of changes to those volume fractions; "pseudo-compositions" created using the $DMOD_N$ as volume fractions exist in the same composition data modules. This record correlates pseudo and actual compositions. (Card 23.) LSPR = NCMP.

<u>Variable Name</u>	<u>Description</u>
(MC(I), I=1, NCMP)	MC (I) is the composition number which is to be used as pseudocompositions with composition I. MC (I) is 0 if the Ith composition is not one of the basic compositions assigned to regions or if it is not to be altered in this search.
(3) <u>Record Type 3.</u> For dimension searches. Here $DMOD_N$ is a mesh increment. (Card 24.) $LSPR = NINTI + NINTJ$.	
NINTI	Number of intervals, I-direction.
NINTJ	Number of intervals, J-direction.
(DIMOD(I), I=1, NINTI)	I-direction modifiers. [†]
(DJMOD(I), I=1, NINTJ)	J-direction modifiers. [†]
(4) <u>Record Type 4.</u> For buckling searches. (Card 25.) $LSPR = NREG * NIL$.	
NREG	Number of regions
NIL	Number of integration limits for this geometry.
((DMOD(I,J), I=1, NREG), J=1, NIL)	Buckling modifiers. [†]

[†]All modifiers are given as 0 if they have not been otherwise specified.

38. Data Module SP.T1NEWa. Data Module Name

SP.T1NEW.

b. Description

Binary translation of part of the data module A.INPTR1.

c. Specifications

Two generations of this data module can exist at a given time.
Two files.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUC003 1D-Transport
X		NUI004 1D-Transport Specifications

e. Structure and Content

File 1 is always present. Logical Record Type 1 of File 2 is always present.

(1) File 1Logical Record 1

<u>Variable Name</u>	<u>Description</u>
MKRDF	0 if there are no density factors, NINTI if there are density factors, where NINTI is defined in Data Module GEOM.
MKRDTH	0 if diffusion-theory option is requested for no group; number of groups for which diffusion theory option is requested.
MKRSKI	0 if no group skipping is requested; number of groups to be skipped.
MKRANS	0 if no ℓ numbers are specified; number of compositions for which ℓ numbers are given explicitly.

<u>Variable Name</u>	<u>Description</u>
MAXII	Maximum number of inner iterations for each group.
MAXOI	Maximum number of outer iterations for this problem.
NUMDIR	Number of directions in the angular integration scheme.
ISN	The S_n order.
EPS	k_{eff} calculation convergence criterion.
PAROD	Parameter oscillation damper for criticality searches only.
CONNF	Normalization factor (0.0 means no normalization is to be performed).

End of file.

(2) File 2

Logical Record 1

(DIRWGT(I), DIRWGT(I) is a weight.
I=1, NUMDIR)

(DIRMU(I), DIRMU(I) is a direction cosine.
I=1, NUMDIR)

Logical Record 2 (Present only when MKRANS > 0)

(NAMANS(I), Where MKRANS is the number of compositions for
LNOANS(I), which an ℓ number is given explicitly,
I=1, MKRANS)

NAMANS(I) is the composition number of such a composition, and

LNOANS(I) is the ℓ number to be used for this composition.

Logical Record 3 (Present only when MKRDF > 0)

(CSCFAC(I), MKRDF is the number of mesh intervals and CSCFAC(I)
I=1, MKRDF) is the density factor for the Ith interval.

Logical Record 4 (Present only when MKRDTH > 0)

(MKRDT(K), MKRDTH is the number of groups for which diffusion,
K=1, MKRDTH) theory approximation will be used, and MKRDT(K) is
the group number of such a group.

Logical Record 5 (Present only when MKRSKI > 0)

(MKRDT(K), MKRSKI is the number of groups to be skipped, and
K=1, MKRSKI) MKRDT(K) is the group number of such a group.

39. Data Module SP.T2NEWa. Data Module Name

SP.T2NEW.

b. Description

Binary translation of part of the data module A.INPTR2.

c. Specifications

Two generations of this data module can exist at a given time.
Two files.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
	X	NUC005 2D-Transport
X		NUI005 2D-Transport Specifications

e. Structure and Content

File 1 is always present. Logical Record Type 1 of File 2 is always present.

(1) File 1Logical Record 1

<u>Variable Name</u>	<u>Description</u>
MKRDF	0 if there are no density factors, 1 if there are density factors.
MKRDTH	0 if diffusion-theory option is requested for no group; number of groups for which diffusion theory option is requested.
MKRSKI	0 if no group skipping is requested; number of groups to be skipped.
MKRANS	0 if no ℓ numbers are specified; number of compositions for which ℓ numbers are given explicitly.

<u>Variable Name</u>	<u>Description</u>
MAXII	Maximum number of inner iterations for all groups.
MAXOI	Maximum number of outer iterations for this problem.
NUMDIR	Number of directions in the angular integration scheme.
ISN	The S_n order.
EPS	K_{eff} calculation convergence criterion.
PAROD	Parameter oscillation damper for criticality searches only.
CONNF	Normalization factor (0.0 means no normalization is to be performed).

End of file.

(2) File 2

Logical Record 1

<u>Variable Name</u>	<u>Description</u>
(DIRWGT(I), I=1, NUMDIR), (DIRETA(I), I=1, NUMDIR), (DIRMU(I), I=1, NUMDIR)	DIRWGT(I) is a weight, and DIRETA(I) is a direction cosine, and DIRMU(I) is a direction cosine.

Logical Record 2 (Present only when MKRANS > 0)

(NAMANS(I), LNOANS(I), I=1, MKRANS)	NAMANS(I) is the composition number of such a composition LNOANS(I) is the ℓ number to be used for this composition.
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Logical Record 3 (Present only when MKRDF > 0)

(CSCFAC(I,J), I=1, NINTI, J=1, NINTJ)	NINTI and NINTJ are the numbers of mesh intervals in the I and J directions, defined in Data Module GEOM, and CSCFAC(I,J) is the density factor for the (I,J)th interval.
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Logical Record 4 (Present only when MKRDTH > 0)

(MKRDT(K), K=1, MKRDTH)	MKRDTH is the number of groups for which diffusion-theory approximation will be used, and MKRDT(K) is the group number of such a group.
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Logical Record 5 (Present only when MKRSKI > 0)

<u>Variable Name</u>	<u>Description</u>
(MKRDT(K), K=1, MKRSKI)	MRKSKI is the number of groups to be skipped, and MKRDT(K) is the group number of such a group.

40. Data Module XS.C.ANIa. Data Module Name

XS.C.ANI.

b. Description

Anisotropic, composition level total cross sections.

c. SpecificationsTwo files.d. Program Modules That Create (C) or Read (R) Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X	X	NUC001 Cross-section Homogenization
	X	NUI004 1D-Transport Specifications
	X	NUI005 2D-Transport Specifications
	X	NUC003 1D-Transport
	X	NUC005 2D-Transport
	X	NUE001 Neutronics Output Manipulation

e. Structure and Contents

Structure: One descriptive Record Type 1 in File 1 and NCMP Composition Blocks in File 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NCMP	Number of compositions in entire set.
2	NUMANI	Number of compositions with anisotropic components.
3	NGROUP	Number of energy groups.
4	MAXLNO	Maximum scattering order in set. (Scattering order = 1 plus, order of anisotropy.)
5	MAXUPS	Maximum number of groups of up-scattering.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
6	MAXDNS	Maximum number of groups of downscattering.
	(CNAME(I), I=1, NCMP)	Composition labels, indexed as Composition Blocks in File 2.

End of file.

Composition Block: One descriptive Record Type 2 and (LNO-1) records of Type 3.

(2) Record Type 2

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	LNO	Scattering order of this composition. (Scattering order = 1 plus order of anisotropy.)
2	MAXUP	Maximum number of groups of up-scattering, this composition.
3	LASCAT	Length of scattering list, LASCAT = MAXUP + 1 + number of groups of down-scattering.

(3) Record Type 3

One for each order of anisotropy, L = 1, 2, ..., LNO - 1.

<u>Variable Name</u>	<u>Description</u>
((SCAT(K,J), K=1, LASCAT), J=1, NGROUP)	Total anisotropic cross section for order L, into group J from the group indexed by K. K references J + MAXUP, J + MAXUP-1, ..., J, J-1, ..., J - (number groups downscattering).

41. Data Module XS.C.AUXa. Data Module Name

XS.C.AUX.

b. Description

Auxiliary, composition level cross sections; individual capture and scattering types.

c. Specifications

Two files.

d. Program Modules That Create (C) or Read (R) the Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X	X	NUC001	Cross-section Homogenization
	X	AJC001	Neutron Inventory
	X	AJC003	Transport Perturbation

e. Structure and Content

Structure: One descriptive Record Type 1 in File 1 and NCMP Composition Blocks in File 2.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NCMP	Number of compositions.
2	NGROUP	Number of energy groups.
3	MAXLNO	Maximum scatter order in set. (Scattering order = 1 plus order of anisotropy.)
	(CNAME(I), I=1, NCMP)	Composition labels, indexed as Composition Blocks in File 2.

End of File

Composition Block: One descriptive Record Type 2 and a set of LNO Scattering Blocks.

(2) Record Type 2 (Composition description)

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	LNO	Maximum scattering order of this composition. (Scattering order = 1 plus order of anisotropy.)
2	LIN	Inelastic scattering order of this composition.
3	LEL	Elastic scattering order of this composition.
4	LN2N	(n,2n) scattering order of this composition.
	(SCAP(I), I=1, NGROUP)	(n, γ) cross section.
	(SNALF(I), I=1, NGROUP)	(n, α) cross section.
	(SNP(I), I=1, NGROUP)	(n,p) cross section.

Scattering Block: One for each scattering order from 1 up to LNO (not present for LNO = 0). Consists of descriptive Record Type 3 and records of Types 4-9 according to values of LIN, LEL, and LN2N for this composition.

(3) Record Type 3 (Scattering description)

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NUP	Number of groups of upscattering for this order and composition.
2	LSCAT	Length of scattering list for this order and composition.

(4) Record Type 4 (Present only when order of Block is $\leq$ LIN)

<u>Variable Name</u>	<u>Description</u>
((XINEL(K,J), K=1, LSCAT), J=1, NGROUP)	Inelastic scattering cross section into group J from the group indexed by K, for this scattering order. K references J+NUP, J+NUP-1, ..., J, J-1, ..., J-(number groups of downscattering).

(5) Record Type 5 (Present only when order of Block is $\leq$ LEL)

<u>Variable Name</u>	<u>Description</u>
((XEL(K,J),K=1,LSCAT,J=1, NGROUP)	Elastic scattering cross section ordered as XINEL, Record Type 4.

(6) Record Type 6 (Present only when order of Block is $\leq$ LN2N)

((XN2N(K,J),K=1,LSCAT),J=1, NGROUP)	(n,2n) scattering cross section ordered as XINEL, Record Type 4.
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(7) Record Type 7 (Present only when order of Block is $\leq$ LIN)

(XTIR(J),J=1,NGROUP)	Total inelastic removal cross section.
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(8) Record Type 8 (Present only when order of Block is $\leq$ LEL)

(XTER(J),J=1,NGROUP)	Total elastic removal cross section.
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(9) Record Type 9 (Present only when order of Block is $\leq$ LN2N)

(XTN2NR(J),J=1,NGROUP)	Total (n,2n) removal cross section.
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42. Data Module XS.C.MINa. Data Module Name

XS.C.MIN.

b. Description

Minimal, composition level cross-section data.

c. Specifications

Two files.

d. Program Modules That Create (C) or Read (R) the Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X	X	NUC001	Cross-section Homogenization
	X	NUI002	Geometry Specifications
	X	NUI003	Neutronics Specifications
	X	NUI004	1D-Transport Specifications
	X	NUI005	2D-Transport Specifications
	X	All NUC Modules	
	X	NUE001	Neutronics Output Manipulation

e. Structure and Content

Structure: File 1 contains one descriptive record. File 2 may contain a Record Type 2. This is followed by NCMP Composition Blocks; each Composition Block contains a descriptive Record Type 3 and a Group Block of NGROUP Records.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NCMP	Number of compositions in entire set.
2	NGROUP	Number of energy groups.
3	ISCHI	Fission spectrum flag:
	$\text{ISCHI} = \begin{cases} 0 & \text{if there is no set-wide } \chi; \\ 1 & \text{if Record Type 2 is a vector;} \\ \text{NGROUP} & \text{if Record Type 2 is a matrix.} \end{cases}$	

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
4	NFCMP	Number of fissionable compositions.
5	NFAM	Number of families of delayed neutrons.
6	MAXUP }	Maximum number of groups of scattering, up and down, respectively, of all compositions in set.
7	MAXDN }	
	(CNAME(I), I=1, NCMP)	Composition labels, indexed as Composition Blocks in File 2.

End of File

(2) Record Type 2 (Present only when ISCHI > 0)

<u>Variable Name</u>	<u>Description</u>
((CHI(I,J), I=1, ISCHI), J=1, NGROUP)	Fission-fraction spectrum, from group I into group J.

Composition Block: One Record Type 3 immediately followed by NGROUP records of Type 4.

(3) Record Type 3

Composition Description

<u>Variable Name</u>	<u>Description</u>
ICHI	Fission spectrum flag of this composition: - 1, composition uses Set χ , Record Type 2; 0, composition not fissionable; 1, χ vector appears in records of Type 4; NGROUP, χ matrix given in records of Type 4.
(NUP(I), I=1, NGROUP)	
(NDN(I), I=1, NGROUP)	

Group Block(4) Record Type 4

Groups Constants

<u>Variable Name</u>	<u>Description</u>
J	Group number.
XA	Absorption cross section.
XTOT	Total cross section.
XREM	Removal cross section.
XTR	Transport cross section.
XF	Fission cross section, given only when $ICHI \neq 0$.
XNF	Number of neutrons emitted per fission times XF, given only when $ICHI \neq 0$.
(CHI(I), I=1, ICHI)	Fission fraction into group J from group I, given only when $ICHI > 0$.
(XSCATU(I), I=1, NUP(J))	Total scattering into group J from groups J + NUP(J), J + NUP(J) - 1, ..., J + 2, J + 1 (given only when $NUP(J) > 0$).
XSCATJ	Total self-scattering.
(XSCATD(I), I=1, NDN(J))	Total scattering into group J from groups J - 1, J - 2, ..., J - NDN(J) (given only when $NDN(J) > 0$).
PXNF	Number of prompt neutrons emitted per fission times XF, given only when $NFAM > 0$ and $ICHI \neq 0$.
DNCHI(I=1, NFAM)	Delayed-neutron fission-fraction spectrum (given only when $NFAM > 0$ and $ICHI \neq 0$).

43. Data Module XS.C.RESa. Data Module Name

XS.C.RES.

b. Description

Homogenized macroscopic resolved resonance fission, nu times fission and capture cross sections.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X		CSC001	Resonance Cross Sections
	X	CSC002	Nonresonant Cross Sections and Fundamental-mode Spectrum

e. Structure and Content

Structure: One record ordered from low-energy groups to high-energy groups.

Record Type 1

NINT1R,(HOMCAP(I),HOMBRG(I),HOMFIS(I),I=1,NINT1R)

<u>Variable Name</u>	<u>Description</u>
NINT1R	Number of resolved resonance groups.
HOMCAP(I)	Homogenized resonance capture cross section.
HOMBRG(I)	Homogenized resonance $\nu\sigma_f$.
HOMFIS(I)	Homogenized resonance fission cross section.

44. Data Module XS.I.RESa. Data Module Name

XS.I.RES.

b. Description

Resolved-resonance microscopic ultrafine-group cross sections.

c. Specifications

Two files.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		CSC001 Resonance Cross Sections
	X	CSC004 Broad-group Cross Sections and Fundamental-mode Spectrum

e. Structure and Content

Structure: One Record Type 1; one Record Type 2 for each resolved resonance group, ordered by increasing energy; one Record Type 3. End of file after Record Type 1.

(1) File 1Record Type 1

NINT1R,NOI

<u>Variable Name</u>	<u>Description</u>
NINT1R	Number of resolved resonance groups.
NOI	Number of isotopes.

(2) File 2Record Type 2

(AMICAP(I),AMIFIS(I),I=1,NOI)

<u>Variable Name</u>	<u>Description</u>
AMICAP(I)	Resolved capture resonance microscopic cross section.
AMIFIS(I)	Resolved fission resonance microscopic cross section.

Record Type 3

(PHIIN(I),PHIOUT(I),I=1,NINT1R)

<u>Variable Name</u>	<u>Description</u>
PHIIN(I)	Weighting spectra for resonance cross sections, inside fuel pin.
PHIOUT(I)	Weighting spectra for resonance cross sections, outside fuel pin

45. Data Module XS.ISOa. Data Module Name

XS.ISO.

b. Description

Microscopic group cross sections.

c. Specifications

Two files.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		CSC004 Broad-group Cross Sections and Fundamental-mode Spectrum
	X	NUC001 Cross-section Homogenization

e. Structure and Content

(1) File 1 Structure. Three or four records conditional on parameter ICHI.

(a) Record Type 1. NGROUP, NISO

<u>Variable Name</u>	<u>Description</u>
NGROUP	Number of groups in set.
NISO	Number of isotopes in set.

(b) Record Type 2. (ISONME(I), I=1, NISO), (LOCA(I), I=1, NISO)

<u>Variable Name</u>	<u>Description</u>
ISONME(I)	Name of Ith isotope (Real*8).
LOCA(I)	Number of records in second file to be skipped to read data for isotope I. (LOCA(1) = 0).

(c) Record Type 3. ICHI,(E(I), I=1, NGP1), (U(I), I=1, NGP1), (VEL(I), I=1, NGROUP) NGP1 = NGROUP + 1.

<u>Variable Name</u>	<u>Description</u>
ICHI	Fission spectrum flag for set (0, 1 or NGROUP).
E(I)	Energy boundaries of groups (E(I) is maximum energy).
U(I)	Lethargy boundaries of groups (U(I) = 0).
VEL(I)	Velocity of group I.

(d) Record Type 4. (If ICHI $\neq$ 0) ((CHI(I,J), I=1, ICHI), J=1, NGROUP).

<u>Variable Name</u>	<u>Description</u>
CHI(I,J)	Fission spectrum incident in group I, born in group J.

End of File

(2) File 2 Structure. One complete block for each isotope consisting of Record Type 1; Record Type 2; Record Type 3 (Conditional); Record Type 4 for each of NGROUP groups; Record 5, 6, 7, 8 for each of NGROUP groups for each of LMAX orders of scattering. LMAX=MAXO (LIN, LEL, LN2N).

(a) Record Type 1. ISONME.

<u>Variable Name</u>	<u>Description</u>
ISONME	Isotope name. (Real*8.)

(b) Record Type 2. ICHI, LIN, LEL, LN2N.

<u>Variable Name</u>	<u>Description</u>
ICHI	Fission flag for isotope: -1 Fissionable, use CHI for set; 0 Nonfissionable; 1 Not incident energy dependent; NGROUP incident energy dependent.
LIN	Maximum order of inelastic scattering: 0 None; 1 Isotropic; 2 Linear anisotropy.

<u>Variable Name</u>	<u>Description</u>
LEL	Maximum order of elastic scattering.
LN2N	Maximum order of n, 2n scattering.

(c) Record Type 3. (If ICHI > 0) ((CHI(I,J), I=1, ICHI), J=1, NGROUP).

<u>Variable Name</u>	<u>Description</u>
CHI(I,J)	Fission spectrum incident in group I, born in group J.

(d) Record Type 4. J,STR,SCAP,SNALF,SNP,ANISO,SFIS, FISNU.

<u>Variable Name</u>	<u>Description</u>
J	Group index.
STR	σ_{tr} transport cross section.
SCAP	σ_c radiative capture (n, γ) cross section.
SNALF	$\sigma_{n,\alpha}$ n, α cross section.
SNP	$\sigma_{n,p}$ n,p cross section.
ANISO	$\sigma_{e\ell}^0(j \rightarrow j)$ Isotropic elastic self-scattering consistent with anisotropic total cross section.
SFIS	σ_f fission cross section.
FISNU	$\nu\sigma_f$ Number of fission neutrons per fission times fission cross section.

(e) Record Type 5. (If LIN + LEL + LN2N $\neq$ 0) LINUP,LINDN, LELUP,LELDN, LN2NUP, LN2NDN.

<u>Variable Name</u>	<u>Description</u>
LINUP	Number of inelastic upscatter groups.
LINDN	Number of inelastic downscatter groups.
LELUP	Number of elastic upscatter groups.
LELDN	Number of elastic downscatter groups.
LN2NUP	Number of n, 2n upscatter groups.
LN2NDN	Number of n, 2n downscatter groups.

(f) Record Type 6. (Present if $LIN > 0$) $SINL(J+LINUP)$, ..., $SINL(J)$, ..., $SINL(J-LINDN)$.

<u>Variable Name</u>	<u>Description</u>
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$SINL(K)$	Inelastic scattering, group K to group J.
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(g) Record Type 7. (Present if $LEL > 0$) $SELT(J+LELUP)$, ..., $SELT(J)$, ..., $SELT(J-LELDN)$.

<u>Variable Name</u>	<u>Description</u>
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$SELT(K)$	Elastic scattering, group K to group J.
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(h) Record Type 8. (Present if $LN2N > 0$) $SN2N(J+LN2NUP)$, ..., $SN2N(J)$, ..., $SN2N(J-LN2NDN)$.

<u>Variable Name</u>	<u>Description</u>
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$SN2N(K)$	n, 2n scattering, group K to group J.
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46. Data Module XS.M.ANIa. Data Module Name

XS.M.ANI.

b. Description

Anisotropic, material level total cross sections.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X	X	NUC001 Cross-section Homogenization
	X	NUI004 1D-Transport Specifications
	X	NUI005 2D-Transport Specifications
	X	NUC003 1D-Transport
	X	NUC005 2D-Transport
	X	NUE001 Neutronics Output Manipulation
	X	AJC001 Neutron Inventory

e. Structure and Content

Structure: One descriptive Record Type 1, followed by NMAT Material Blocks.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NMAT	Number of materials in entire set.
2	NUMANI	Number of materials with anisotropic components.
3	NGROUP	Number of energy groups.
4	MAXLNO	Maximum scattering order in set. (Scattering order = 1 plus order of anisotropy.)

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
5	MAXUPS	Maximum number of groups of upscattering.
6	MAXDNS	Maximum number of groups of downscattering.
	(CMNAME(I), I=1, NMAT)	Material labels, indexed as Material Blocks in remainder of Data Module.

Material Block: One descriptive Record Type 2 and (LNO - 1) records of Type 3.

(2) Record Type 2. Material description.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	LNO	Scattering order of this material (Scattering order = 1 plus order of anisotropy).
2	MAXUP	Maximum number of groups of upscattering, this material.
3	LASCAT	Length of scattering list, LASCAT=MAXUP+1+number of groups of downscattering.

(3) Record Type 3. One for each order of anisotropy, L=1, 2, ..., LNO-1.

<u>Variable Name</u>	<u>Description</u>
((SCAT(K,J),K=1,LASCAT),J=1,NGROUP)	Total anisotropic cross section for order L, into group J from the group indexed by K. K references J+MAXUP, J+MAXUP-1, ..., J, J-1, ..., J- (number groups downscattering).

47. Data Module XS.M.AUXa. Data Module Name

XS.M.AUX.

b. Description

Auxiliary, material level cross sections; individual capture and scattering types.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X	X	NUC001	Cross-section Homogenization
	X	AJC001	Neutron Inventory
	X	AJC003	Transport Perturbation

e. Structure and Content

Structure: One descriptive Record Type 1 and NMAT Material Blocks.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NMAT	Number of materials.
2	NGROUP	Number of energy groups.
3	MAXLNO	Maximum scattering order in set. (Scattering order = 1 plus order of anisotropy.)
	(CMNAME(I),I=1,NMAT)	Material labels, indexed as Material Blocks in remainder of Data Module.

Material Block: One descriptive Record Type 2 and a set of LNO Scattering Blocks.

(2) Record Type 2. Material description.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	LNO	Maximum scattering order of this material. (Scattering order = 1 plus order of anisotropy.)
2	LIN	Inelastic scattering order of this material.
3	LEL	Elastic scattering order of this material.
4	LN2N	(n,2n) Scattering order of this material.
	SCAP(I=1,NGROUP)	(n, γ) cross section.
	SNALF(I=1,NGROUP)	(n, α) cross section.
	SNP(I=1,NGROUP)	(n,p) cross section.

Scattering Block: One for each scattering order from 1 up to LNO (not present for LNO = 0). Consists of descriptive Record Type 3 and records of Types 4-9 according to values of LIN, LEL, and LN2N for this material.

(3) Record Type 3. Scattering description.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NUP	Number groups of upscattering for this order and material.
2	LSCAT	Length of scattering list for this order and material.

(4) Record Type 4. (Present only when order of Block is $\leq$ LIN).

<u>Variable Name</u>	<u>Description</u>
((XINEL(K,J),K=1,LSCAT),J=1,NGROUP)	Inelastic scattering cross section into group J from the group indexed by K, for this scattering order. K references J+NUP, J+NUP-1, ..., J, J-1, ..., J- (number groups of downscattering).

(5) Record Type 5. (Present only when order of Block is $\leq$ LEL.)

<u>Variable Name</u>	<u>Description</u>
((XEL(K,J),K=1,LSCAT),J=1,NGROUP)	Elastic scattering cross section ordered as XINEL, Record Type 4.

(6) Record Type 6. (Present only when order of Block is $\leq$ LN2N.)

<u>Variable Name</u>	<u>Description</u>
((XN2N(K,J),K=1,LSCAT),J=1,NGROUP)	(n,2n) scattering cross section ordered as XINEL, Record Type 4.

(7) Record Type 7. (Present only when order of Block is $\leq$ LIN.)

<u>Variable Name</u>	<u>Description</u>
XTIR(J=1,NGROUP)	Total inelastic removal cross section.

(8) Record Type 8. (Present only when order of Block is $\leq$ LEL.)

<u>Variable Name</u>	<u>Description</u>
XTER(J=1,NGROUP)	Total elastic removal cross section.

(9) Record Type 9. (Present only when order of Block is $\leq$ LN2N.)

<u>Variable Name</u>	<u>Description</u>
XTN2NR(J=1,NGROUP)	Total (n,2n) removal cross section.

48. Data Module XS.M.MINa. Data Module Name

XS.M.MIN.

b. Description

Minimal, material level cross-section data.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Set

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>	
X	X	NUC001	Cross-section Homogenization
	X	NUI004	1D-Transport Specifications
	X	NUI005	2D-Transport Specifications

e. Structure and Content

Structure: One descriptive Record Type 1, possibly followed by a Record Type 2. Then there are NMAT Material Blocks.

(1) Record Type 1

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
1	NMAT	Number of materials in entire set.
2	NGROUP	Number of energy groups.
3	ISCHI	Fission spectrum flag: $\text{ISCHI} = \begin{cases} 0 & \text{if there is no set-wide } \chi; \\ 1 & \text{if Record Type 2 is a vector;} \\ \text{NGROUP} & \text{if Record Type 2 is a matrix.} \end{cases}$
4	NFCMP	Number of fissionable materials.
5	NFAM	Number of families of delayed neutrons.

<u>Word No.</u>	<u>Variable Name</u>	<u>Description</u>
6	MAXUP	Maximum numbers of groups of scattering, up and down, respectively, of all materials in set.
7	MAXDN	
	(CMNAME(I), I=1, NMAT)	Material labels, indexed as Material Blocks in remainder of Data Module.

(2) Record Type 2. Present only when ISCHI > 0.

<u>Variable Name</u>	<u>Description</u>
((CHI(I,J), I=1, ISCHI), J=1, NGROUP)	Fission fraction spectrum, from group I into group J.

Material Block: One Record Type 3, immediately followed by NGROUP records of Type 4.

(3) Record Type 3

<u>Variable Name</u>	<u>Description</u>
ICHI	Fission spectrum flag of this material: $\text{ICHI} = \begin{cases} -1, & \text{material uses Set } \chi \text{ Record Type 2;} \\ 0, & \text{material not fissionable;} \\ 1, & \chi \text{ vector appears in records of Type 4;} \\ \text{NGROUP, } & \chi \text{ matrix given in records of Type 4.} \end{cases}$
NUP(I=1, NGROUP)	
NDN(I=1, NGROUP)	Number of groups of upscattering given in all records of Type 4 for this material.
	Number of groups of downscattering given in all records of Type 4 for this material.

(4) Record Type 4. Group Constants.

<u>Variable Name</u>	<u>Description</u>
J	Group number.
XA	Absorption cross section.
XTOT	Total cross section.
XREM	Removal cross section.
XTR	Transport cross section.
XF	Fission cross section, given only when ICHI $\neq$ 0.

<u>Variable Name</u>	<u>Description</u>
XNF	Fission reaction rate (ν times XF), given only when $ICHI \neq 0$.
(CHI(I),I=1,ICHI)	Fission fraction into group J from group I, given only when $ICHI > 0$.
(XSCATU(I),I=1,NUP(J))	Total scattering into group J from groups $J \pm NUP(J)$, $J+NUP(J)-1$, ..., $J+2$, $J+1$, given only when $NUP(J) > 0$.
SCATJ	Total self-scattering.
(XSCATD(I),I=1,NDN(J))	Total scattering into group J from groups $J-1$, $J-2$, ..., $J-NDN(J)$, given only when $NDN(J) > 0$.
PXNF	Prompt fission reaction rate = $\nu^P \Sigma_f$ (given only when $NFAM > 0$ and $ICHI \neq 0$).
(DNCHI(I),I=1,NFAM)	Delayed-neutron fission-fraction spectrum (given only when $NFAM > 0$ and $ICHI \neq 0$).

49. Data Module XS.THERMa. Data Module Name

XS.THERM.

b. Description

Thermal cross sections.

c. Specifications

Standard.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		CSI001 Epithermal Cross-section Specifications
	X	CSC002 Nonresonant Cross Sections and Fundamental-mode Spectrum

e. Structure and Content

One record.

Record Type 1: NOI, CTH, FTH, GFTH, SNATH, SNPTH, TRTH,
(THC(I), THF(I), THNA(I), THNP(I), THNU(I), THTR(I), I=1, NOI).

<u>Variable Name</u>	<u>Description</u>
NOI	Number of isotopes.
CTH	Homogenized thermal capture cross section.
FTH	Homogenized thermal fission cross section.
GFTH	Homogenized thermal $\nu\Sigma_f$.
SNATH	Homogenized thermal n, α cross section.
SNPTH	Homogenized thermal n,p cross section.
TRTH	Homogenized thermal transport cross section.
THC(I)	Microscopic thermal group capture cross section for isotope I.
THF(I)	Microscopic thermal group fission cross section for isotope I.

<u>Variable Name</u>	<u>Description</u>
THNA(I)	Microscopic thermal group n, α cross section for isotope I.
THNP(I)	Microscopic thermal group n,p cross section for isotope I.
THNU(I)	Number of neutrons emitted per fission in the thermal group for isotope I.
THTR(I)	Microscopic thermal group transport cross section for isotope I.

50. Data Module XS.UNRESa. Data Module Name

XS.UNRES.

b. Description

Microscopic unresolved resonance capture and fission cross section, energy pairs.

c. Specifications

Two files.

d. Program Modules That Create (C) or Read (R) the Data Module

<u>(C)</u>	<u>(R)</u>	<u>Program Module Name</u>
X		CSC001 Resonance Cross Sections
	X	CSC002 Nonresonant Cross Sections and Fundamental-mode Spectrum

e. Structure and Content(1) File 1: One Record NUNRES.

<u>Variable Name</u>	<u>Description</u>
NUNRES	Number of isotopes with unresolved capture or fission resonances.

(2) File 2: (NUNRES > 0; one record for each isotope.)

LZ, NP, (EN(I), SCUN(I), SFUN(I), I=1, NP)

<u>Variable Name</u>	<u>Description</u>
LZ	Isotope identification number.
NP	Number of points of data.
EN(I)	Energy point.
SCUN(I)	Capture cross section.
SFUN(I)	Fission cross section.

ACKNOWLEDGMENTS

Thanks are due to S. Kyong, now at the Bell Telephone Laboratories, for his perseverance during the initial tedious specification phase of setting up the ARC system concept. Thanks are also due to R. Avery for providing the initial stimulation for development of a computation system and for his continued support and encouragement.

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