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SCALE

A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation

Control Modules

Oak Ridge National Laboratory

Prepared for
U.S. Nuclear Regulatory Commission

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SCALE: A Modular Code System for Performing Standardized Computer Analyses for Licensing Evaluation

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Computing Applications Division

SAS1: A ONE-DIMENSIONAL SHIELDING ANALYSIS MODULE

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*Obsolete with SCALE-4.0 release.

PREFACE

Background

This Manual represents Revision 4 of the user documentation for the modular code system referred to as SCALE. The history of the SCALE code system dates back to 1969 when the current Computing Applications Division at Oak Ridge National Laboratory (ORNL) began providing the transportation package certification staff at the U.S. Atomic Energy Commission with computational support in the use of the new KENO code for performing criticality safety assessments with the statistical Monte Carlo method. From 1969 to 1976 the certification staff relied on the ORNL staff to assist them in the correct use of codes and data for criticality, shielding, and heat transfer analyses of transportation packages. However, the certification staff learned that, with only occasional use of the codes, it was difficult to become proficient in performing the calculations often needed for an independent safety review. Thus, shortly after the move of the certification staff to the U.S. Nuclear Regulatory Commission (NRC), the NRC staff proposed the development of an easy-to-use analysis system that provided the technical capabilities of the individual modules with which they were familiar. With this proposal, the concept of the Standardized Computer Analyses for Licensing Evaluation (SCALE) code system was born.

The NRC staff provided ORNL with some general development criteria for SCALE: (1) focus on applications related to nuclear fuel facilities and package designs, (2) use well-established computer codes and data libraries, (3) design an input format for the occasional or novice user, (4) prepare "standard" analysis sequences (control modules) that will automate the use of multiple codes (functional modules) and data to perform a system analysis, and (5) provide complete documentation and public availability. With these criteria the ORNL staff laid out the framework for the SCALE system and began development efforts. The initial version (Version 0) of the SCALE Manual was published in July 1980. Then, as now, the Manual is divided into three volumes – Volume 1 for the control module documentation (Sections C4, S1– S4, and H1), Volume 2 for the functional module documentation (Sections F1– F16), and Volume 3 for the documentation of the data libraries and subroutine libraries (Sections M1–M16).

System Overview

The original concept of SCALE was to provide "standardized" sequences where the user had very few analysis options in addition to the geometry model and materials. Input for the control modules has been designed to be free-form with extensive use of keywords and engineering-type input requirements. The more flexible functional modules have a more difficult input logic and require the user to interface the data sets necessary to run the modules in a stand-alone fashion. As the system has grown in popularity over the years and additional options have been requested, the control modules have been improved to allow sophisticated users additional access to the numerous capabilities within the functional modules. However, the most important feature of the SCALE system remains the capability to simplify the user knowledge and effort required to prepare material mixtures and to perform adequate problem-dependent cross-section processing.

The modules available in Version 0 of SCALE were for criticality safety analysis sequences (CSAS) that provided automated material and cross-section processing prior to a one-dimensional (1-D) or multidimensional criticality analysis. Since that time the capabilities of the system have been significantly expanded to provide additional CSAS capabilities, new shielding analysis sequences (SAS) that also include depletion/decay capabilities for spent fuel characterization, and a heat transfer analysis sequence (HTAS). At the center of the CSAS and SAS sequences is the library of subroutines referred to as the Material Information Processor or MIPLIB (see Section M7). The purpose of MIPLIB is to allow users to specify problem materials using easily remembered and easily recognizable keywords that are associated with mixtures, elements, and nuclides provided in the Standard Composition Library (see Section M8). MIPLIB also uses other keywords

and simple geometry input specifications to prepare input for the modules that perform the problem-dependent cross-section processing: BONAMI, NITAWL-II, and XSDRNPM. A keyword supplied by the user selects the cross-section library from a standard set provided in SCALE (see Section M4) or designates the reference to a user-supplied library. Several utility modules from AMPX[1] have been added to this version of SCALE to provide users with the capability to edit the cross-section data and reformat user-supplied libraries for use in SCALE.

Over the history of the project several modules have been removed from the system because they are no longer supported by the development staff at ORNL. Tables 1 and 2 provide a summary of the major applications of each of the control modules and functional modules currently in the SCALE code system. The control modules were designed to provide the system analysis capability originally requested by the NRC staff. The CSAS module (sometimes denoted as the CSAS4 module and documented in Section C4) is currently the only control module designed for the calculation of the neutron multiplication factor of a system. Eight sequences enable general analysis of a 1-D system model or a multidimensional system model, capabilities to search on geometry spacing, and problem-dependent cross-section processing for use in executing stand-alone functional modules. The SAS1 and SAS3 modules (see Sections S1 and S3, respectively) provide general 1-D deterministic and 3-D Monte Carlo analysis capabilities. The SAS2 module (see Section S2) was originally developed to perform a depletion/decay calculation to obtain spent fuel radiation source terms that were subsequently input automatically to a 1-D, radial shielding analysis in a cylindrical geometry. Over time the depletion/decay portion of the SAS2 module has been significantly enhanced and interfacing to the other shielding modules has been provided. The SAS4 module (see Section S4) enables automated particle biasing for a Monte Carlo analysis of a transportation package-type geometry. The HTAS1 module (see Section H1) is the only heat transfer control module and uses the various capabilities of the HEATING code to perform different sequences of steady-state and transient analysis that enable the normal and accident conditions of a transportation package to be evaluated. Like SAS4, the HTAS1 module is limited to a package-type geometry.

Portability

Version 4.2 of the SCALE system has been developed to ensure portability among various computing platforms. The system is maintained and enhanced at ORNL under quality assurance and configuration management plans. The system has been routinely tested on IBM mainframe and IBM workstations. In addition, the system has been applied at ORNL on DEC and SUN workstations. Information needed to install SCALE on each of these systems is included with the software package distributed by the code centers. Advice for installation on HP workstations is also included in the software package. A separate SCALE software package, designated SCALE-PC, is available for the execution of select portions of the SCALE system on a personal computer.

Related Developments

The definition of "easy-to-use" has changed considerably since the late 1970s. As funding has allowed, the ORNL development staff has sought to develop user interfaces that provide a distinct aid to novice or occasional users of the system. These full-screen input processors were developed to work on a personal computer and provide interactive help to the user in preparing accurate input for a SCALE module. Currently, input processors are available only for the criticality control sequences[2] and the ORIGEN-S functional module.[3]

The capability to perform a point-kernel shielding analysis within the SCALE system has been developed[4] and will be provided within SCALE-PC in the next release of the software package.

A 238-energy-group neutron cross-section library based on ENDF/B-V has recently been prepared for the SCALE system.[5] All the nuclides that are available in ENDF/B-V are in the library. A 44-group

library has been collapsed from this 238-group library and validated against numerous critical measurements.[6] These libraries are available as separate data packages from the software distribution centers.

Availability

The SCALE code system and the other software designated under Related Developments have been packaged by the Radiation Shielding Information Center (RSIC) under cooperative agreement with the Energy Science and Technology Software Center. The SCALE system and the related software may be obtained by contacting either

Energy Science and Technology Software Center
P.O. Box 1020
Oak Ridge, TN 37831-1020
Telephone: (615) 576-2606
FAX: (615) 576-2865

or

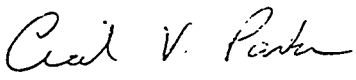
Radiation Shielding Information Center
Oak Ridge National Laboratory
P.O. Box 2008
Oak Ridge, TN 37831-6362
Telephone: (615) 574-6176
FAX: (615) 574-6182

Acknowledgments

The SCALE system is maintained at ORNL and enhanced to keep pace with normal technical advancements in the analysis areas of interest. Although the NRC continues its role as the controlling sponsor of the SCALE system, the U.S. Department of Energy (DOE) began assisting in the maintenance of the SCALE system in 1987. Over the years numerous individuals within these sponsoring organizations have played key roles in ensuring that the SCALE system remained a readily available, reliable system for the analysis of nuclear fuel facilities and packages. The individuals who have worked with the ORNL staff to coordinate maintenance and development activities include R. H. Odegaarden (NRC, ret.), G. H. Bidinger (NRC, ret.), C. Mauck (DOE, ret.), E. P. Easton (NRC), W. H. Lake (NRC and DOE), M. E. Wangler (DOE), and M. G. Bailey (NRC).

As demonstrated by this Manual, there are also numerous individuals from the ORNL staff who have contributed significantly to the development and enhancement of the SCALE system. Most are credited by their authorship of the sections in this Manual that correspond to their work. A few individuals have been essential to the development and maintenance of SCALE but are not credited by authorship. These individuals include: S. M. Bowman, who is responsible for proper configuration and testing of the development and production systems at ORNL and is the principal contact for general user assistance and training; S. K. Martin, who is responsible for implementing system changes; C. H. Shappert, who provided the editorial review of this Manual; and L. F. Norris, who prepared the entire manuscript. Special acknowledgement is also due to R. M. Westfall and G. E. Whitesides who, together with R. H. Odegaarden of the NRC, developed the concept and long-range goals of the SCALE system in the late 1970s. Finally, this Project Leader will always be grateful to L. M. Petrie, who for nearly 20 years has consistently provided consultation and advice on the technical

direction that should be taken in development of nearly every module and cross-section library that are in the present system.



Cecil V. Parks
SCALE Project Manager
March 1995

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Table 1 Analysis capabilities summary of the SCALE control modules

Control module	Analysis function(s)	Functional modules executed	Section reference
CSAS	1-D deterministic calculation of neutron multiplication 3-D Monte Carlo calculation of neutron multiplication Problem-dependent cross-section processing Multiplication search or spacing	BONAMI NITAWL-II XSDRNPM KENO V.a ICE	C4
SAS1	1-D deterministic calculation of radiation transport through shield and dose evaluation at a point Calculation of dose at detector based on leakage from critical volume	BONAMI NITAWL-II XSDRNPM XSDOSE	S1
SAS2	Point depletion/decay of nuclear fuel 1-D radial shielding analysis in cylindrical geometry	BONAMI NITAWL-II XSDRNPM COUPLE ORIGEN-S XSDOSE	S2
SAS3	Dose evaluation using MORSE Monte Carlo code	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S3
SAS4	Calculation of dose outside of transportation package using MORSE code and automated biasing techniques	BONAMI NITAWL-II XSDRNPM MORSE-SGC	S4
HTAS1	R-Z steady-state and transient analyses of a transportation package	OCULAR HEATING	H1

Table 2 Analysis capabilities summary of the SCALE functional modules

Module	Function	Section reference
BONAMI	Resonance self-shielding of cross sections with Bondarenko factors	F1
NITAWL-II	Resonance self-shielding of cross sections with resolved resonance data	F2
XSDRNPM	General 1-D, discrete-ordinates code for: • zone-weighting of cross sections • eigenvalue calculations for neutron multiplication • fixed-source calculation for shielding analysis • adjoint calculation for determining importance functions	F3
XSDOSE	Module for calculation of dose at a point based on the 1-D leakage flux from a finite shield	F4
COUPLE	Interface module for preparation of cross-section and spectral data for ORIGEN-S	F6
ORIGEN-S	General-purpose point-depletion and decay code to calculate isotopic, decay heat, radiation source terms, and curie levels	F7
ICE	Cross-section utility module for mixing cross sections	F8
MORSE-SGC	Monte Carlo code with combinatorial and array geometry features used to perform radiation shielding analysis	F9
HEATING7.2	Finite-volume, multidimensional code for conduction and radiation heat transfer	F10
KENO V.a	Monte Carlo code for calculation of neutron multiplication factors	F11
OCULAR	Calculation of radiation exchange factors	F16

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Computing Applications Division

CSAS: CONTROL MODULE FOR ENHANCED CRITICALITY SAFETY ANALYSIS SEQUENCES

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ABSTRACT

The Criticality Safety Analysis Sequences (CSAS) were developed within the SCALE code system to provide automated, problem-dependent, cross-section processing followed by calculation of the neutron multiplication factor for the system being modeled. This document describes the program that contains the available sequences.

These control sequences activate the cross-section processing codes BONAMI and NITAWL-II to provide resonance-corrected cross sections. Control sequences ending with "X" utilize XSDRNPM to provide a cell-weighted mixture cross section and/or the neutron multiplication factor (k-effective) for a one-dimensional system model. ICE is used by CSASI and CSASIX to provide a Monte Carlo-formatted mixed cross-section library. KENO V.a uses the processed cross sections and calculates the k-effective of three-dimensional system models. The geometric modeling capabilities available in KENO V.a coupled with the automated cross-section processing within the control sequences allow complex, three-dimensional systems to be easily analyzed. A search capability is achieved by repeatedly activating the control module MODIFY to alter the pitch or other dimensions and the functional module KENO V.a to calculate the k-effective for the new pitch or dimensions.

The control sequences (sometimes referred to as modules) described within this document were developed simultaneously and are closely related. These sequences are listed in the following table with the modules they invoke:

Control module	Search function	Functional modules executed by the control module				
CSASI	No search	BONAMI	NITAWL-II		ICE	
CSASIX	No search	BONAMI	NITAWL-II	XSDRNPM	ICE	
CSASN	No search	BONAMI	NITAWL-II			
CSAS1X	No search	BONAMI	NITAWL-II	XSDRNPM		
CSAS25	No search	BONAMI	NITAWL-II		KENO V.a	
CSAS2X	No search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	
CSAS4	Search	BONAMI	NITAWL-II		KENO V.a	MODIFY[a]
CSAS4X	Search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	MODIFY[a]

[a]MODIFY is a control module.

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ACKNOWLEDGMENTS

CSAS and its related Criticality Safety Analysis Sequences are based on the old CSAS2 control module, which was not written in VS FORTRAN and, therefore, is not included in this version of SCALE, and the KENO V.a functional module described in Sect. F11. Therefore, special acknowledgment is made to J. A. Bucholz, R. M. Westfall, and J. R. Knight who developed CSAS2. G. E. Whitesides is acknowledged for his contributions through early versions of KENO. Appreciation is expressed to C. V. Parks for his guidance in developing CSAS.

C4.1 INTRODUCTION

Within the life cycle of the SCALE system, the CSAS program has superseded earlier programs that contained criticality safety analysis sequences. Embedded within the CSAS program are numerous sequences that enable automated cross-section processing and criticality analyses with and without the search option. All the criticality analysis sequences (sometimes referred to as modules) within SCALE are contained within the CSAS program.

Criticality Safety Analysis Sequence No. 4 (CSAS4) was developed to provide a search capability for three-dimensional (3-D) configurations in the SCALE system. Because it encompassed all the options and functional modules available in earlier SCALE criticality sequences, the program was initially called by the same name, CSAS4. In order to distinguish the program from the numerous sequences that it contained (including CSAS4), the program name was later changed to CSAS. The reader should be aware that the documentation has not been completely revised, and the program is still referred to as CSAS4 in much of the documentation that follows.

The standardized automated procedures process SCALE cross sections using the Bondarenko method (via BONAMI) and the Nordheim integral method (via NITAWL-II) to provide a resonance-corrected cross-section library based on the physical characteristics of the problem being analyzed. This cross-section library can be utilized by KENO V.a, a 3-D multigroup Monte Carlo criticality program, or XSDRNPM, a one-dimensional (1-D) discrete-ordinates code for transport analysis. The search capability utilizes KENO V.a and is performed by activating CSAS4 or CSAS4X. The type of search is defined by the input data, and a parameter search is performed on k-effective as a function of pitch or other dimensions. The two basic search options offered are (1) an optimum search seeking a maximum or minimum and (2) a critical search seeking a fixed value of k-effective.

The user may select the CSAS4 or the CSAS4X sequence to perform a search sequence. An X in the module name specifies that XSDRNPM will be used to provide cell-weighted cross sections. CSAS4 should be used for 3-D searches when the fuel pins are modeled individually in the KENO V.a geometry. CSAS4X should be used for 3-D searches when cell-weighted cross sections are used to provide a homogeneous representation of the fuel pins in the KENO V.a geometry. Cell-weighting is accomplished by describing a unit cell, as in a fuel assembly, for which a 1-D eigenvalue calculation of the unit cell is made to determine the spatially dependent flux spectrum. This flux spectrum is used to cell-weight the microscopic cross-section data. The nuclide number densities in the unit cell are homogenized, and the resultant homogenized cell-weighted cross sections are identified as mixture 500 and utilized in the KENO V.a geometry. Note that only one mixture 500 can be created per problem.

The codes utilized in Criticality Safety Analysis Sequence No. 4 start with an AMPX master format cross-section library and generate a self-shielded, group-averaged library applicable to the specific problem configuration. These cross sections are then used in the Monte Carlo determination of the effective neutron multiplication factor. The codes and their functions are given below.

1. BONAMI — performs resonance self-shielding calculations for nuclides that have Bondarenko data associated with their cross sections.
2. NITAWL-II — applies a Nordheim resonance self-shielding correction to nuclides having resonance parameters.
3. XSDRNPM — provides cell-weighted cross sections based on the specified unit cell and, in addition, can calculate the effective neutron multiplication (k-effective) for a 1-D system.
4. ICE — creates a Monte Carlo formatted mixed cross-section library for use by KENO V.a.
5. KENO V.a — calculates k-effective of a 3-D system.

6. MODIFY — alters the pitch and redefines the geometry data used by KENO V.a. The optimum pitch search is achieved by repeatedly changing the geometry data and executing KENO V.a until the optimum pitch is determined or the calculation is terminated for other reasons.

All the control sequences in the CSAS program are listed in the following table with the modules they invoke. The first seven sequences are subsets of the CSAS4X sequence. This section of the SCALE manual describes all eight sequences.

Control module	Search function	Functional modules executed by the control module				
CSASI	No search	BONAMI	NITAWL-II		ICE	
CSASIX	No search	BONAMI	NITAWL-II	XSDRNPM	ICE	
CSASN	No search	BONAMI	NITAWL-II			
CSAS1X	No search	BONAMI	NITAWL-II	XSDRNPM		
CSAS25	No search	BONAMI	NITAWL-II		KENO V.a	
CSAS2X	No search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	
CSAS4	Search	BONAMI	NITAWL-II		KENO V.a	MODIFY*
CSAS4X	Search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	MODIFY*

*MODIFY is a control module.

C4.2 TECHNIQUES

Criticality Safety Analysis Sequence No. 4 (CSAS) is designed to perform a search utilizing the Monte Carlo Criticality code KENO V.a. Related sequences (see Table C4.2.1) can bypass the search and provide k-effective for the system being analyzed or simply prepare a cross-section library for subsequent use. In order to minimize human error, the SCALE data handling is automated as much as possible. CSAS and many other SCALE sequences apply a standardized procedure to provide appropriate cross sections for the calculation. This procedure is carried out by the Material Information Processor that generates number densities and related information, prepares geometry data for resonance self-shielding and flux-weighting cell calculations, and creates data input files for the cross-section processing codes. Sequences that execute KENO V.a include a KENO V.a Data Processor to read and check the KENO V.a data. Sequences that execute a search use a Search Data Processor to read and check the search data. When the data checking has been completed, the control sequence executes BONAMI and NITAWL-II to prepare a resonance-corrected microscopic cross-section library in the AMPX working library format. If cell-weighted cross sections are requested, XSDRNPM performs the necessary calculations and produces a cell-weighted microscopic cross-section library in the AMPX working library format. ICE may be executed to produce mixture libraries (macroscopic cross-section libraries) in the ICE Monte Carlo format and the AMPX working library format. KENO V.a may be executed to calculate the k-effective or neutron multiplication factor using the cross-section library that was prepared by the control sequence. MODIFY may be invoked to perform a search* by repeatedly altering the KENO V.a data and executing KENO V.a.

Table C4.2.1 CSAS and related criticality sequences

Control module	Search function	Functional modules executed by the control module				
CSASI	No search	BONAMI	NITAWL-II		ICE	
CSASIX	No search	BONAMI	NITAWL-II	XSDRNPM	ICE	
CSASN	No search	BONAMI	NITAWL-II			
CSAS1X	No search	BONAMI	NITAWL-II	XSDRNPM		
CSAS25	No search	BONAMI	NITAWL-II		KENO V.a	
CSAS2X	No search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	
CSAS4	Search	BONAMI	NITAWL-II		KENO V.a	MODIFY[a]
CSAS4X	Search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	MODIFY

[a]MODIFY is a control module.

The Material Information Processor is described in Sect. M7. It is responsible for reading the standard composition data and other engineering-type specifications, including volume fraction or percent theoretical density, temperature, and isotopic distribution. The techniques used in the Material Information Processor and their applications and limitations are discussed in Sect. M7.2. The input data for the Material Information Processor is the same for all eight analytical sequences available through CSAS. For convenience, the Material Information Processor input data guide is included in Sect. C4.4.

*This search technique is discussed in detail in the report by M. J. Lorek, *Improved Criticality Search Techniques for Low- and High-Enriched Systems*, NUREG/CR-2122, ORNL/NUREG/CSD/TM-13, NUREG/CR-2122, 1981.

The Material Information Processor checks the input data pertaining to cross-section preparation and prepares binary input files for the applicable functional modules. Depending on the specified sequence, data is prepared for BONAMI, NITAWL-II, XSDRNPM, and ICE as appropriate.

The Bondarenko method is discussed in the Material Information Processor document, Sect. M7.2.5.1, and BONAMI is described in Sect. F1. The Nordheim method and NITAWL-II are described in Sects. M7.2.5.2 and F2 respectively. The Dancoff treatment is discussed in Sect. M7.2.5.3. The automatic mesh generator, the automatic quadrature generator, and the convergence criteria for control sequences that execute XSDRNPM are described in Sects. M7.2.5.6, M7.2.5.7, and M7.2.5.8 respectively. XSDRNPM is described in Sect. F3. ICE is described in Sect. F8, and KENO V.a is described in Sect. F11. See Sect. M7A for an explanation of many of the techniques used in processing the cross sections.

The search capability is implemented by the control module MODIFY. It performs operations according to the specified search data to determine (1) the maximum (or minimum) value of k-effective as a function of pitch or dimensions or (2) the pitch or dimensions corresponding to a specified value of k-effective. An iterative procedure is used, making use of all previous information to modify the pitch or dimensions to achieve the desired result. The procedures for conducting optimum searches and critical searches are summarized below.

C4.2.1 OPTIMUM SEARCH

Because only an initial value of k-effective and a set of boundary constraints are available, four initial points are generated spanning the range defined by the constraints. The search package identifies the type of cubic equation [i.e., a cubic with no local extrema (type A) or a cubic with two local extrema (type B)] and utilizes this knowledge in determining the pitch or dimensions corresponding to the maximum (or minimum) value of k-effective. The optimum search procedure is summarized as follows:

1. Calculate k-effective for the specified problem.
2. Calculate k-effective for the minimum constraint.
3. Calculate k-effective for the maximum constraint.
4. Calculate k-effective for a fourth point that lies approximately equidistant between the initial guess and the constraint that is farthest from it.
5. Utilize a weighted least-squares fit to a cubic polynomial on the data points.
6. Determine the type of cubic. For a type A cubic, go to step 11.
7. Take the first derivative of the least-squares cubic.
8. Solve the quadratic for its roots.
9. Take the second derivative of the least-squares cubic to determine which root is the maximum (or minimum), and if it falls within the constraints, use this root as the next guess. Otherwise, convergence has been defined as occurring at the constraint with the maximum (or minimum) k-effective.
10. Calculate the k-effective corresponding to the next guess. Go to step 5. Repeat this procedure until convergence is achieved.

11. If the cubic equation is a type A cubic, the optimum lies on one of the boundaries. If the fit shows that the cubic is actually a type B cubic, go to step 7 and continue.

Convergence is defined as occurring when a k-effective has been calculated for a point on the curve where the value of the curve is within epsilon of the maximum (or minimum) of the curve. Additionally, the calculated k-effective must be within two standard deviations of the value of the curve at that point. The search is terminated when convergence is achieved or when the code determines there is no local maximum within the constraints.

NOTE: The entire search is performed using the problem-dependent cross sections that were created using data derived from the initial cell description. Therefore, if the search converges with a configuration that is significantly different from the initial cell, the search should be rerun using the converged cell configuration to ensure that the cross-section treatment was adequate.

C4.2.2 CRITICAL SEARCH

The critical search option searches for the pitch or dimensions corresponding to a specified value of k-effective. If the calculated value of k-effective is within the specified search tolerance (EPS) of the desired k-effective, the search is considered to be complete. The critical search procedure is summarized as follows:

1. Calculate k-effective for the specified problem. If it is within EPS of the specified k-effective, convergence has been achieved.

2. Calculate k-effective for one of the constraints. If the specified problem coincided with one of the constraints, calculate k-effective at a point halfway to the other constraint. If the calculated k-effective is within EPS of the specified k-effective, convergence has been achieved.

3. Calculate k-effective for a point chosen from a linear fit of the two existing points closest to the specified k-effective. If the calculated k-effective is within EPS of the specified k-effective, convergence has been achieved.

4. Repeat step 3.

5. Calculate k-effective for a point determined from fitting the previous points to a cubic and solving the cubic for the point closest to the desired k-effective. If all roots lie outside the constraints, the problem is terminated and an appropriate message is written. If the calculated k-effective is within EPS of the specified k-effective, convergence has been achieved. Repeat step 5 until the problem converges, exceeds the specified number of passes, or determines that a feasible solution does not exist.

It should be noted that the entire search is performed using the problem-dependent cross sections that were created using data derived from the initial cell description. Therefore, if the search converges with a configuration that is significantly different from the initial cell, the search should be rerun using the converged cell configuration to ensure that the cross-section treatment was adequate.

C4.2.3 CSAS LIMITATIONS

The CSAS control module was developed to use simple input data and prepare problem-dependent cross sections for use in calculating the effective neutron multiplication factor of a 1-D or 3-D system using XSDRNPM or KENO V.a. An attempt was made to make the system as general as possible within the constraints of the standardized methods chosen to be used in SCALE. Standardized methods of data input

were adopted to allow easy data entry and for quality assurance purposes. Some of the limitations of the CSAS sequences are due to assumptions in the Nordheim integral treatment[1] as implemented in CSAS. Inherent limitations in the NITAWL-II Nordheim integral treatment of resonance nuclides are as follows:

1. The treatment assumes no resonance overlap from other resonances or other material regions.

2. The treatment of an external moderator assumes an asymptotic flux present at the absorber-moderator interface.

3. The treatment of spatial transport uses the first-flight escape probability for the absorber, the two-region reciprocity theorem, and Dancoff[2] factors.

In many cases, the Nordheim integral treatment is an excellent method for processing resonance cross sections for use in the analysis of light-water reactor (LWR) fuel pin cells and for many other applications commonly used in neutronics analysis. However, caution should be used in applications involving several isotopes with large resonances or complicated absorber-moderator geometries. Another area of probable inadequacy involves the analysis of machinery for dissolving spent fuel elements. Such a system usually requires the simultaneous consideration of resonance absorbers located in both the solid fuel pellets and the acid solution, thereby resulting in an inadequate treatment by NITAWL-II.

The major limitations of the analytical model used by the Nordheim integral treatment in CSAS are as follows:

1. A lattice system whose fuel or moderator contains an absorber that has rapidly varying cross sections across the resonance region may be inadequately treated. Examples include gadolinium, silver, indium, and hafnium.

2. The presence of more than one resonance isotope in a material can lead to an effect called resonance overlap, which can result in enhanced or reduced group-averaged cross sections, depending on the predominance of resonance scattering or absorption and the relative locations of the resonances within the energy groups. The resonance overlap effect is discussed in more detail in Sect. M7.A.7.

3. Resonance interference between two different media is not correctly treated.

4. Fissile lumps in fissile solutions are not correctly treated.

5. The determination of parameters used in processing the cross sections are derived from the geometry of the cell description. CSAS does not allow multiple cell descriptions.

6. It is strongly recommended that CSAS calculations be made of benchmark experiments similar to the problem being calculated in order to demonstrate the validity of the code/cross-section combination for that type of problem.

CSAS uses cross sections created using data derived from the cell description specified in the Material Information Processor data. The cell description is not updated, and the cross sections are not reprocessed even when convergence is achieved. Therefore, it is strongly recommended that once convergence is achieved, the materials information processor cell be updated to use the converged configuration and the search be rerun to ensure that the cross sections were adequate. The new search should converge immediately if the initial cell was adequate for the cross-section treatment. Otherwise, the search will continue until convergence is achieved.

C4.2.4 REFERENCES

1. L. W. Nordheim, "The Theory of Resonance Absorption," *Proceedings of Symposia in Applied Mathematics*, Vol XI, p. 58, G. Birkhoff and E. P. Wigner, Eds., Am. Math. Soc. (1961).

2. S. M. Dancoff and M. Ginsburg, *Surface Resonance Absorption in a Close-Packed Lattice*, CP-2157, Clinton Plant, U.S. Atomic Energy Commission (September 1944).

C4.3 LOGICAL PROGRAM FLOW

The general flow of Criticality Safety Analysis Sequence No. 4 is given in this section. The program flow is divided into several sections. An abbreviated representation, rather than a formal flowchart, is used to outline the program flow of each section. A flowchart may show a subroutine or library routine only once, even though it may be called multiple times in that portion of the program. The corresponding text usually states when multiple calls are made to a routine. Accompanying each abbreviated flowchart is an explanation of the purpose of that segment of the program and text describing each of the referenced subroutines.

Criticality Safety Analysis Sequence No. 4 has been written in a general form to allow maximum flexibility. Data are transferred from one module to another via sequential data files and direct-access data files. Table C4.3.1 lists the data files utilized by this program. CSAS is used to represent the control module defining the available sequences. Data files utilized by the individual functional modules are included in Table C4.3.2.

The flowchart representation for Criticality Safety Analysis Sequence No. 4 is defined as follows:

The SCALE DRIVER is contained in a diamond, subroutines initiating control modules are contained in circles, functional modules are contained in hexagons, major program segments are contained in rectangularized ovals, subroutine names are contained in boxes, and library routines are represented as bare names. An arrow in the flowchart indicates that the subroutine or module associated with the arrow will be discussed later in the section.

C4.3.1 INITIATION OF CSAS4 (CRITICALITY SAFETY ANALYSIS SEQUENCE NO. 4)

This portion of the program is the initiation of the criticality safety analysis sequence. The SCALE DRIVER, described in Sect. M1, obtains the name of the module to be accessed from the first card (module specification card) in the user input data file. The control modules available in Criticality Safety Analysis Sequence No. 4 are shown in Fig. C4.3.1. These control modules, with the exception of MODIFY, use the Material Information Processor data as described in Sect. M7.3.

SCALE DRIVER allows implementation of a modular code system which includes Criticality Safety Analysis Sequence No. 4. See Sect. M1 for additional information about the driver.

CSAS4 performs a search for three-dimensional (3-D) problems that do not need a cell-weighted mixture cross section. The search is conducted by sequentially activating the functional modules BONAMI, NITAWL-II, and KENO V.a to process the required cross sections and calculate the k-effective. The control module MODIFY then performs operations to alter the pitch or other geometric dimensions repeatedly and to activate KENO V.a until the search requirements are met or the job is terminated for other reasons.

CSAS4X performs a search for 3-D problems that require a cell-weighted mixture cross section. The search is achieved by sequentially activating the functional modules BONAMI, NITAWL-II, XSDRNPM-S, and KENO V.a to process the required cross sections and calculate the k-effective. The control module MODIFY then performs operations to alter the pitch or other geometric dimensions repeatedly and to activate KENO V.a until the search requirements are met or the job is terminated for other reasons.

Table C4.3.1 Description of units utilized by the Criticality Safety Analysis Sequence No. 4 control module

Unit No.	Type of data	Creating module	User module	Type of file
5	Input	DRIVER	CSAS	Sequential
8	Scratch file	CSAS	CSAS	Direct or random-access data
11	Short master cross-section library	CSAS	BONAMI	Sequential
16	Scratch file	CSAS	CSAS	Sequential
17	Scratch file	CSAS	CSAS	Sequential
18	Scratch file	CSAS	CSAS	Sequential
19	Scratch file	CSAS	CSAS	Sequential
70	User-supplied cross sections		CSAS	AMPX master format library
81	16-group cross sections		CSAS	AMPX master format library
82	27-group cross sections		CSAS	AMPX master format library
83	123-group cross sections		CSAS	AMPX master format library
84	218-group cross sections		CSAS	AMPX master format library
85	22 neutron-18 gamma cross sections		CSAS	AMPX master format library
86	18-gamma cross sections		CSAS	AMPX master format library
87	27-group cross sections for burnup		CSAS	AMPX master format library
88	27 neutron-18 gamma cross sections		CSAS	AMPX master format library
89	Standard Composition Library		CSAS	Direct or random-access data file
90	Search data	CSAS	MODIFY	Direct or random-access data
92	ICE input data	CSAS	ICE	Sequential
95	KENO V.a restart data	CSAS MODIFY KENO V.a	KENO V.a MODIFY	Sequential
96	BONAMI input data	CSAS	BONAMI	Sequential
97	NITAWL-II input data	CSAS	NITAWL-II	Sequential
98	XSDRN input data	CSAS	XSDRNPM	Sequential
99	Printed output	CSAS MODIFY	CSAS MODIFY	Sequential

Table C4.3.2 Description of units used by the functional modules of CSAS

Unit no.	Module	Action	Type of file
1	BONAMI	WRITE	Microscopic master working format cross sections
	NITAWL-II	READ	Microscopic master working format cross sections
2	ICE	WRITE	Macroscopic working format cross sections
3	XSDRNPM	WRITE	Microscopic cell-weighted working format cross sections
	ICE	READ	Microscopic cell-weighted working format cross sections
	KENO V.a	READ	Microscopic cell-weighted working format cross sections
4	NITAWL-II	WRITE	Microscopic working format cross sections
	ICE	READ	Microscopic working format cross sections
	KENO V.a	READ	Microscopic working format cross sections
	XSDRNPM	READ	Microscopic working format cross sections
6	BONAMI	WRITE	Printed output
	ICE	WRITE	Printed output
	KENO V.a	WRITE	Printed output
	NITAWL-II	WRITE	Printed output
	XSDRNPM	WRITE	Printed output
8	BONAMI	WRITE/READ	Direct or random-access scratch files
	ICE	WRITE/READ	Direct or random-access scratch files
	KENO V.a	WRITE/READ	Direct or random-access scratch files
	XSDRNPM	WRITE/READ	Direct or random-access scratch files
9	BONAMI	WRITE/READ	Direct or random-access scratch files
	ICE	WRITE/READ	Direct or random-access scratch files
	KENO V.a	WRITE/READ	Direct or random-access scratch files
	NITAWL-II	WRITE/READ	Direct or random-access scratch files
	XSDRNPM	WRITE/READ	Direct or random-access scratch files
10	ICE	WRITE/READ	Direct or random-access scratch files
	KENO V.a	WRITE/READ	Direct or random-access scratch files
	XSDRNPM	WRITE/READ	Direct or random-access scratch files
11	BONAMI	READ	Short AMPX master format cross sections
14	ICE	WRITE	Monte Carlo-formatted macroscopic cross sections
	KENO V.a	READ/WRITE	Monte Carlo-formatted macroscopic cross sections
16	KENO V.a	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Angular flux file
17	XSDRNPM	WRITE/READ	Sequential scratch file
18	BONAMI	WRITE/READ	Sequential scratch file
	NITAWL-II	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Sequential scratch file
19	BONAMI	WRITE/READ	Sequential scratch file
	NITAWL-II	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Sequential scratch file
79	KENO V.a	READ	KENO V.a albedo file
80	KENO V.a	READ	KENO V.a weighting file
92	ICE	READ	Binary input file
95	KENO V.a	READ	Binary input file
96	BONAMI	READ	Binary input file
97	NITAWL-II	READ	Binary input file
98	XSDRNPM	READ	Binary input file

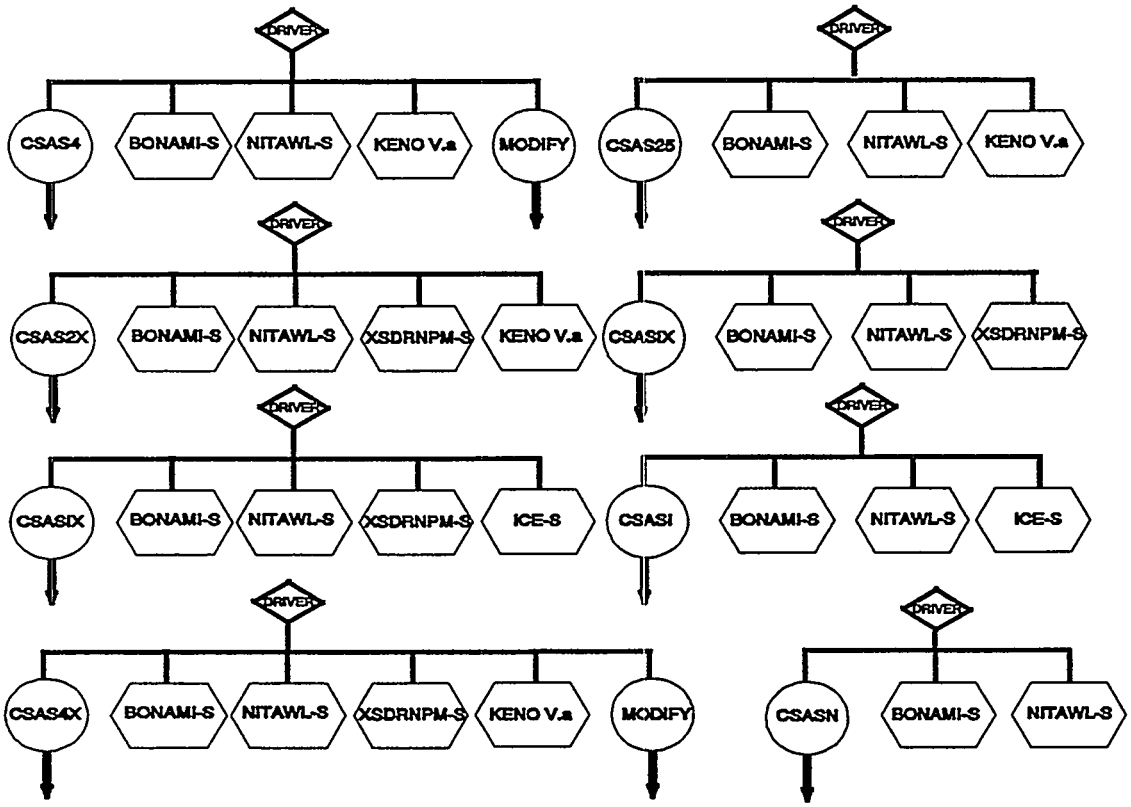


Figure C4.3.1 Control modules available in Criticality Safety Analysis Sequence No. 4

CSAS25 calculates the k-effective for 3-D problems. This module sequentially activates the functional modules BONAMI, NITAWL-II, and KENO V.a to process the required cross sections and calculate the k-effective. Note that a cell-weighted mixture cross section cannot be used.

CSAS2X calculates the k-effective for 3-D problems that require a cell-weighted mixture. It is the same as CSAS25 except a cell-weighted mixture cross section is always created. This control module sequentially activates the functional modules BONAMI, NITAWL-II, XSDRNPM-S, and KENO V.a to process the required cross sections and calculate the k-effective.

CSAS1X creates a microscopic cell-weighted library in the AMPX working library format. This control module sequentially activates the functional modules BONAMI and NITAWL-II to process the necessary cross sections and calculates the k-effective of the one-dimensional (1-D) problem using the discrete-ordinates code XSDRNPM-S.

CSASN creates a resonance-corrected microscopic cross-section library in the AMPX working library format by sequentially activating the functional modules BONAMI and NITAWL-II.

CSASI provides a resonance-corrected macroscopic mixture cross-section library in the MORSE/KENO (ICE Monte Carlo-processed) format by sequentially activating the functional modules BONAMI, NITAWL-II, and ICE.

CSASIX provides a resonance-corrected, cell-weighted, macroscopic mixture cross-section library in the MORSE/KENO (ICE Monte Carlo-processed) format by sequentially activating the functional modules BONAMI, NITAWL-II, XSDRNPM-S, and ICE. The discrete ordinates code XSDRNPM-S also computes the k-effective for the 1-D problem.

BONAMI is a functional module in the SCALE system that performs resonance self-shielding calculations for nuclides that contain Bondarenko data in their cross sections. See Sect. F1 for detailed information concerning BONAMI.

NITAWL-II is a functional module in the SCALE system. It applies a Nordheim resonance self-shielding correction to nuclides having resonance parameters associated with the cross-section data. See Sect. F2 for detailed information.

XSDRNPM-S is a functional module in the SCALE system. It provides cell-weighted cross sections based on the specified unit cell. It can also calculate the k-effective for 1-D problems. See Sect. F3 for additional information.

ICE is a functional module in the SCALE system. It creates a Monte Carlo-formatted mixed cross-section library for use by KENO V.a or MORSE. See Sect. F8 for additional details.

KENO V.a is a functional module in the SCALE system. It calculates the effective neutron multiplication of a 3-D problem. See Sect. F11 for a detailed description of KENO V.a.

MODIFY is a control module in the SCALE system. It is responsible for conducting a search by repeatedly altering the geometry specifications and executing KENO V.a. Section C4.3.6 contains more detail about MODIFY.

C4.3.2 OVERALL FLOW DIAGRAM

Figure C4.3.2 illustrates the overall flow of Criticality Safety Analysis Sequence No. 4. The control modules CSAS4, CSAS4X, CSAS25, CSAS2X, and CSAS1X communicate with the driver and dictate the order in which other modules are to be executed.

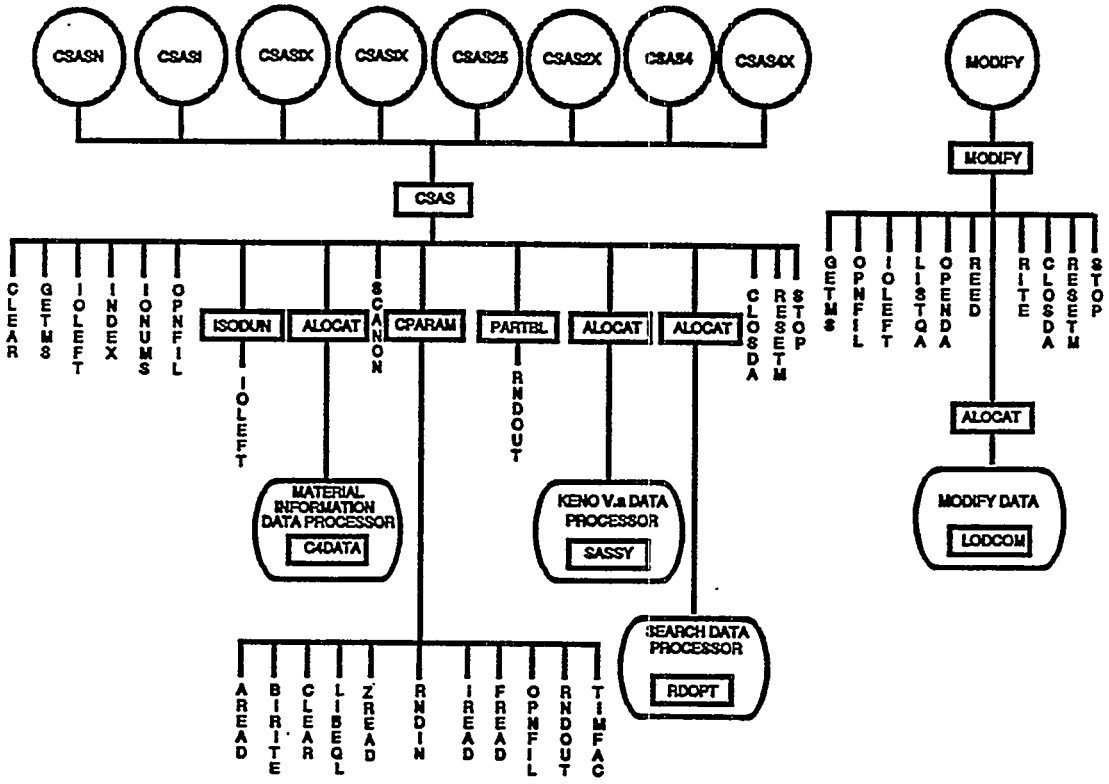


Figure C4.3.2 Overall flow of Criticality Safety Analysis Sequence No. 4

CSAS4 - This control module is responsible for conducting a search for 3-D problems that do not need a cell-weighted cross section.

CSAS4X - This control module is responsible for conducting a search for 3-D problems that require a cell-weighted cross section.

CSAS25 - This control module calculates k-effective for a 3-D system, using KENO V.a, when a cell-weighted mixture cross section is not needed.

CSAS2X - This control module calculates k-effective for a 3-D system, using KENO V.a, when a cell-weighted mixture cross section is required.

CSAS1X - This control module is responsible for performing a 1-D criticality calculation and providing a resonance-corrected, cell-weighted, microscopic cross-section library in the AMPX working library format.

CSASI - This control module generates both a resonance-corrected, microscopic, cross-section library in the AMPX working library format and a resonance-corrected, macroscopic mixture cross-section library in the MORSE/KENO (ICE Monte Carlo-processed) format by sequentially activating the functional modules BONAMI, NITAWL-II, and ICE.

CSASIX - This control module generates both a resonance-corrected, cell-weighted, microscopic cross-section library in the AMPX working library format and a resonance-corrected, cell-weighted, macroscopic mixture cross-section library in the MORSE/KENO (ICE Monte Carlo-processed) format by sequentially activating the functional modules BONAMI, NITAWL-II, XSDRNPM-S, and ICE. The discrete-ordinates code XSDRNPM-S also provides the k-effective for the 1-D problem.

CSASN - This control module generates a resonance-corrected, microscopic cross-section library in the AMPX working library format. This is accomplished by sequentially activating the functional modules BONAMI and NITAWL-II.

CSAS - This is the main program for CSAS and its associated control modules. GETMS is called to read the analytical sequence specification and the parameters associated with it. The sequence specification is used to set flags to cause the desired functional modules to be executed in the proper order. IOLEFT is called to initialize the counter that keeps track of the number of I/Os that are done. INDEX is a FORTRAN-supplied intrinsic function used to determine if a variable matches a specified character string. IONUMS is called to set the input and output units for the free-form reading routines. OPNFIL is called to open the input and output units that are used by the control module. IOSDUN is called several times to determine the number of I/Os that have been used in various operations. C4DATA is called from ALOCAT with the requested storage allocation. This accesses the MATERIAL INFORMATION PROCESSOR. SCANON is called to activate the feature that allows scanning the input data for the word END. If KENO V.a is to be executed, CPARAM is called to read the KENO V.a title and to read and initialize the KENO V.a parameter data. SASSY is called from ALOCAT to read the KENO V.a data and write the information in a form that can be utilized by the CSAS module. If a search is to be made, RDOPT is called from ALOCAT to read and check the search data and transmit it to the CSAS module. If errors are encountered during reading, preparing, and checking the data, execution is terminated without activating any of the functional modules. The direct-access files are closed out when the problem is completed or terminated. This program makes use of error flags in an effort to continue reading and checking input data even after errors are found. However, some errors are severe enough to cause immediate termination.

CLEAR - This library routine is called to initialize the logical unit numbers used by CSAS.

GETMS - This assembly language library routine is called to read the analytical sequence specification and any associated parameter data. It establishes communication with the SCALE driver and enters data obtained from the SCALE driver into common. An example of an analytical sequence specification is given on the following page. This particular example specifies that the control module CSAS is to be executed. The associated parameters are entered following the word "PARM=," starting beyond column 10. In this example the parameters specify that the data are to be checked without executing the problem, and a maximum of 200,000 words is requested to complete this task.

```
=CSAS4    PARM=  (CHECK,SIZE=200000).
```

IOLEFT - This library routine is called to store the initial I/O count in common for determining the number of I/Os used in certain parts of the program.

IONUMS - This library routine sets the I/O units or devices for the free-form data reading routines.

OPNFIL - This library routine is called to open the I/O units or devices used by the specified CSAS control module and all of the functional modules it invokes.

IOSDUN - This subroutine is called several times to indicate the number of I/Os used in various operations.

ALOCAT - This assembly language library routine is called with three arguments. The first argument is a subroutine name, the second argument is the maximum number of words of core storage to be allocated, and the third argument is the statement number to return to if the available core storage is less than that requested by the second argument. ALOCAT is used to call C4DATA, SASSY and, if a search is to be made, RDOPT. In each call an array name, the length of the array, and a statement number in a nonstandard return are passed to the subroutine.

MATERIAL INFORMATION PROCESSOR - This segment of the program is accessed by calling subroutine C4DATA via ALOCAT. It is responsible for reading the standard compositions specification data and associated engineering-type specifications used to generate the mixing table and in performing the cell-weighting calculations. It checks the data for obvious errors and generates information necessary for processing the cross sections. It continues checking and preparing data for use in the functional modules activated by the sequence. The MATERIAL INFORMATION PROCESSOR is described in more detail in Sect. M7.3.

SCANON - This library routine is called to activate the feature that allows scanning for the word END during data reading.

CPARAM - This subroutine is called only if KENO V.a is to be executed. It is responsible for reading the KENO V.a title, initializing certain default values for the KENO V.a parameter data, reading the KENO V.a parameter data, and writing the parameter data on the restart data file to communicate it to the KENO V.a functional module. AREAD, IREAD, FREAD and ZREAD are used to read the parameter data. BIRITE is used to write the parameter data on the restart data file, which is used by the functional module KENO V.a to define the problem. CLEAR is called to zero a common. LIBEQL determines the unit from which cross sections are to be read. RNDIN is called to load the random number if it is entered as parameter data. OPNFIL opens the I/O units that will be used, RNDOUT stores the current random number, and TIMFAC adjusts the time estimate.

AREAD - This library routine may be called many times from subroutine PARAM. It is used to read parameter names and alphanumeric parameter data.

BIRITE - This library routine is used to write the binary data used by the functional modules.

CLEAR - This library routine is called to zero common DIMEN.

LIBEQL - This subroutine is called to determine which unit or device will be used to read the resonance-corrected microscopic library.

ZREAD - This library routine can be called from subroutine PARAM to read a hexadecimal random number that will be used as a kernel for the random number package.

RNDIN - This library routine is called from subroutine PARAM to transfer the random number read by ZREAD to the random number package. It is called only if a random number is entered as parameter data.

IREAD - This library routine can be called many times from subroutine PARAM. It is used to read integer parameter data.

FREAD - This library routine can be called many times from subroutine PARAM. It is used to read floating-point parameter data.

OPNFIL - This library routine opens the I/O units or devices that will be utilized in the problem.

RNDOUT - This library routine is used to preserve the current random number so it can be written on the restart data file.

TIMFAC - This library routine provides the proper adjustment factor by which the allotted time is multiplied to adjust the execution time for execution for different computers.

PARTBL - This subroutine is called only if KENO V.a is to be executed. It is responsible for printing the KENO V.a numeric and logical parameter tables. RNDOUT is called to preserve the current random number so that it can be printed in the numeric parameter table.

KENO V.a DATA PROCESSOR - This segment of the program is accessed by calling subroutine SASSY via ALOCAT. It reads and checks the remainder of the KENO V.a data used by CSAS. It writes the data on the restart data file to be used by the functional module KENO V.a. This segment of the program is described in detail in Sect. C4.3.4.

SEARCH DATA PROCESSOR - This segment of the program is accessed by calling subroutine RDOPT via ALOCAT. It reads the search data and writes it on a data set for use by the CSAS control module. It is described in more detail in Sect. C4.3.5.

CLOSDA - This library routine is called to close out each direct-access file when the problem is completed in a normal manner.

RESETM - This library routine is an entry point in the assembly language library routine GETMS. It transmits control data back to the SCALE driver.

STOP - This library routine is called several times to write error messages. It can be instructed to provide a traceback and can terminate execution or allow execution to continue, depending on the arguments provided to it.

MODIFY - This is the MAIN program for the search control module. GETMS establishes communication between the SCALE driver and the search control module, MODIFY. OPNFIL opens the input and output units for the search. IOLEFT is used to monitor the I/Os used by the code. LISTQA is called to print a program verification information table for quality assurance purposes. OPENDA opens the direct-access units; REED is used to load data from direct access. LODCOM is called via ALOCAT to process the search data and alter the appropriate data accordingly. RITE writes data on the direct-access unit.

CLOSDA is called to close out the direct-access file. RESETM transmits control data back to the SCALE driver. STOP is called if additional core storage is required. If the problem has converged or become unsolvable, an appropriate message is written, and flags are set to terminate execution. Otherwise, a flag is set so that the driver will execute KENO V.a using the modified data.

ALOCAT - This assembly language library routine is used to call LODCOM with an array name, the length of the array, and a statement number for a nonstandard return.

MODIFY DATA - This segment of the program alters the data for the optimum pitch search. It is accessed by calling subroutine LODCOM. Section C4.3.6 contains a detailed description of this segment of the program.

C4.3.3 THE MATERIAL INFORMATION PROCESSOR

The Material Information Processor is responsible for reading data that specifies the cross-section library, defines the materials to be used in the problem, and provides data used to apply geometric and resonance corrections to the cross sections. After the data are read and checked, calculations are performed to create a mixing table and provide data to the functional modules that are invoked by the control module to perform cross-section processing to prepare a problem-dependent cross-section library. Section M7.3 contains the program flow for the Material Information Processor.

C4.3.4 KENO V.a DATA PROCESSOR

This portion of the program, as shown in Fig. C4.3.3, is responsible for processing the KENO V.a input data. All the KENO V.a data, except the title and parameters, are read in this portion of the program. The data are carefully checked for errors and are written on the restart data file to be used by the functional module KENO V.a.

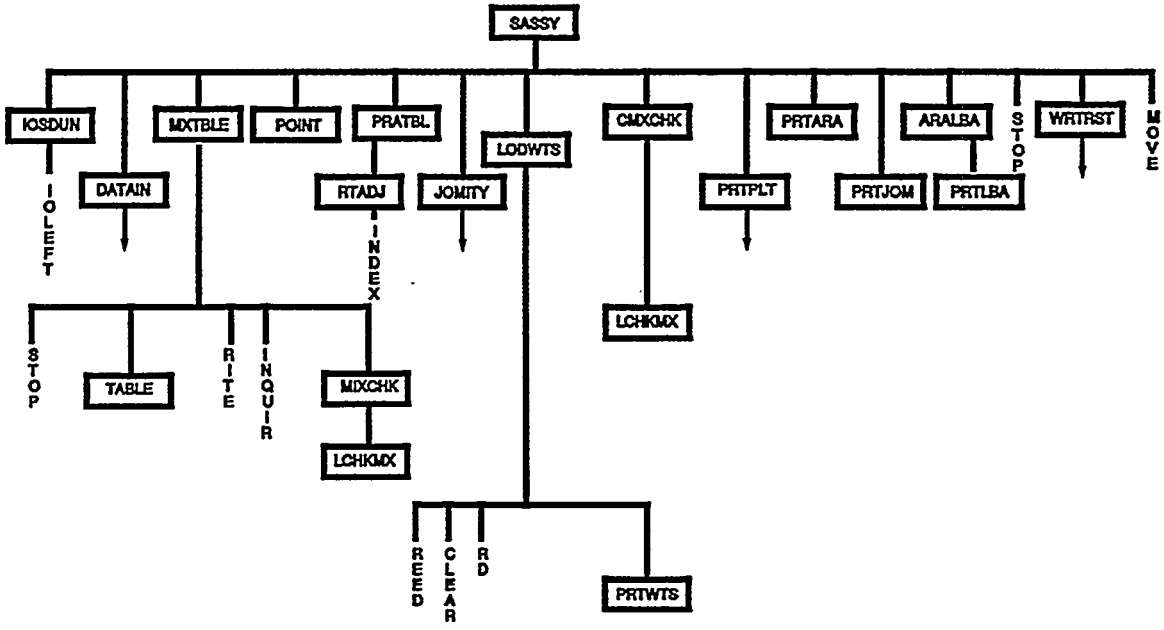


Figure C4.3.3 Flowchart of KENO V.a data processor

SASSY - This subroutine controls the processing of the KENO V.a data. It calls CLEAR to zero the direct-access pointer and length arrays. IOSDUN is called to indicate the number of I/Os used in the different operations involved in processing the KENO V.a data. Then RITE is used to load the direct-access pointer and length arrays on the direct-access data file. Various subroutines are called to read and check the KENO V.a data. If an error is recognized in the data, STOP is called to write a message, and control is returned to the MAIN program. If the data are found to be error free, a restart data file is written by subroutine WRTRST before returning to MAIN.

IOSDUN - This subroutine is called several times to indicate the number of I/Os used for various operations.

IOLEFT - This library routine stores the I/O count in common.

DATAIN - This subroutine controls the reading of all the KENO V.a input data except the title card and parameters. It is explained in more detail in Sect. C4.3.4.1.

MXTBLE - This subroutine initializes the threshold for printing cross-section processing error messages for invalid moments if it was not entered as data, sets up pointers for mixing table data for KENO V.a, calls STOP if more storage is required, and calls TABLE to read the mixing table data. RITE is used to write the mixing table data to a random-access file, and INQUIR is called to set the next block for a direct or random-access device. MIXCHK is called to

ensure that the mixtures used in the geometry data were also specified in the Material Information Processor data.

TABLE - This subroutine is responsible for reading the mixing table data created by the Material Information Processor and storing it in the proper arrays for KENO V.a.

MIXCHK - This subroutine reads the KENO V.a mixing table data and writes an error message if a mixture utilized in the geometry data was not created by the Material Information Processor.

LCHKMX - This logical function is called by MIXCHK to return a value of true if a mixture specified on a KENO V.a geometry card is not specified in the mixing table and a value of false if it is.

POINT - This subroutine calculates pointers for storing and accessing KENO V.a data in memory.

PRATBL - This subroutine prints the KENO V.a table of additional data.

RTADJ - This subroutine right-adjusts the albedo boundary condition names that are read in as left-adjusted data. RTADJ utilizes the FORTRAN-supplied intrinsic function INDEX to locate the first blank character.

JOMITY - This subroutine is primarily responsible for generating additional geometry data, checking the geometry data, writing appropriate geometry error messages, and printing the geometry that is used in the problem. See Sect. C4.3.4.9 for additional information.

LODWTS - This subroutine is called only if PWT=YES is specified in the KENO V.a parameter data. LODWTS prints the bias IDs versus the material I/Os used in the problem. It also loads and prints the biasing or weighting data. The library routine REED is used to load the bias IDs from the direct-access device. CLEAR is used to zero the weighting arrays. RD is used to load the biasing data, and subroutine PRTWTS is called to print it.

PRTWTS - This subroutine prints the group-dependent weight average array for each biasing region in a compact fashion.

CMXCHK - This subroutine is used to ensure that a component of the cell-weighted mixture is not used in the KENO V.a geometry data. If it is, an error message is written, and an error flag is set.

LCHKMX - This logical function is called by CMXCHK to return a value of true if a mixture specified on a KENO V.a geometry card is not a component of the cell-weighted mixture and a value of false if it is.

PRTPLT - This subroutine is called to generate and print 2-D printer plots representing slices through the geometrical representation of the physical problem. See Sect. C4.3.4.14 for details.

PRTARA - This subroutine prints a table listing the array number, the number of units in the x, y, and z directions, and the nesting level for each array utilized in the problem.

PRTJOM - If a geometry error is recognized, this subroutine is called to print the KENO V.a geometry data that is used in the problem.

ARALBA - This subroutine calls PRTLBA for each unit orientation array used in the problem. Subroutine PRTLBA checks each array for geometrical consistency and prints the array data.

STOP - This library routine is called to print an error message and terminate if errors were found in the CSAS or KENO V.a data.

PRTLBA - If a geometry error is recognized, and more than one unit or box type is entered in the geometry data, this subroutine is called to print the KENO V.a unit orientation array data. STOP is called to write an error message if too many units are used in the KENO V.a geometry description.

WRTRST - This subroutine controls the writing of all the KENO V.a data on the restart data file for use by the KENO V.a functional module. MOVE is called to load the required common information into COMMON/REC1/, a common that is used by the analytical sequence. The array that contains the IDs of the 1-D cross sections is written on the restart data file. REED and IO are then used to write the geometry data, unit orientation data, biasing data, and start data on the restart data file.

MOVE - This library routine is called to load data into common.

C4.3.4.1 Control of the Data Input for KENO V.a

This section of the program, shown in Fig. C4.3.4, is responsible for reading the input data that will be used by KENO V.a, with the exception of the title and parameter data.

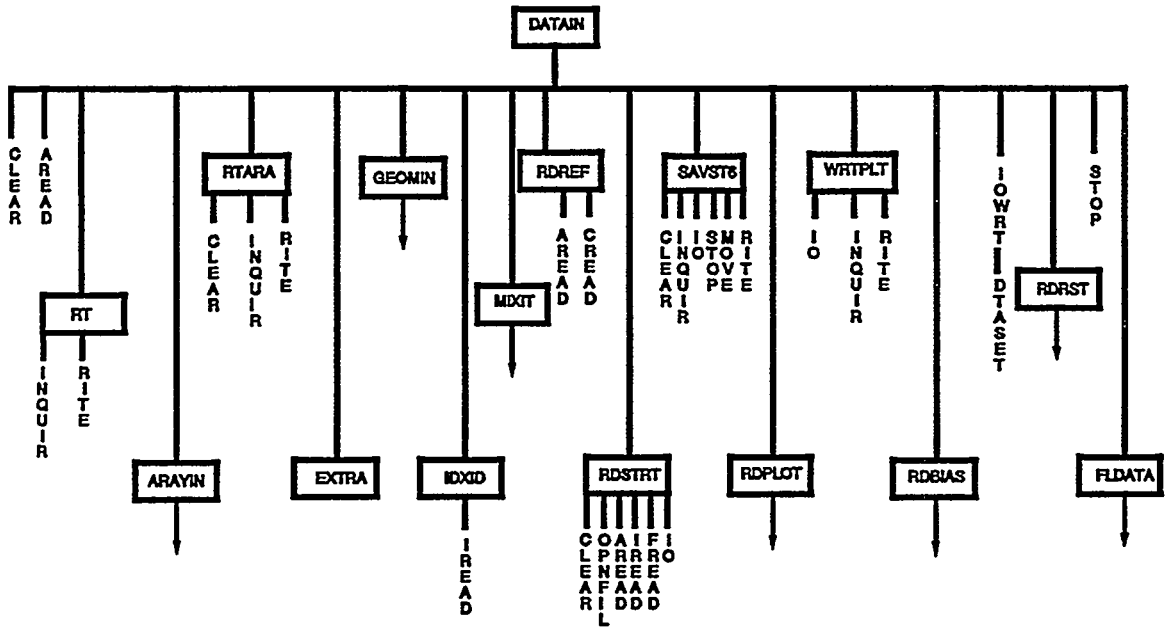


Figure C4.3.4 Flowchart of KENO V.a data reading routines

DATAIN - This subroutine controls the reading of all the KENO V.a data except the title card and parameter data. It initializes COMMON/STDATA/, the common that contains the start data, and initializes the array that contains the IDs of the 1-D cross sections that are to be utilized in the problem. The data reading is accomplished by reading blocks of data. Each block of

data is preceded by a keyword that indicates the type of data being entered. After reading the keyword, the appropriate subroutine is called to read the accompanying data. After the data has been read, it is written on the direct-access data file. IOWRT is called several times to generate a table that lists the unit numbers used by KENO V.a, their names, data set names, and the volume containing the data set. This table can be valuable for quality assurance applications. The library routine STOP is called to write error messages. Subroutine FLDATA is then called to supply information that was not entered as data.

CLEAR - This library routine is called to initialize COMMON/STDATA/. If biasing data are entered, it is also called to clear the space that will contain the biasing data. CLEAR is called with two arguments, a beginning location and a length. It initializes all included locations to zero.

AREAD - This library routine is used to read the READ flag and the keyword defining the type of associated data as well as the END flag and the associated keyword. It can be called many times from DATAIN.

RT - This subroutine may be called many times to write data on the direct-access data file. It passes information between DATAIN and RITE. INQUIR is called to return the value of the next direct-access record after the geometry data and/or the extra 1-D cross sections are written on the direct-access device.

RITE - This library routine is called from RT to write an array of data on the direct-access data file.

ARAYIN - This subroutine is called to read data defining the array size. It also reads the unit orientation data if it is entered. ARAYIN is not called for a single unit problem. See Sect. C4.3.4.2 for a more complete description.

RTARA - This subroutine is called only if ARAYIN is called. CLEAR is called to zero the array before RTARA reads the array data from the scratch unit and writes them on the direct-access device. INQUIR is called to return the value of the next direct-access record after the array data are written on the direct-access device.

EXTRA - This dummy subroutine is provided to allow the user to input extra data that is not normally processed by KENO V.a. The user must provide the programming to read and utilize the data.

GEOMIN - This subroutine is called to read the geometry region data. See Sect. C4.3.4.3 for additional information. The geometry region data are described in detail in Sect. F11.4.4.

IDX1D - This subroutine is called if the number of extra 1-D cross sections is greater than zero and extra 1-D data are entered. It reads the extra 1-D IDs and loads them into the MT array. The data reading is accomplished using the library routine IREAD.

MIXIT - This subroutine is called to read the mixing table data block that defines the mixtures that are to be created. Section C4.3.4.4 explains the mixing procedure in more detail.

RDREF - This subroutine is called to read the boundary conditions (or albedo options) that are to be applied at the outer boundaries of the system described by the KENO V.a geometry data and unit orientation data. The boundary condition data are read using the library routine AREAD. The library routine CREAD is used to read the albedo names. Some preliminary

data checks are made to detect invalid face code names and incompatible boundary conditions. Section F11.4.6 describes the input data for defining the KENO V.a boundary conditions.

RDSTRT - This subroutine is called to read start data for KENO V.a. This data are used to define the spatial distribution of the initial generation. The library routine CLEAR is called to zero the array that will contain the start data. The library routine AREAD is used to read the keywords associated with the start data. IREAD and FREAD are used to read the integer and floating-point start data, respectively. The library routine IO is used to write the start data associated with start type 6 on the scratch data file. The library routine INQUIR returns the value of the next direct-access record after writing the start data on the direct-access device. Data input for defining the initial source distribution is described in Sect. F11.4.8.

SAVST6 - This subroutine is called to save the data associated with start type 6. SAVST6 is called only if start type 6 is specified in the start type data. See Sect. F11.5.8 for information concerning the specification of start data. The library routine CLEAR is called to initialize the arrays that will contain the start data. The library routine IO is used to read the start data array from the scratch data file and load it into memory. The library routine MOVE is used to move the start data array into the neutron bank. The library routine RITE is called to write the neutron bank data on the direct-access data file. The library routine INQUIR returns the value of the next direct-access record after writing the start type 6 data on the direct-access device.

RDPLOT - This subroutine is called to read the plot data block that is used to generate printer plots. Section C4.3.4.5 explains the processing of the plot data in more detail. Section F11.4.11 describes the plot input data in detail.

WRTPLT - This subroutine reads the plot data block from the scratch data file and loads it on direct access. IO reads the data from the scratch data file and loads it in memory. RITE writes the data on the direct-access data file. INQUIR returns the value of the next direct-access record.

RDBIAS - This subroutine is called to read the biasing or weighting data to be used in the problem. See Sect. C4.3.4.6 for more information. The biasing input data block is described in detail in Sect. F11.4.7.

IOWRT - This subroutine is called with five arguments. In sequence they are (1) the output unit, (2) a four-character hollerith name representing a unit name, (3) the unit number represented by the second argument, (4) the number of words of hollerith information contained in the fifth argument, and (5) hollerith information to be printed. IOWRT is called several times to generate a table of the unit numbers, their names, the data set names, and the volumes on which each resides.

DTASET - This library routine is called from IOWRT to provide the data set name of the requested I/O unit and the volume on which it resides.

RDRST - After the data reading is complete, this subroutine is called if a unit containing data for restarting the problem has been defined. It loads data from the restart data file as described in Sect. C4.3.4.7.

FLDATA - This subroutine is called to supply default data for arrays that were not entered as input. Section C4.3.4.8 contains a more detailed account of the exact procedure.

C4.3.4.2. Read KENO V.a Array Data

This section explains the procedure involved in reading the KENO V.a array data utilized by the analytical sequence, as shown in Fig. C4.3.5.

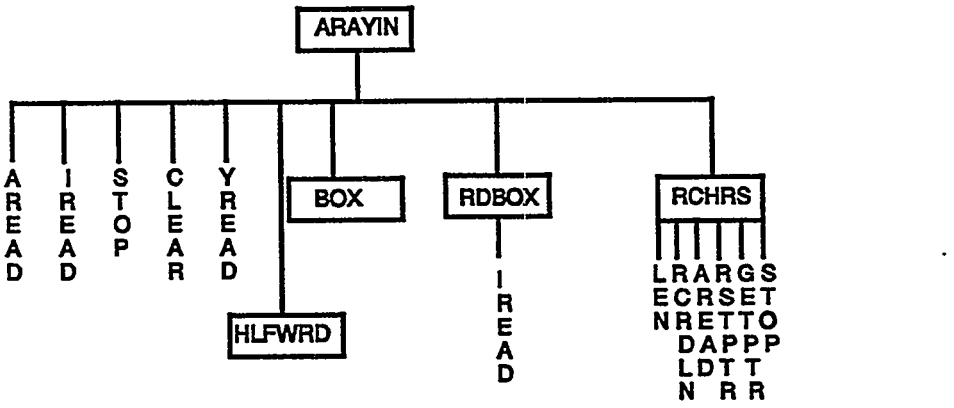


Figure C4.3.5 Flowchart for reading KENO V.a array data

ARAYIN - This subroutine is called from DATAIN when the words READ ARRA are encountered. It is responsible for reading the data that define the size of each unit orientation array. It reads the unit orientation data for each array using subroutine HLFWRD for the FILL option and subroutine RDBOX for the loop option. BOX then writes the array data on the scratch data file. CLEAR is called to zero the unit orientation array. The data are read using the library routines AREAD, IREAD, and YREAD. The data read by this subroutine is described in Sect. F11.4.5.

AREAD - This library routine is used to read the keywords associated with the array data.

IREAD - This library routine is used to read the integer data associated with the array data.

STOP - This library routine is called to write an error message and stop if insufficient memory is available to accommodate the unit orientation array.

CLEAR - This library routine is used to zero arrays.

YREAD - This library routine is called to read the unit orientation data for the FILL option.

HLFWRD - This subroutine is called only if the FILL option is used for entering the unit orientation data. The purpose of HLFWRD is to convert the unit orientation array data from full-word integers to half-word integers.

BOX - This subroutine is called to write the array data on the scratch data file.

RDBOX - This subroutine is called only if the LOOP option is used for entering the unit orientation data. It uses the library routine IREAD to read the unit orientation data. Some data consistency checks are made, and appropriate error messages are written if errors are encountered. If the input geometry is to be printed, RDBOX prints the unit orientation for each array.

RCHRS - This subroutine is used to read the comment associated with an array. LEN is a FORTRAN-supplied function that sets the length of the data string. GETPTR is used to return the current pointer in the input buffer. RSTPTR resets the pointer. AREAD is used to read the input data, and RCRDLN sets the length of the input buffer. STOP is called to write an error message and stop if the array comment is too long (i.e., the ending delimiter is missing).

C4.3.4.3. Read KENO V.a Geometry Data

This section of the program reads the KENO V.a geometry data required for the problem as shown in Fig. C4.3.6.

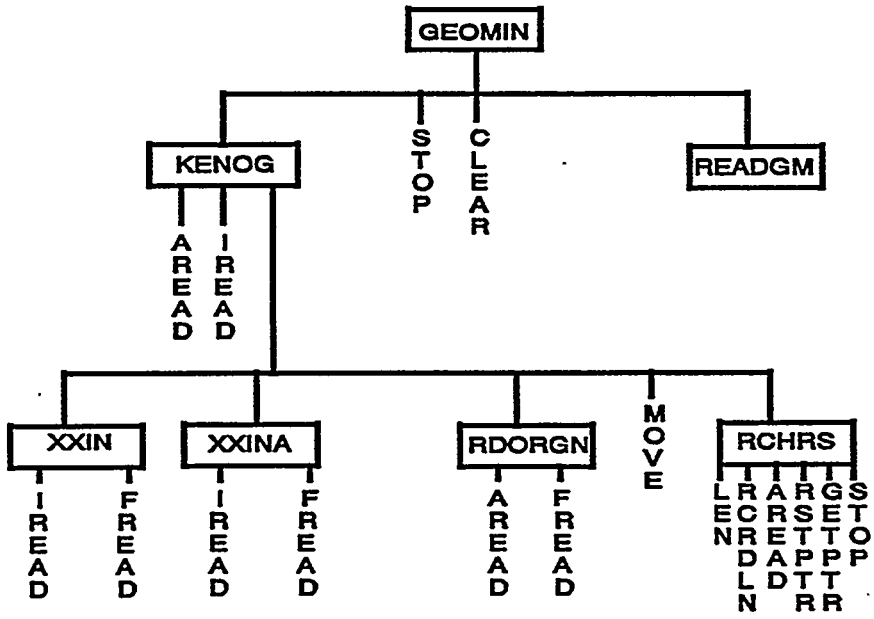


Figure C4.3.6 Flowchart of routines to read the KENO V.a geometry data

GEOMIN - This subroutine controls the reading of the KENO V.a geometry data. KENOG is called to read the data and write it on the scratch data file. Pointers are then calculated. STOP is called to print a message and terminate if more computer storage is required. CLEAR is called to zero the arrays that hold the geometry data. READGM is called to read the data

from the scratch data file and load it into the appropriate arrays. STOP is called to write an error message if more storage is needed. Section F11.4.4 describes the KENO V.a geometry input data in detail.

KENOG - This subroutine uses AREAD to read the geometry word. IREAD is called to read the unit number for a unit or box type. It is also used to read the number of reflector regions on a reflector card. XXIN is called to read the mixture number, the bias ID number, and the geometry dimensions. XXINA is an entry point in XXIN. It reads the mixture number and geometry dimensions. The origin specification, if any, associated with a sphere, hemisphere, cylinder, or hemicylinder is read by RDORGN. The chord specification, if any, associated with a hemisphere or hemicylinder is also read by RDORGN. The necessary geometry data block is written on the scratch data unit. If the input geometry data block is to be printed, KENOG does this as the data are read.

XXIN - This subroutine is called to read the mixture number, the bias ID number, and the geometry dimensions. IREAD is used to read the mixture number and bias ID number. FREAD is used to read the geometry region dimensions.

XXINA - XXINA is an entry point in XXIN. It is called when the geometry word ARRA or ARRAY is encountered. It reads the mixture number and the geometry dimensions. IREAD is used to read the mixture number. FREAD is used to read the geometry region dimensions.

RDORGN - This subroutine uses AREAD to read a word. If the word is ORIGIN, it uses FREAD to read the points defining the origin. If the word is CHORD, it uses FREAD to read the offset of the plane with respect to the origin. If the word is not ORIGIN or CHORD, a flag is set to prevent KENOG from attempting to read another geometry word.

RCHRS - This subroutine is used to read the comment associated with a unit in the geometry region data. LEN is a FORTRAN-supplied function that sets the length of the data string. GETPTR is used to return the current pointer in the input buffer. RSTPTR resets the pointer. AREAD is used to read the input data, and RCRDLN sets the length of the input buffer. STOP is called to write a message and terminate the problem if the comment is too long.

READGM - This subroutine reads the geometry data from the scratch data unit and loads them into the proper arrays.

C4.3.4.4. Read KENO V.a Mixing Table Data

This section deals with reading the mixing table data, as shown in Fig. C4.3.7.

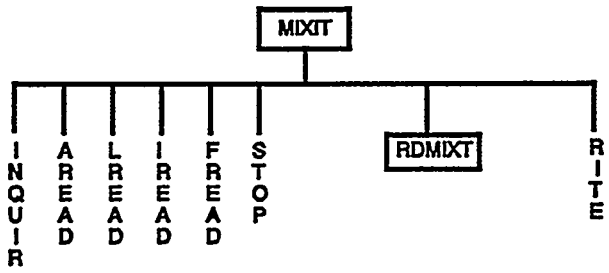


Figure C4.3.7 Flowchart for reading KENO V.a mixing table data

MIXIT - This subroutine uses AREAD to read the mixture keywords and the scattering keyword. IREAD is used to read the mixture numbers and the number of scattering angles as well as the nuclide IDs. FREAD reads the number densities. LREAD is used to determine if the next item is a keyword rather than a number. The necessary data arrays are written on the scratch data file. Pointers are calculated for the necessary storage arrays, and RDMIXT is called to load the data from the scratch file into the storage arrays.

The library routine RITE is called to write the mixing table information on the direct-access device, and INQUIR is called to return the value of the next direct-access record.

LREAD - This library routine returns a value of "true" if the next character is a numeric digit. Otherwise, a value of "false" is returned.

STOP - This library routine is called from MIXIT if the storage space is insufficient to hold the mixing table arrays.

RDMIXT - This subroutine reads the mixing table data arrays from the scratch data file and loads them into the storage arrays.

C4.3.4.5. Read KENO V.a Plot Data

This section of the program, shown in Fig. C4.3.8, reads the plot or picture data used to generate printer plot maps of the mixtures, units, and/or bias IDs used in the problem. The plot input data block is described in Sect. F11.4.11.

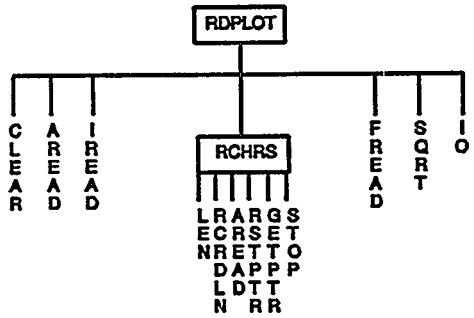


Figure C4.3.8 Flowchart for reading KENO V.a plot data

RDPLOT - This subroutine uses CLEAR to initialize the data arrays. RCHRS is used to read the plot title and the character string of symbols to be used in the plot. AREAD, IREAD, and FREAD are used to read the plot or picture input data. SQRT is used to determine the normalization factor for the direction cosines, and IO is called to load the plot data on the scratch data file.

RCHRS - This subroutine is used to read the plot title and the character string that defines the symbols to be used in the plot. LEN is a FORTRAN-supplied routine that sets the length of the data string. GETPTR is used to return the current pointer in the input buffer. RSTPTR resets the pointer. AREAD is used to read the input data, and RCRDLN sets the length of the input buffer. STOP is called to write an error message if the plot title is too long and terminate the problem.

C4.3.4.6. Read KENO V.a Biasing Data

This section of the program reads the biasing data used in the problem. The biasing input data block is described in Sect. F11.4.7 and illustrated in Fig. C4.3.9.

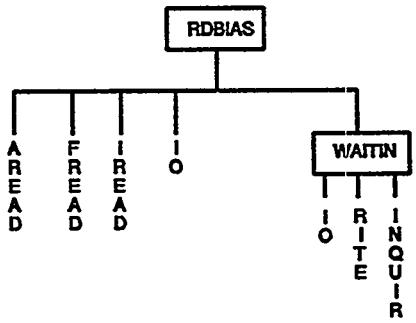


Figure C4.3.9 Flowchart for reading KENO V.a biasing data

RDBIAS - This subroutine is responsible for reading the biasing data block and writing it on the scratch data file. AREAD is used to read the keywords used in the biasing data and a title for the biasing material if the energy- and space-dependent values of the biasing function are entered from cards. IREAD and FREAD are used to read the numerical data. Pointers for the storage arrays needed to process the biasing data are determined, and WAITIN is called to load the data from the scratch data file into the storage arrays and write them on the direct-access data file.

RDPLOT - This subroutine uses CLEAR to initialize the data arrays. RCHRS is used to read the plot title and the character string of symbols to be used in the plot. AREAD, IREAD, and FREAD are used to read the plot or picture input data. SQRT is used to determine the normalization factor for the direction cosines, and IO is called to load the plot data on the scratch data file.

RCHRS - This subroutine is used to read the plot title and the character string that defines the symbols to be used in the plot. LEN is a FORTRAN-supplied routine that sets the length of the data string. GETPTR is used to return the current pointer in the input buffer. RSTPTR resets the pointer. AREAD is used to read the input data, and RCRDLN sets the length of the input buffer. STOP is called to write an error message if the plot title is too long and terminate the problem.

WAITIN - This subroutine reads the biasing data block from the scratch data file and loads it into the storage arrays. IO is used to load the energy- and space-dependent biasing function (*wtavg*) into the storage arrays. RITE is used to write the biasing data on the direct-access data file. The library routine INQUIR is called to set the next block on a direct- or random-access device.

C4.3.4.7. Read KENO V.a Restart Data

This section of the program reads restart information from the restart data file. The flowchart for this procedure is given in Fig. C4.3.10.

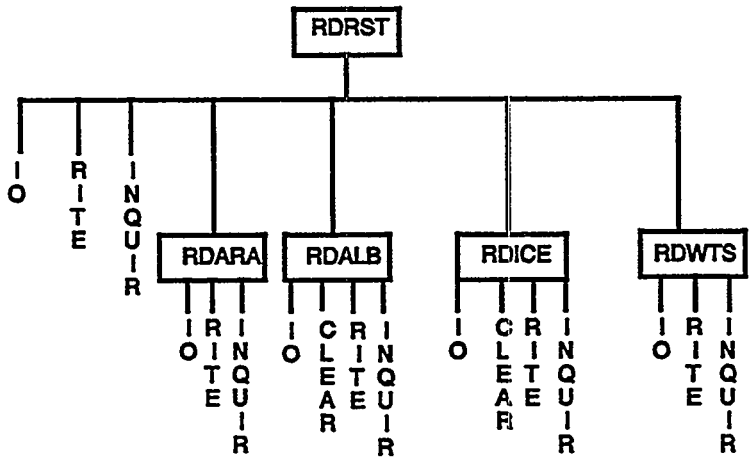


Figure C4.3.10 Flowchart for reading KENO V.a restart data

RDRST - This subroutine is called only if the problem is to use data from the restart data file. The program recognizes that restart data will be read if the restart unit is defined as a number greater than zero. IO is used to load the array that contains the 1-D IDs from the restart data file. Each type of data is loaded from the restart data file using IO and is written on the direct-access data file by RITE. All restart data except the mixed cross-section data, the differential albedo data, the array data, and the biasing data are processed directly in RDRST. RDICE is called to load the cross-section data on the direct-access data file, RDALB is called to load the differential albedo data on the direct-access data file, RDARA is called to load the array data on the direct-access data file, and RDWTS is called to load the biasing data on the direct-access data file. The library routine INQUIR is called to return the value of the next direct-access record.

RDALB - This subroutine is called from RDRST to read the albedo data block from the restart data file and write it on the direct-access data file. IO is used to load the albedo pointer and length arrays into memory from the restart data file. CLEAR is called to zero the albedo pointer and length arrays, and RITE writes them on the direct-access data file. INQUIR stores the next direct-access block number. Each record of albedo data is read from the restart data file, loaded into memory using IO, and written on the direct-access data file using RITE. When all the records of albedo data have been processed, the updated pointer and length arrays are rewritten over the initial ones using RITE.

RDICE - This subroutine is called from RDRST to read the cross-section data block from the restart data file and write it on the direct-access data file. CLEAR is called to zero the pointer and length arrays. The length array is then read from the restart data file. RITE is used to write the pointer array and the length array on the direct-access data file. INQUIR stores the next direct-access block number. Then IO and RITE are used to load the cross-section data from the restart data file and write them on the direct-access data file. This procedure is repeated for every record of each mixture. The updated pointer and length arrays are then rewritten over the initial ones using RITE.

RDARA - This subroutine is called from RDRST to read the array data block from the restart data file and write it on the direct-access data file. IO is used to load the data from the restart data file, and RITE is used to write them on the direct-access data file. INQUIR stores the next direct-access block number.

RDWTS - This subroutine is called from RDRST to read the biasing data block from the restart data file and write it on the direct-access data file. IO is used to load the data from the restart data file, and RITE is used to write them on the direct-access data file. INQUIR stores the next direct-access block number.

C4.3.4.8. Generate Remaining KENO V.a Data

This section of the program, shown in Fig. C4.3.11, is responsible for generating data that are required for a KENO V.a problem but are not entered directly as data.

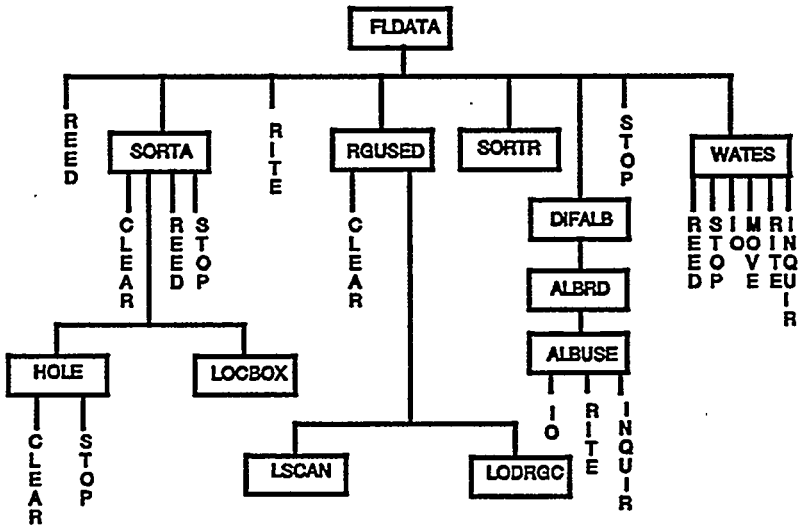


Figure C4.3.11 Flowchart for generating remaining KENO V.a data

FLDATA - The library routine REED is used to load data arrays from the beginning of the mixtures used in the geometry through the geometry data. The library routine STOP may be called to print an error message. SORTA is called to determine which arrays and holes are used as well as the array and hole nesting levels. RITE is called to write the geometry data on the direct-access data file. RGUSED is called to determine which geometry regions are used in the problem. SORTR is called to generate the mixture correspondence array. It is called again to generate the bias region correspondence array. These correspondence arrays are used to avoid storing mixture cross sections and biasing data that are entered as data but are not actually used in the problem. If boundary conditions specify differential albedo data, and they are not available from the restart data file, DIFALB is called to read the albedo data block

and load the requested data on the direct-access file. If the requested biasing data were unavailable from the restart data file, WATES is called to load the energy and position-dependent biasing function (*wtavg* array) on the direct-access data file.

SORTA - This subroutine checks to see that the global array is properly defined. It determines the array correspondence array and the nesting levels for holes and arrays. SORTA uses CLEAR to initialize arrays. REED is used to load the array data, and STOP is used to write an error message and terminate if more computer storage is needed for the problem.

HOLE - This subroutine is called from SORTA to determine what holes occur at the next nesting level and to adjust the array nesting level for arrays that occur in holes. It also checks to ensure holes are not recursively nested.

LOCBOX - This function subprogram is called from SORTA to determine the unit or box type at a given position in the unit orientation array.

RGUSED - This subroutine determines which geometry regions are used in the problem. The library routine CLEAR is called to zero the space for the region correspondence array. LSCAN determines if a particular unit or box type has been used in the unit orientation array, and if it has, LODRGC is called to load the region number into the region correspondence array.

LSCAN - This is a logical function that returns a value of true if the specified unit or box type is used in the unit orientation array. A value of false is returned if the unit or box type was not used in the unit orientation array.

LODRGC - This subroutine loads the region number in the region correspondence array.

SORTR - This subroutine is called twice from FLDATA to create a mixture correspondence array and a biasing correspondence array. These correspondence arrays are used to avoid storing mixture cross sections and biasing information that are defined in the input data but were not referenced in the geometry data utilized in the problem. They are also used throughout the code for accessing the proper mixture cross sections and biasing information.

DIFALB - This subroutine is called if differential albedos are specified as a boundary condition but are not available from the restart data file. It rewinds the albedo data file, reads the header record, and calculates pointers. ALBRD is called to load the albedo data.

ALBRD - This subroutine searches through the albedo data file to locate the requested albedo name or boundary condition. If it is not found, an error message is written. If it is found, the number of different differential albedos that were requested are tabulated and ALBUSE is called.

ALBUSE - This subroutine writes the albedo pointer array on the direct-access data file. IO is used to load data from the albedo data file, and RITE is used to write the data on the direct-access data file. Then the pointer and length arrays are rewritten on the direct-access data file. INQUIR stores the next direct-access block number.

WATES - This subroutine reads the biasing input data block from the direct-access data file and reads the KENO V.a weights library. STOP is called if the computer storage space is too small to contain the energy- and position-dependent biasing function (*wtavg*). IO is used to load the

biasing function into a temporary storage array. If a specific biasing function is to be used, MOVE is called to load it into the *wtavg* array. If biasing or weighting data are entered from cards, REED is used to load the data into a temporary storage array. If a specific biasing function that was loaded from cards is to be used in the problem, MOVE is called to load it into the *wtavg* array. When all the data have been processed, RITE is called to load the biasing input data on the direct-access data file. RITE is called again to load the *wtavg* array on the direct-access data file. INQUIR is used to store the next direct-access block number.

C4.3.4.9. Process the KENO V.a Geometry Data

This portion of the program, shown in Fig. C4.3.12, is primarily responsible for loading the geometry data, generating additional geometry data, checking the geometry for consistency, writing error messages related to the geometry, and printing the geometry that is used in the problem.

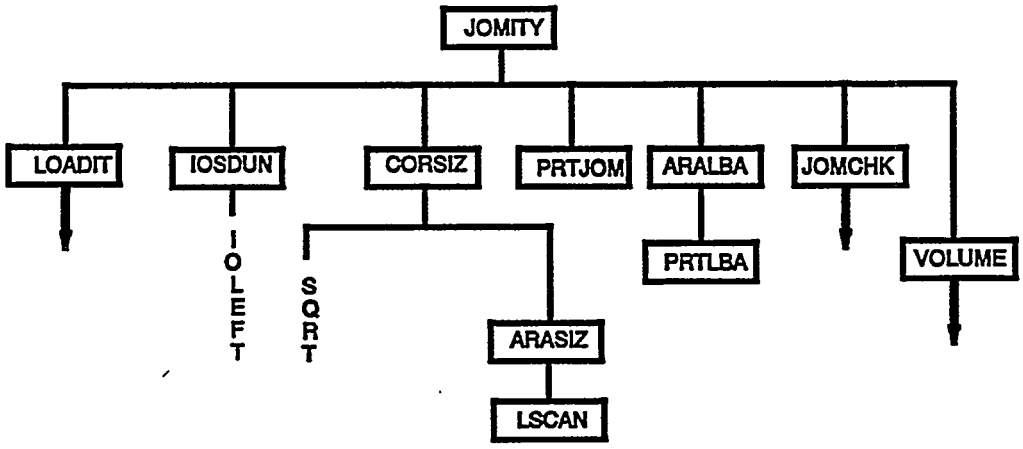


Figure C4.3.12 Flowchart for processing KENO V.a geometry data

JOMITY - This subroutine is responsible for generating additional geometry data, checking the geometry data, writing geometry error messages, and printing the geometry.

LOADIT - This subroutine loads the geometry data and the nonsupergrouped portion of the albedo data. Section C4.3.4.10 contains a more detailed description of the procedure.

IOSDUN - This subroutine returns the numbers of I/Os used. The library routine IOLEFT returns the numbers of I/O requests remaining before the system cancels the job.

CORSIZ - This subroutine sends the appropriate lattice or array information to ARASIZ for each lattice that is used in the problem. Using this information, it calculates the overall positive dimensions of the global array. The library routine, SQRT, is utilized to calculate the maximum chord length of an unreflected array, a reflected array, or a single unit problem.

ARASIZ - This subroutine uses the array unit orientation data to calculate the positive dimensions of the core boundary for that array or lattice. The function LSCAN is called to determine if a specified unit or box type has been used in the array. ARASIZ also checks to ensure that the faces of adjacent units are the same size and shape. Several error messages are written if errors are encountered.

LSCAN - This is a logical function that returns a value of true if the specified unit or box type is used in the unit orientation array. A value of false is returned if the unit or box type was not used in the unit orientation array.

PRTJOM - This subroutine prints the geometry data used in the problem.

ARALBA - This subroutine calls PRTLBA for each array that is used in the problem.

PRTLBA - This subroutine is called to print the unit orientation data for each lattice or array that is used in the problem. It may print a warning message associated with one or more lattices.

JOMCHK - The purpose of this subroutine is to perform consistency checks on the geometry data and write the appropriate error messages. See Sect. C4.3.4.11 for additional details.

VOLUME - This subroutine is responsible for calculating the volume of each geometry region and the cumulative volumes for each unit that is used in the problem. See Sect. C4.3.4.12 for additional details.

C4.3.4.10. Load KENO V.a Data from the Direct-Access File

This portion of the program loads data from the direct-access data file into permanent memory as shown in Fig. C4.3.13.

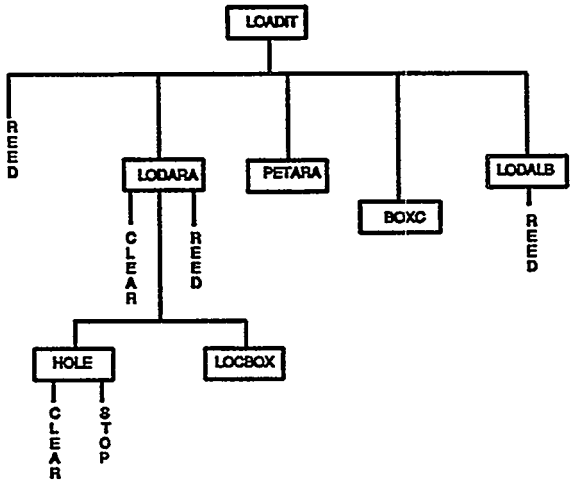


Figure C4.3.13 Flowchart for loading data from direct access

LOADIT - This subroutine calls the library routine REED to load the geometry data. If the problem is an array problem (lattice geometry), LODARA is called to load the lattices that are used

in the problem and recompute and readjust the array nesting level array and hole nesting array. If multiple boxes are used in the problem, PRTARA is called to print the unit orientation array for each lattice used in the problem. BOXC is called to load the box correspondence array, and LODALB is called to load the nonsupergrouped portion of the albedo data.

LODARA - This subroutine is responsible for loading the lattices (unit orientation arrays) that are used in the problem, computing the hole nesting level array, and computing and adjusting the array nesting level array. CLEAR is used to initialize the arrays, and REED is used to load the unit orientation arrays. HOLE and LOCBOX are both called by LODARA.

HOLE - This subroutine is called from LODARA to determine which holes occur at the next nesting level and to adjust the array nesting level for arrays that occur in holes. It also checks to ensure that holes are not recursively nested. CLEAR is used for initialization purposes, and STOP is called if holes are recursively nested.

LOCBOX - This function is called from LODARA to return the unit or box type at a given position in the unit orientation array.

PRTARA - This subroutine prints a table of the arrays used in the problem. The array number, the number of units in the x, y, and z directions, and the nesting level are printed for each array.

BOXC - This subroutine uses the number of units or box types and the geometry region number corresponding to the first and last geometry region of each unit to generate the box correspondence array that contains the unit or box type number for each geometry region. This is loaded in the appropriate position as it is generated.

LODALB - This subroutine calls the library routine REED to load the pointer and length arrays for the albedo data from the direct-access data file. REED is used to load the nonsupergrouped albedo data, for each albedo that is used, into a temporary array. A loop over the number of angles is then used to load these data into the appropriate arrays. When all of the albedos used in the problem have been processed, REED is called to load the pointer arrays for the cross sections and albedos as well as the arrays defining the albedo to cross-section energy group correlation.

C4.3.4.11. Check the KENO V.a Geometry Data

This portion of the program checks the KENO V.a geometry for inconsistencies, surface intersections, and other errors. The flowchart is shown in Fig. C4.3.14.

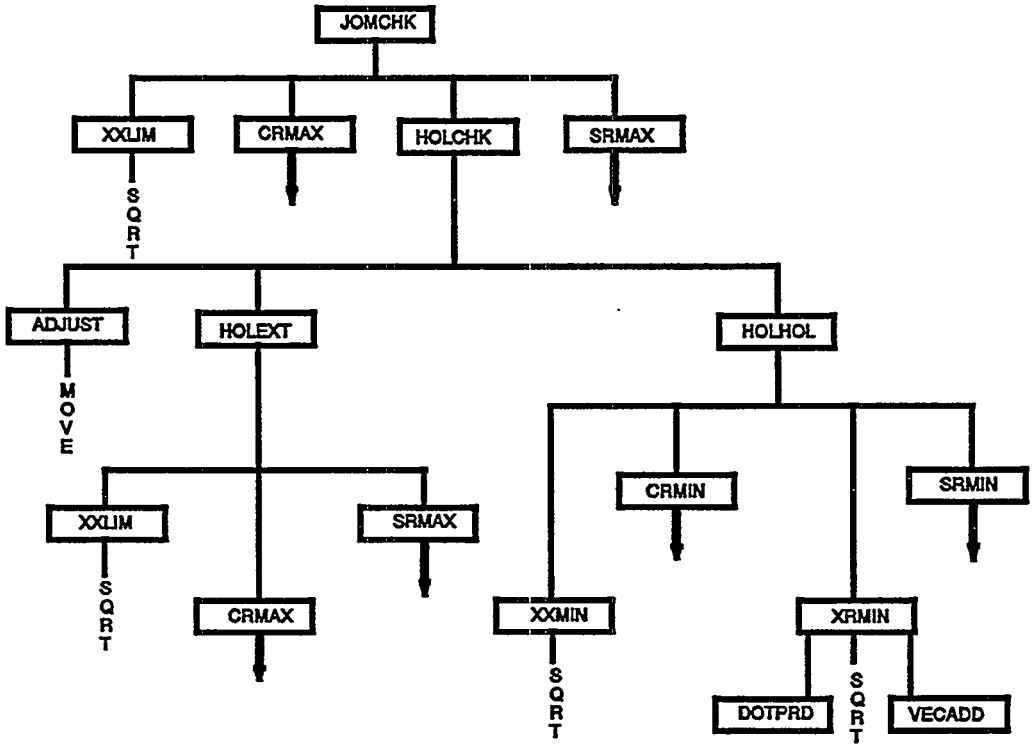


Figure C4.3.14 Flowchart of geometry-checking procedure

JOMCHK - This subroutine checks each geometry region to ensure that it does not intersect the next outer region. If an intersection occurs, an error flag is set and an error message is written. JOMCHK checks each surface of the outer region for an intersection. If the surface is a planar surface, XXLIM is used to return the farthermost point of the inner region in the direction of the plane specified in the call (i.e., for the -x face, XXLIM returns the most negative x value of the inner region). For a spherical surface, SRMAX is used to return the length of the maximum radius vector of the inner region with respect to the origin of the outer region. For a cylindrical surface, CRMAX is used to return the length of the maximum radius vector of the inner region with respect to the axis of the outer region. Subroutine HOLCHK is called to check for intersections between holes and other geometry regions and for holes with other holes.

CRMAX - This function determines the maximum cylindrical radius vector of a geometry region with respect to a given axis and then returns the magnitude of that vector. See Sect. C4.3.4.12 for additional details.

XXLIM - This routine returns the maximum coordinate of an interior region corresponding to a particular face direction (for negative face directions, maximum means most negative).

SRMAX - This function determines the maximum radius vector of a geometry region with respect to a given origin and then returns the magnitude of that vector. See Sect. C4.3.4.12 for additional details.

HOLCHK - This subroutine is responsible for ensuring that a hole does not intersect any other geometry region. ADJUST is called to adjust the dimensions of the hole with respect to the origin of the unit that contains the hole. HOLEXT is called to check for a hole intersecting the region external to it. HOLHOL is used to check for a hole intersecting the region internal to the region that contains the hole. It is also used for checking for the intersection of two holes.

ADJUST - This subroutine corrects the dimensions of a region represented as a hole with respect to the origin of the unit that contains the hole.

HOLEXT - This subroutine checks for a hole intersecting the region external to it. XXLIM is used to return the farthermost point of the hole in the direction of the plane specified in the call. CRMAX is used for a cylindrical surface to return the length of the maximum radius vector of the hole with respect to the axis of the outer region. SRMAX is used for a spherical surface to return the length of the maximum radius vector of the hole with respect to the outer region.

HOLHOL - This subroutine is responsible for ensuring that a hole does not intersect the geometry region internal to the region that contains the hole. It also checks for holes intersecting each other. XXMIN is used to return the nearest point of the hole in the direction of the plane specified in the call. CRMIN is used for a cylindrical surface to return the length of the minimum radius vector of the hole with respect to the axis of the surface. XRMIN determines the minimum coordinate of a hole with respect to a flat circular face. SRMIN is used for a spherical surface to return the length of the minimum radius vector of the hole with respect to the origin of the surface.

XXMIN - This function returns the minimum coordinate of the hole with respect to the fact of the cuboid specified in the call. SQRT is utilized in determining the minimum coordinate of spherical or cylindrical holes.

CRMIN - This function returns the magnitude of the minimum cylindrical radius vector of a hole with respect to a given axis. See Sect. C4.3.4.12 for additional details.

XRMIN - This function determines the minimum coordinate of a hole with respect to a flat circular face. SQRT is used in processing spherical and cylindrical holes. The functions DOTPRD and VECADD are called to perform vector arithmetic.

DOTPRD - This function returns the dot product of two vectors.

VECADD - This function returns the vector sum of two vectors.

SRMIN - This function returns the magnitude of the minimum radius vector from the center of a sphere to another geometry region. See Sect. C4.3.4.12 for additional details.

C4.3.4.12. Determine Distances

This section of the KENO V.a geometry checking procedure is utilized in checking for geometry surface intersections. The flowcharts of the routines utilized in this procedure are given in Fig. C4.3.15.

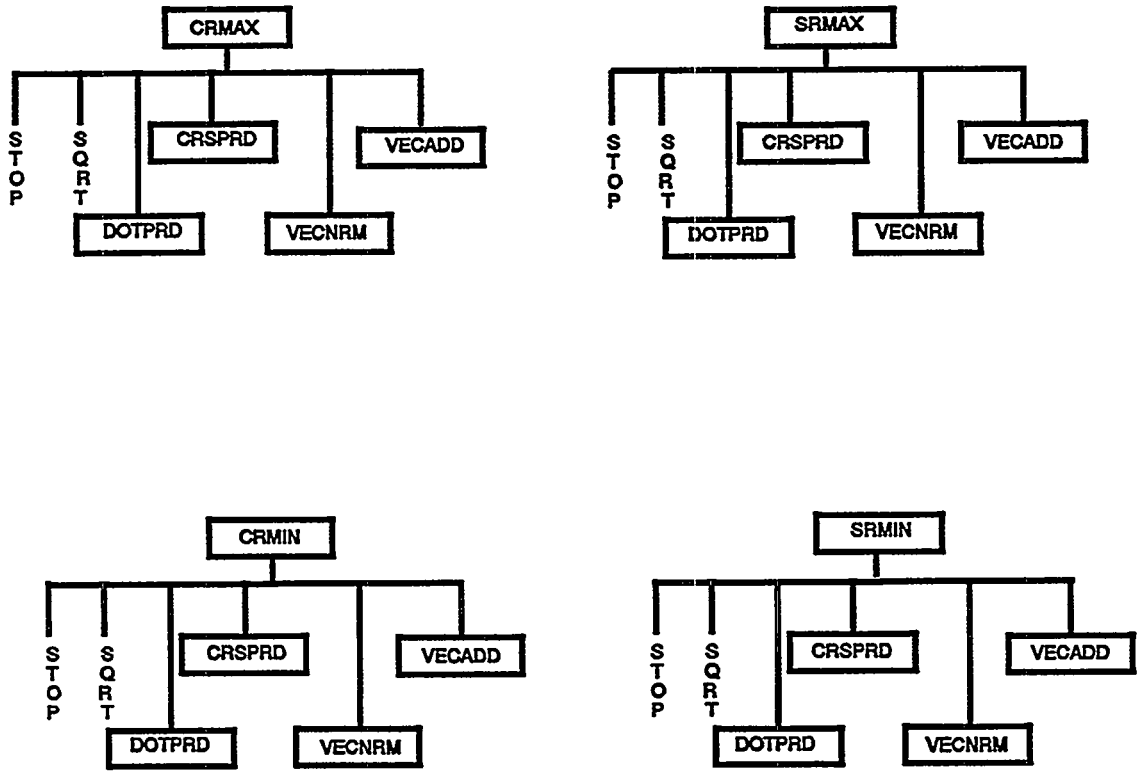


Figure C4.3.15 Flowchart for distance to intersection

CRMAX - This function determines the maximum cylindrical radius vector of a geometry region with respect to a given axis and then returns the magnitude of that vector. Depending on the geometry type, CRMAX may call CRSPRD to generate the cross production of two vectors, DOTPRD to generate the dot product of two vectors, VECADD to add two vectors together, and VECNRM to multiply a vector by a scalar. STOP is called if geometry inconsistencies are encountered.

SRMAX - This function determines the maximum radius vector of a geometry region with respect to a given origin and then returns the magnitude of that vector. Depending on the geometry type, SRMAX may call CRSPRD to take the cross production of two vectors, DOTPRD to take the dot product of two vectors, VECADD to add two vectors together, and VECNRM to multiply a vector by a scalar. STOP is called if geometry inconsistencies are encountered.

CRMIN - This function determines the minimum cylindrical radius vector of a geometry region with respect to a given axis and returns the magnitude of that vector. The geometry type determines which functions will be used to calculate the minimum radius vector. DOTPRD is used to generate the dot product of two vectors, CRSPRD generates the cross product of two vectors, VECNRM multiplies a vector by a scalar, and VECADD adds two vectors together. STOP is called if geometry inconsistencies are encountered.

SRMIN - This function determines the minimum radius vector of a geometry region with respect to a given origin (center of a sphere) and returns the magnitude of that vector. Depending on the geometry type, SRMIN may call DOTPRD to take the dot product of two vectors, CRSPRD to take the cross production of two vectors, VECNRM to multiply a vector by a scalar, and VECADD to add two vectors. STOP is called if geometry inconsistencies are encountered.

CRSPRD - This is a utility routine to generate the cross product of two vectors.

DOTPRD - This function returns the dot product of two vectors.

VECADD - This subroutine returns the result of adding two vectors.

VECNRM - This routine scales a vector by a constant.

C4.3.4.13. Calculate KENO V.a Geometry Volumes

This portion of the program, illustrated in Fig. C4.3.16, is responsible for calculating the volume of each KENO V.a geometry region used in the problem, the cumulative volumes for each unit used in the problem, the number of times each unit was used in the problem, and the total volume of each region summed over all occurrences.

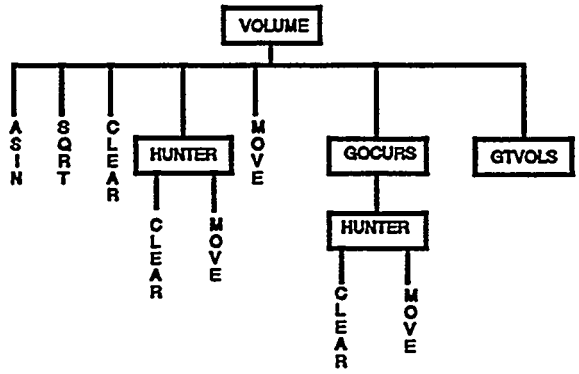


Figure C4.3.16 Flowchart for calculating KENO V.a geometry volumes

VOLUME - This subroutine calculates the volume of each region for every unit that is used in the problem. It then calculates the cumulative volumes for each unit. The intrinsic functions ASIN, which returns the arc sign of a variable, and SQRT, which returns the square root of an expression, are used when calculating the volume of a hemicylinder. CLEAR is used to initialize arrays. If an external reflector is present, HUNTER is called to determine the number of times each array and/or hole is used in the reflector. GOCURS is used to determine the number of times each unit, array, and hole is used in the problem. GTVOLS is called to calculate and print the number of occurrences for each unit and the corresponding total volumes for the entire system. CLEAR is called to initialize the array for the total volume of each mixture used in the problem prior to calculating and printing those totals.

HUNTER - This subroutine determines the number of times each unit, array, and hole is used. CLEAR is used to initialize storage arrays for the present hole level and the next hole level. MOVE is used to move the storage arrays.

GOCURS - This subroutine loops over the array size and calls HUNTER to determine the number of times each unit, lattice or array, and hole is used in the problem.

GTVOLS - This subroutine calculates the total volume of each region for the entire problem by multiplying the volume of the region by the number of times the region is used in the problem.

C4.3.4.14. Generate Printer Plot

This portion of the program, illustrated in Fig. C4.3.17, generates printer plots of a 2-D slice through the KENO V.a geometry. As many plots as are desired can be printed.

PRTPLT - This subroutine controls the generation of the printer plots. The library routine CLEAR is called to zero the necessary space. Subroutine UNTCRS is called to generate a unit correspondence array. REED is used to load the picture data from direct access. INQUIR is called to return the value of the next direct-access data block. The picture title is printed, and subroutine RELATE is called to print a heading for the symbol map and print the symbol map. The picture coordinates, direction cosines, and number of symbols across and down the page, as well as the step intervals, are printed. Then subroutine PRINT is called to generate the actual picture.

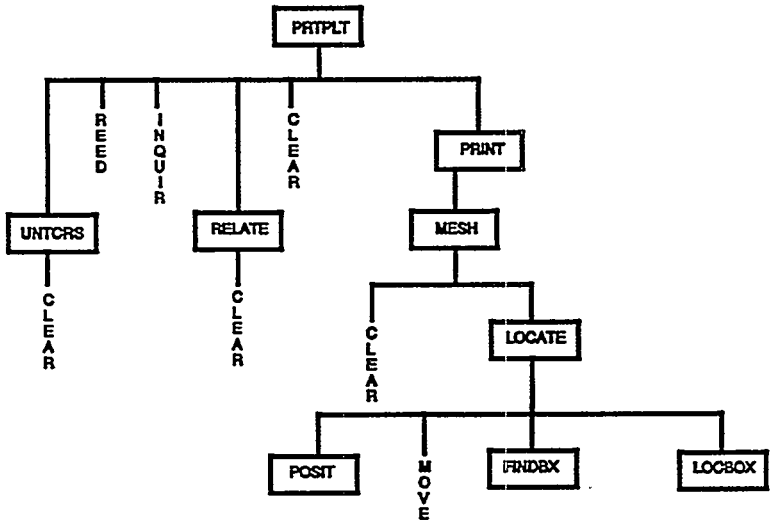


Figure C4.3.17 Flowchart for printer plots

UNTCRS - This subroutine calls CLEAR to zero the unit correspondence array. It then loads the appropriate unit number in the appropriate position of the array.

RELATE - This subroutine calls CLEAR to zero the reverse correspondence array. It then prints the plot header and loads the array that correlates the symbols.

PRINT - This subroutine determines the number of pages that will be needed to print the printer plot picture. Subroutine MESH is called to load the appropriate mixture numbers, unit numbers, or bias ID numbers for each line of print for the picture. Then PRINT prints the line of symbols corresponding to them.

MESH - This subroutine loads an array that contains the appropriate mixture number, unit number, or bias ID number for each character in a line. CLEAR is called to initialize arrays if nested holes or nested arrays are present in the problem. LOCATE is called to determine the geometry region and unit or box type that contains each mesh point. MESH then loads the mixture number unit number, or bias ID number.

LOCATE - This subroutine is responsible for determining the geometry region for each mesh point in the picture. Subroutine POSIT is called to determine the region that contains the specified mesh point. If array data are used, MOVE is called to load the current array data into the array stack. If the mesh point is within an array, FINDBX is called to determine the position within the lattice or array that contains the mesh point. LOCBOX is then called to determine the unit or box type that contains the mesh point. POSIT is used to determine the geometry region that contains the mesh point. If the mesh point is in a region that contains a hole, the coordinate of the mesh point is translated to the hole and POSIT is called again.

FINDBX - This subroutine locates the position in an array that contains a specified point.

LOCBOX - This function returns the unit or box type at a given position in an array.

POSIT - This subroutine determines the region within a unit that contains a specified point.

C4.3.4.15. Write KENO V.a Input Data on Restart File

This portion of the program, illustrated in Fig. C4.3.18, is responsible for writing all data except the calculated results on the restart data file. This section of the program is omitted if a unit number has not been assigned for the restart data file. This information is entered as parameter data, WRS=, as described in Sect. F11.5.3. The calculated results are written on the restart data file later in the program. The restart data file is used for restarting a problem.

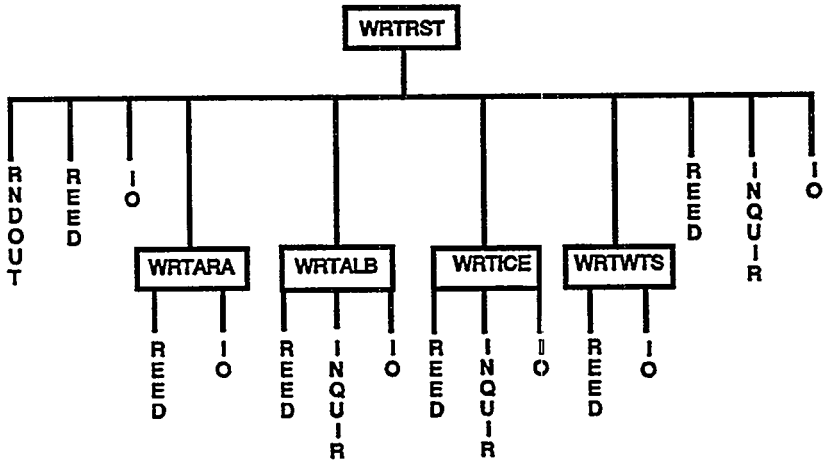


Figure C4.3.18 Flowchart for writing data on the restart data file

WRTRST - This subroutine writes the input data on the restart data file. RNDOUT is called to return the seed of the next random number. The problem title and parameter data are in the first record written on the restart data file. The array containing the IDs of the 1-D cross sections is then written. The geometry region data, mixing table data, extra 1-D data, biasing data, start data, plot data, and energy and inverse velocities are written.

The unit orientation header record is written, and WRTARA is called to write the unit orientation data. The albedo header record is written, and WRTALB is called to write the albedo data. The cross-section header record is written, and WRTICE is called to write the cross sections. The header record for user-supplied weighting data is written, and WRTWTS is called to write out the user-supplied weighting or biasing data.

WRTARA - This subroutine is called from WRTRST to write the array number, array size, and corresponding unit orientation array on the restart data file for each array that is entered in the problem. The library routine REED is called to load the direct-access pointers for the albedo data block. INQUIR is called to return the value of the next direct-access record. REED is used to read the data from the direct-access data file, and IO is used to write it on the restart data file.

WRTALB - This subroutine is called from WRTRST to write the albedo data on the restart data file. The library routine REED is used to read the albedo data from the direct-access data file, and IO is used to write the data on the restart data file.

WRTICE - This subroutine is called from WRTRST to write the cross-section data block on the restart data file. REED is called to load the direct-access pointers for the cross-section data blocks. INQUIR is called to return the value of the next direct-access record. The library routine REED is used to read the rest of the cross-section information from the direct-access data file, and IO is used to write it on the restart data file.

WRTWTS - This subroutine is called from WRTRST to write the biasing input data block on the restart data file. The library routine REED is used to read the data block from the direct-access data file, and IO is used to write it on the restart data file.

C4.3.5 THE SEARCH DATA PROCESSOR

This portion of the program, shown in Fig. C4.3.19, is responsible for processing search data to be used by module MODIFY.

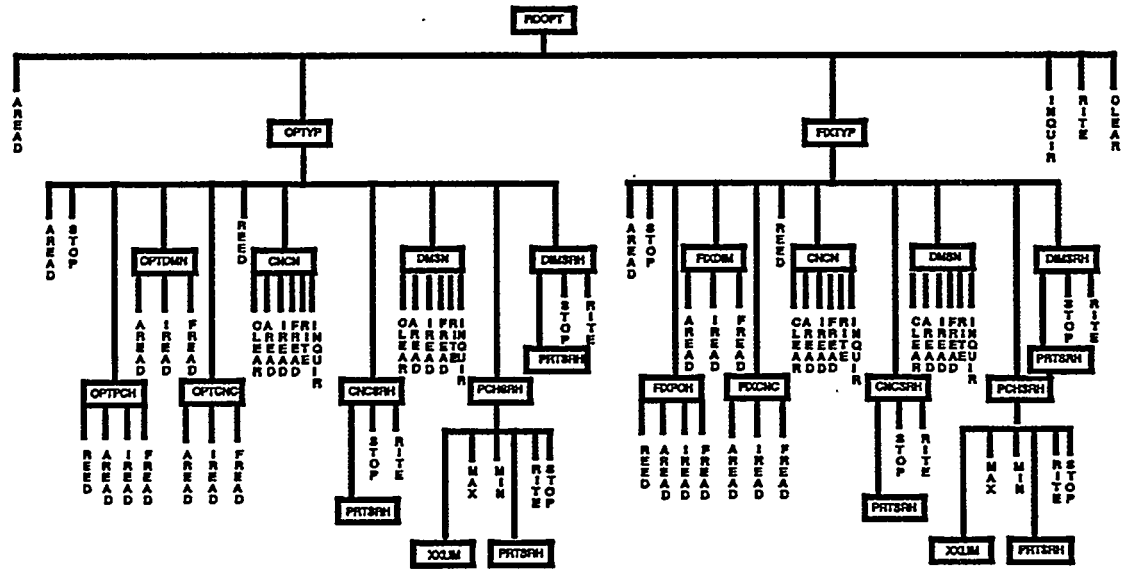


Figure C.4.3.19 Flowchart of the Search Data Processor

RDOPT - This subroutine is responsible for reading and processing the search data. AREAD is used to read the keywords READ, SEARCH, and the search type. Two calls are made to subroutine OPTYP to read and process data for an optimum value search and to read and process data for a minimum value search. Subroutine FIXTYP reads and processes data for a fixed value search. The library routine INQUIR is called twice to set the next direct-access block number. The library routine RITE is called to write common information for the control module MODIFY on the direct-access data file. The library routine CLEAR is called to clear space for data that is saved from pass to pass, such as the k-effective and search parameters. RITE is called twice more to rewrite the direct-access pointer and length arrays for the KENO V.a and CSAS data.

The KENO V.a pointers and their associated data are:

LPOINT(1) is the pointer for the current geometry region data
LPOINT(2) is the pointer for the unit orientation data
LPOINT(3) is the pointer for the mixing table information
LPOINT(4) is the pointer for the extra data
LPOINT(5) is the pointer for the weighting importance region data

LPOINT(6) is the pointer for the data defining start type 6
LPOINT(7) is the pointer for the albedo data
LPOINT(8) is the pointer for the mixed cross sections
LPOINT(9) is the pointer for the energy and inverse velocities
LPOINT(10) is the pointer for the plot or picture data
LPOINT(11) is the pointer for the biasing data
LPOINT(12) is the pointer for the albedo cross-section energy correspondence data

The CSAS pointers and their associated data are:

LPOINT(1) is the pointer for COMMON/REC1/
LPOINT(2) is the pointer for the original geometry region data
LPOINT(3) is the pointer for the original mixing table
LPOINT(4) is the pointer for the search data arrays
LPOINT(5) is the pointer for the calculated data that are saved from pass to pass

OPTYP - This subroutine is responsible for providing data for both optimum value searches and minimum value searches. AREAD is used to read the search type (pitch, dimension, or concentration). Pointers are created for the data arrays required for the search, and STOP is called to write a message if more computer storage is required. OPTPCH, OPTDMN, OPTCNC, CNCN, CNCSRH, DMSN, PCHSRH, and DIMSRH are used to read and process the search data. REED is called to load data from the direct-access device.

OPTPCH - This subroutine uses REED to reload the geometry data from the direct-access data file. The library routines AREAD, IREAD, and FREAD are used to read the optional search parameters for an optimum pitch search. The processed data are written on the scratch unit.

OPTDMN - This subroutine uses the library routines AREAD, IREAD, and FREAD to read the optional search parameters for an optimum dimension search.

OPTCNC - This subroutine uses the library routines AREAD, IREAD, and FREAD to read the optional search parameters for an optimum concentration search.

CNCN - This subroutine calls CLEAR to zero arrays that hold concentration search data. AREAD, IREAD, and FREAD are used to read the concentration search data that are then written on the scratch unit. RITE is called to load the mixing table data on the direct-access data file. INQUIR is called to set the next direct-access block number.

CNCSRH - This subroutine reads concentration search data from the scratch unit, checks data, sets the maximum and minimum constraints, calls PRTSRH to print the search data table, calls STOP to write an error message if no valid search commands are found, and uses RITE to write the search data on the direct-access data file.

PRTSRH - This subroutine prints the search data table that includes the search parameters and the search commands.

DMSN - This subroutine reads the search commands for a search that alters the geometry dimensions. CLEAR is used to zero data arrays. AREAD, IREAD, and FREAD are used to read the data. After reading the data, some of it is written on the scratch unit. The geometry data are written to a direct-access data file using RITE. INQUIR is used to set the next direct-access data block.

PCHSRH - This subroutine reads optimum pitch search data from the scratch unit and fills the search data arrays for an optimum pitch search. XXLIM, MIN, and MAX are used to determine the maximum and minimum search constraints. PRTSRH is called to print the search data table. STOP is called to write an error message if no valid search commands are found. The library routine RITE is used to write the search data arrays to a direct-access data file.

XXLIM - This function is used to determine the maximum coordinate of the geometry region interior to the specified face of the unit.

DIMSRH - This subroutine reads dimension search data from the scratch unit, sets the maximum and minimum constraints, calls PRTSRH to print the search data table, calls STOP to write an error message if no valid search commands are found, and uses RITE to write the search data arrays to a direct-access data file.

FIXTYP - This subroutine is responsible for providing data for a "critical" or "fixed k" search. AREAD is used to read the search type (pitch, dimension, or concentration). Pointers are created for the data arrays required for the search, and STOP is called to write a message if additional computer storage is required. FIXPCH, FIXDIM, FIXCNC, CNCN, CNCSRH, DMSN, PCHSRH, and DIMSRH are used to read and process the search data. REED is called to read data from the direct-access device.

FIXPCH - This subroutine uses REED to reload the geometry data from the direct-access data file. The library routines AREAD, IREAD, and FREAD are used to read the optional search parameters for a critical pitch search. The processed search data arrays are written on the scratch unit.

FIXDIM - This subroutine uses the library routines AREAD, IREAD, and FREAD to read the optional search parameters for a critical dimension search.

FIXCNC - This subroutine uses the library routines AREAD, IREAD, and FREAD to read the optional search parameters for a critical concentration search.

C4.3.6 MODIFY, THE SEARCH MODULE

This segment of the program, shown in Fig. C4.3.20, is part of a control module that is responsible for altering data for a search. CSAS4 and CSAS4X activate both MODIFY and KENO V.a to achieve a search. MODIFY provides new geometry data that are used by KENO V.a to calculate the corresponding k-effective. This procedure is repeated numerous times, and the data resulting from the calculations are analyzed until convergence is achieved, the specified number of search passes have been completed, or the problem uses up the allotted time. See Figs. C4.3.1 and C4.3.2 for the flowcharts that illustrate this procedure. LODCOM is called via ALOCAT from SEARCH, the main program of the control module, MODIFY. SEARCH is activated by the control module MODIFY. Figure C4.3.20 shows the subroutines that are part of the control module MODIFY and are responsible for actually altering the data.

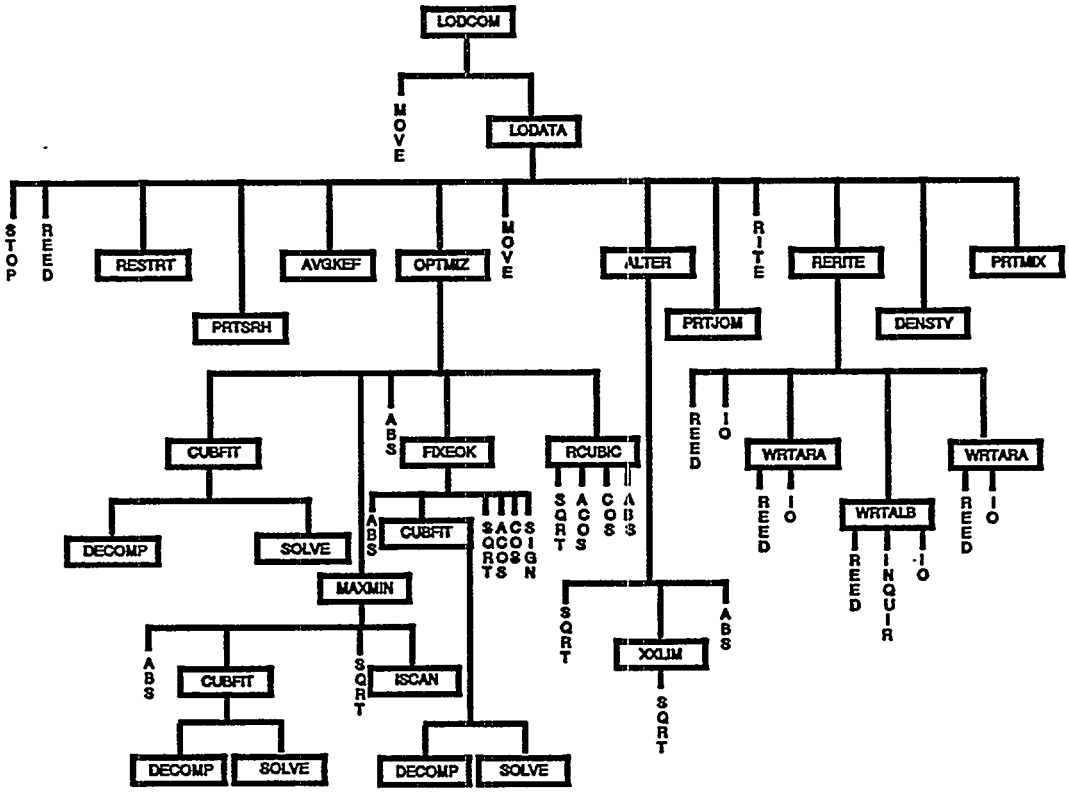


Figure C4.3.20 Flowchart of the search module, MODIFY

LODCOM - This subroutine initiates the data modification procedure of module MODIFY. It strips the individual commons out of COMMON/REC1/ using the library routine MOVE, sets up storage for the required data arrays, and calls subroutine LODATA to load the data into arrays.

LODATA - This subroutine calls the library routine STOP to write an error message if incorrect search data are entered. LODATA uses REED to load the pass-to-pass data into storage from the direct-access data file. RESTRT is called to load data from the restart data file. PRTSRH is called to print the table of search data. AVGKEF is called to load the data that are saved from pass to pass. REED is used to load the search command arrays before calling OPTMIZ to evaluate the parameter values corresponding to values of k-effective. If a pitch or dimension search is to be made, REED is called to load the geometry data and temporary pointers are created for the geometry data. MOVE is called to load the new dimensions into the old dimensions array. ALTER is called to alter the geometry data based on the parameter values returned by OPTMIZ. If convergence has been achieved, a message is written and PRTJOM is called to print the corresponding KENO V.a geometry information. After convergence is achieved, ALTER is called to calculate the best estimate of the dimensions and PRTJOM is called to print them. RITE is used to write the new geometry data on the direct-access data file. REWRITE is called to rewrite the restart data file for

KENO V.a, and RITE is used to rewrite the pass-to-pass search data on unit 90. If a concentration search is to be made, REED is called to load the permanent pointers and temporary pointers are created for the mixing table data. MOVE is used to load the new densities into the old density array. DENSTY is called to modify the concentrations, and if convergence is achieved, PRTMIX is called to print the converged mixing table data. After convergence is achieved, DENSTY is called to calculate the best estimate for the mixing table and PRTMIX is called to print it. RITE is used to rewrite the pass-to-pass data on unit 90.

RESTRT - This subroutine reads the restart data file from unit 95 and loads the k-effective by generation array for processing by subroutine AVGKEF.

AVGKEF - This subroutine loops over the number of generations. It determines the average k-effective and corresponding deviation, skipping an additional generation each time but never skipping more than half the generations. SQRT is used in determining the deviations. The minimum deviation and its corresponding k-effective are stored for use by subroutine OPTMIZ.

OPTMIZ - This subroutine includes methods for an optimization search and a fixed value search. The optimization search[1] is capable of determining a maximum or a minimum. For an optimum pitch search, it searches for the value of a parameter that corresponds to the maximum k-effective. The fixed value search finds the value of a parameter that corresponds to a fixed value of k-effective. Both searches rely on least squares curve fitting to obtain the information needed to make an estimate. The data points are least squares fitted to a cubic polynomial, which is solved analytically for parameter values. CUBFIT is called to determine the coefficients of the cubic polynomial. MAXMIN is called to provide the parameter value corresponding to the optimum k-effective, using a cubic fit. If a fixed k calculation is to be made, FIXEDK is called to solve the cubic equation. RCUBIC provides the analytic solution of the cubic equation. The FORTRAN-supplied function ABS provides the absolute value of a variable, and DSQRT returns the square root of a double-precision variable.

CUBFIT - This subroutine fits the input data to a cubic equation by determining the coefficients of the cubic polynomial. DECOMP decomposes the matrix, and SOLVE provides the solution for a linear system.

DECOMP - This subroutine decomposes a real matrix by Gaussian elimination and estimates the condition of the matrix.

SOLVE - This subroutine uses the triangularized matrix and pivot vector provided from DECOMP to determine the solution of the linear system.

MAXMIN - This subroutine uses a least-squares fit to a cubic polynomial to determine the parameter value corresponding to the maximum value of k-effective. It is also capable of determining the parameter value corresponding to the minimum k-effective. One portion of the subroutine is devoted to determining the optimum for a cubic having a maximum and a minimum; another portion of the subroutine determines the optimum for a cubic with only a point of inflection. CUBFIT is utilized in both portions to fit the input data to a cubic equation. SQRT is used in the first portion to evaluate the discriminate. The library routine ABS is used to provide the absolute value of a variable. ISCAN is called to ensure that calculations are not duplicated.

ISCAN - This function scans a vector for a specific value and returns the index if the value is found.

FIXEDK - This subroutine performs a fixed value search. It utilizes an extended mean value theorem method to determine the value of the parameter corresponding to the desired value of k-effective. CUBFIT supplies a least squares fit to a cubic polynomial. The library routines ABS, SQRT, ACOS, COS, and SIGN are used in providing the analytical solution of the cubic.

RCUBIC - This subroutine is responsible for determining the analytical solution to a cubic. It utilizes the library routines SQRT, ACOS, COS, and ABS.

ALTER - This subroutine translates changes in the search parameters into changes in the geometric dimensions. CLEAR is used to zero the region correspondence array. The search command array is used to determine which geometry regions will be altered. For pitch or dimension search, the geometry region data are altered. For a pitch search, the function XXLIM is used to provide the maximum coordinate of the interior region corresponding to the specified face of the unit. This capability ensures that the pitch does not decrease beyond the point of tangency. The new dimensions are calculated from the original dimensions and the parameters provided by OPTMIZ.

XXLIM - This function provides the maximum coordinate of the interior region corresponding to the specified face of the unit. SQRT is used to return the square root of a variable.

PRTJOM - When convergence has been achieved, this subroutine is called to print the geometry data. The corresponding parameter, pass number, and k-effective are printed by LODATA.

RERITE - This subroutine is called to rewrite the restart data file used by KENO V.a. It contains the new geometry data for which a k-effective will be calculated. REED is used to read the data from the direct-access data file, and IO is used to write it on the restart data file. WRTARA, WRTALB, and WRTWTS are used to write the KENO V.a array, albedo, and weighting data on the restart data file.

WRTARA - This subroutine is called from WRTRST to write the array number, array size, and corresponding unit orientation array on the restart data file for each array that is entered in the problem. The library routine REED is used to read the data from the direct-access data file, and IO is used to write it on the restart data file.

WRTALB - This subroutine is called from WRTRST to write the albedo data on the restart data file. The library routine REED is used to read the albedo data from the direct-access data file, INQUIR is called to return the value of the next direct-access record, and IO is used to write the albedo data on the restart data file.

WRTWTS - This subroutine is called from WRTRST to write the biasing input data block on the restart data file. The library routine REED is used to read the data block from the direct-access data file, and IO is used to write it on the restart data file.

DENSTY - This subroutine modifies the number densities of the mixture components according to search commands for a concentration search.

PRTMIX - This subroutine prints the new mixing table resulting from the concentration search.

C4.3.7 REFERENCE

1. M. J. Lorek, *Improved Criticality Search Techniques for Low- and High-Enriched Systems*, ORNL/NUREG/CSD/TM-13, Union Carbide Corp., Nucl. Div., Oak Ridge Natl. Lab., 1981.

C4.4 INPUT DATA GUIDE

This section describes the input data required for Criticality Safety Analysis Sequence No. 4 (CSAS4X). Several subsets of the CSAS4X sequence are available to achieve several different levels of processing. These are listed in Table C4.4.1 with the functional modules they invoke. Note that modules with an "X" in their names create cell-weighted libraries by using XSDRNPM-S.

Table C4.4.1 Functional modules executed by CSAS control modules

Control module	Search function	Functional modules executed by the control module				
CSASI	No search	BONAMI	NITAWL-II		ICE	
CSASIX	No search	BONAMI	NITAWL-II	XSDRNPM	ICE	
CSASN	No search	BONAMI	NITAWL-II			
CSAS1X	No search	BONAMI	NITAWL-II	XSDRNPM		
CSAS25	No search	BONAMI	NITAWL-II		KENO V.a	
CSAS2X	No search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	
CSAS4	Search	BONAMI	NITAWL-II		KENO V.a	MODIFY[a]
CSAS4X	Search	BONAMI	NITAWL-II	XSDRNPM	KENO V.a	MODIFY

[a]MODIFY is a control module.

Each sequence generates various libraries that may be saved for future use. Table C4.4.2 lists the various I/O units that may be saved and their definitions. Table C4.4.3 lists those I/O units containing cross-section libraries that are generated by each sequence. See Table C4.5.1 in Sect. C4.5 for a complete list of I/O units utilized by Criticality Safety Analysis Sequence No. 4 and Table C4.5.2 for the I/O units utilized by the associated functional modules.

The input data for these CSAS modules are composed of three broad categories of data. The first (Material Information Processor, including Standard Composition Specification Data and Unit Cell Geometry Specification) specifies the cross-section library and defines the composition of each mixture and the unit cell geometry that is used to process the cross sections. This data block is necessary for CSASN, CSAS1X, CSASI, and CSASIX. The second category of data, the KENO V.a input data, are used to specify the geometric and boundary conditions that represent the physical 3-D configuration of the problem. Both data blocks are necessary for CSAS25 and CSAS2X. The last category of data is the search data. All three data blocks are required for CSAS4 and CSAS4X.

All data are entered in free form, allowing alphanumeric data, floating-point data, and integer data to be entered in an unstructured manner. Eighty columns of data entry are allowed, simulating a card of data. Data can usually start or end in any column. Each data entry must be followed by one or more blanks to terminate the data entry. For numeric data, either a comma or a blank can be used to terminate each data entry. Integers may be entered for floating values. For example, 10 will be interpreted as 10.0. Imbedded blanks are not allowed within a data entry unless an E precedes a single blank as in an unsigned exponent in a floating-point number. For example, 1.0E 4 would be correctly interpreted as 1.0×10^4.

The word "END" is a special data item. An "END" may have a name or label associated with it. The name or label associated with an "END" is separated from the "END" by a single blank and is a maximum of 12 characters long. *At least 2 blanks MUST follow every labeled and unlabeled "END." It is the user's responsibility to ensure compliance with this restriction. Failure to observe this restriction can result in the use of incorrect or incomplete data without the benefit of warning or error messages.*

Table C4.4.2 I/O units on which cross-section libraries are written

Unit	Type of data	Creating module
2	Resonance-corrected mixed working library	ICE
3	Resonance-corrected, cell-weighted working library	XSDRNPM
4	Resonance-corrected working library	NITAWL-II
14	Resonance-corrected, mixed cross-section, MORSE/KENO library. If the invoked sequence contains an X in its name, this library contains a cell-weighted mixture identified as mixture 500	ICE, KENO V.a

Table C4.4.3 I/O units generated by CSAS and associated modules

		Unit numbers of generated cross-section libraries			
Module name	Primary product	2	3	4	14
CSASN	Resonance-corrected working			X	
CSAS1X	library		X	X	
CSASI	XSDRNPM eigenvalue calculation	X		X	X
CSASIX	Resonance-corrected, mixed cross-section MORSE/KENO library	X	X	X	X
CSAS25	Resonance-corrected, cell-weighted, mixed cross-section, MORSE/KENO library			X	X
CSAS2X	KENO V.a k-effective		X	X	X
CSAS4	KENO V.a k-effective using homogenized cell			X	X
CSAS4X	Dimension alterations		X	X	X
	Dimension alterations using homogenized cell				

Multiple entries of the same data value can be achieved by specifying the number of times the data value is to be entered, followed by either R, *, or $, followed by the data value to be repeated. Imbedded blanks are not allowed between the number of repeats and the repeat flag. For example, 5R12, 5*12, 5$12, or 5R 12, etc., will enter five successive 12s in the input data. Multiple zeros can be specified as nZ where n is the number of zeroes to be entered. The SCALE free-form reading routines are described in more detail in Sect. M3.

The purpose of this section is to define the input data in discrete subsections relating to a particular type of data. Tables of the input data are included in each subsection, and the entries are described in more detail after the tables illustrated in Fig. C4.4.1. Section C4.4.1 is provided for experienced users and contains all the tables that are used to describe the input data. Section C4.4.2 describes input data requirements and the data-checking capability. Sections C4.4.3 through C4.4.8 describe the Material Information Processor data, Sect. C4.4.9 summarizes the KENO V.a data that are explained in detail in Sect. F11.4, and Sect. C4.4.10 describes the search data.

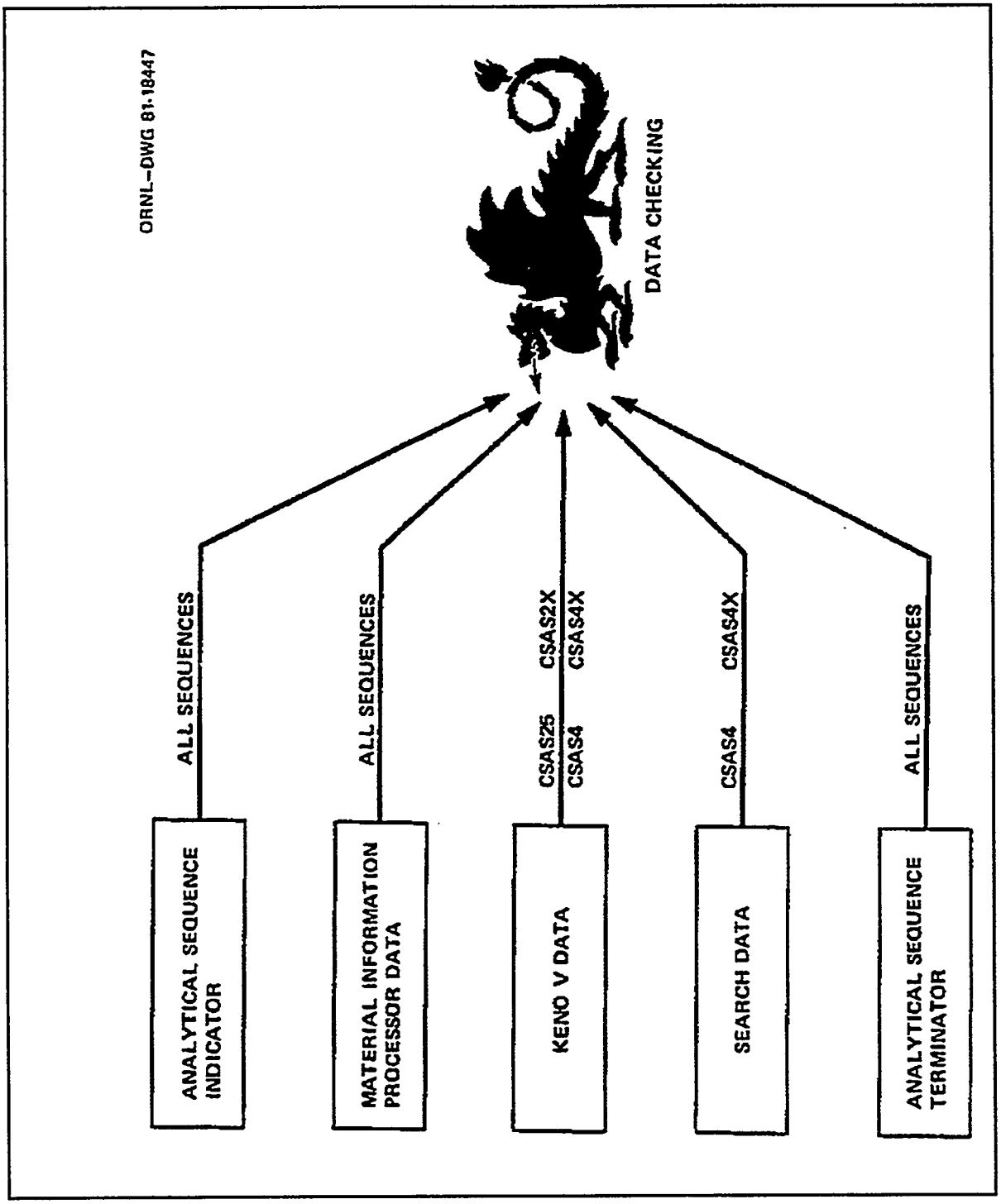


Figure C4.4.1 Outline of CSAS input data

Resonance-corrected cross sections utilize Dancoff corrections based on the unit cell specification. Because only one unit cell can be specified in the data, resonance corrections can only be applied to one mixture via conventional methods. However, if multiple resonance-corrected mixtures are required, the necessary data can be entered via the OPTIONAL PARAMETER DATA described in Sect. C4.4.8 and Tables C4.4.4 and C4.4.13.

To check the input data without actually processing the cross sections, the words "PARM=CHECK" or "PARM=CHK" should be entered, starting in column 11 of the analytical sequence specification for IBM versions as shown below.

```
=CSAS4    PARM=CHK
            or
#CSAS4    PARM=CHK
```

This would cause the input data for CSAS to be checked and appropriate error messages to be printed. If plots are specified in the data, they will be printed. This feature allows the user to debug and verify the input data while using a minimum of computer time. Many problems can be checked in 10 s or less. The number of words of storage requested by CSAS and its associated sequences is defaulted to 100,000 words of storage. This can be respecified through the use of the PARM command on the analytical sequence specification. For example, if 150,000 words of storage are required for the problem, "PARM=SIZE=150,000" should be entered, starting in column 11 of the analytical sequence specification as shown below.

```
=CSAS4    PARM=SIZE=150000
```

To combine checking and size specification, specify "PARM=(CHECK,SIZE=nnn)" or "PARM=(CHK,SIZE=nnn)" starting in column 11 or beyond on the analytical sequence specification. The value of nnn is given in words of storage. The minimum value of nnn is the amount of storage required by the problem, and the maximum value of nnn is the available computer storage.

C4.4.1 INPUT DATA SUMMARY FOR EXPERIENCED USERS

Section C4.4.1 is provided for the convenience of experienced users. Other users should skip to Sect. C4.4.2, page C4.4.26. All of the input data for Criticality Safety Analysis Sequence No. 4 are illustrated in Fig. C4.4.1, and are summarized in Table C4.4.4. This table is provided as an input data guide for users who are familiar with CSAS data requirements. Each component table of Table C4.4.4 is repeated and discussed in detail in Sects. C4.4.4 through C4.4.12. The KENO V.a data are included in this table in very general terms. Table C4.4.5 contains a summary of the KENO V.a input data. They are described in detail in Sect. F11.4 with additional information contained in Sect. F11.5. Table C4.4.6 contains a summary of the SEARCH data for CSAS4 and CSAS4X.

The Material Information Processor now allows terse data input for all data except the standard composition names and the keyword entries in the optional parameter data (MORE DATA). Terse data entry requires the user to enter only as many characters as is necessary to uniquely define the data entry. However, as many characters as are specified by the user must match the name allowed by the code.

For example, refer to Table C4.4.4, **Outline of Material Information Processor data**, data position 3. The available choices for the type of calculation are: INFHOMMEDIUM, LATTICECELL, and MULTIREGION. Therefore, I would be sufficient to specify an infinite homogeneous medium, L would be sufficient for lattice cell, and M would specify multiregion. If it is desirable to use more characters, the user is free to do so. However, as many characters as are entered must match the name allowed by the code. For example, if INFHOMMEDIUM is to be specified, INFH is correct, but INFI is not.

WARNING: If several choices begin with the same letters, sufficient characters should be entered to uniquely define the name. For example, ASPHSQUAREP and ASPHTRIANGP are identical through the first four characters. If only ASPH is entered, the code will accept the first name whose first four characters are ASPH. This may not be the one the user intended to use.

Table C4.4.4 Input data requirements

Summary of data input requirements (see Sect. C4.4.2 for details)

	Type of data	Analytical sequence							
1	Analytical sequence specification	=CSASN	=CSAS1X	=CSASI	=CSASIX	=CSAS25	=CSAS2X	=CSAS4	=CSAS4X
2	Material Information Processor data	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
3	KENO V.a data	No	No	No	No	Yes	Yes	Yes	Yes
4	Search data	No	No	No	No	No	No	Yes	Yes
5	END for the analytical sequence	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

Outline of Material Information Processor data (see Sect. C4.4.3 for details)

Data position	Type of data	Data entry	Comments
1	TITLE	Enter a title	80 characters
2	Cross-section library name	HANSEN-ROACH 27GROUPNDF4 123GROUPGMTH 218GROUPNDF4 27BURNUPLIB etc.	The currently available libraries are listed in Table M8.8.2.
3	Type of calculation	INFHOMMEDIUM LATTICECELL MULTIREGION	These are the available options. See the explanation in Sect. C4.4.3.
4	Standard Composition specification data	Enter the appropriate data	Terminate this data block with END COMP. See Sect. C4.4.4.
5	Unit cell geometry specification	Enter the appropriate data (optional for INFHOMMEDIUM)	Optional for INFHOMMEDIUM. See Sect. C4.4.5 for INFHOMMEDIUM. See Sect. C4.4.6 for LATTICECELL. See Section C4.4.7 for MULTIREGION.
6	Optional parameter data	Enter the desired data	Precede this data block by MORE DATA if more parameter data are to be entered. Otherwise, omit these data entirely. See Sect. C4.4.8.

Table C4.4.4 (continued)

Outline of standard compositions specification data (see Sect. C4.4.4 for details)

Entry number	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Table M8.2.1. Additional allowed names include those beginning with ARBM for arbitrary materials and SOLN for solutions
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each standard composition component that is an arbitrary material
A2	NEL	Number of elements in the material	ARBM	Enter once for each standard composition component that is an arbitrary material
A3	IVIS	Multiple isotope indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 for a material that does not contain multiple isotope elements. Enter 1 if the material contains a multiple isotope element. An arbitrary material cannot have more than one multiple isotope element. If necessary, several arbitrary materials may be used in a single mixture
A4	ICP	Compound indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 1 for a compound, 0 for alloys, mixtures, etc.
A5	IRS	Resonance indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 if all the nuclides in the material are non-resonance nuclides; enter 1 if one or more have resonance data. See Sect. M8.2, Table M8.2.1
A6	NCZA	ID number (from far right column of Table M8.2.1)	ARBM	Repeat the sequences A6 and A7 for each element in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1. (Premixed standard compositions cannot be used in an arbitrary material definition)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material	ARBM & ICP=1	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP=1
		or	or	or
		Weight percent of this element in this arbitrary material	ARBM & ICP=0	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP=0

Table C4.4.4 (continued)

Outline of standard compositions specification data (continued)

Entry number	Variable name	Type of data	Entry requirement	Comments
2	MX	Mixture ID number	Always	Enter once for each standard composition component
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML=0 if there is no acid in the solution
O1	SPGR or ROTH	Specific gravity of the solution or Density of the basic standard composition	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR or if the density of a basic standard composition (ROTH) is to be entered, use DEN=ROTH
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF=0 is not allowed for SOLN or ARBM
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF=0	Enter only if VF=0.0
5	TEMP	Temperature, in K	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted
6a	IZA	Isotope's ZA number	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
6b	WTP	Weight percent of the isotope	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0.0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
7[a]	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP

[a]NOTE: Entry 7 should not begin in column 1 unless a name is associated with it.
At least two blanks should separate the last entry 7 from the END COMP.

Table C4.4.4 (continued)

Optional unit cell specifications for INFHOMMEDIUM problems (see Sect. C4.4.5 for details)

Entry number	Variable name	Type of data	Data entry	Comments
1	NAME	Keyword	CELLMIX	Initiate reading cell data for INFHOMMEDIUM
2	MFUEL	Mixture number in the cell	Mixture number	Specifies the mixture number to be used in the cell. Defaults to the smallest mixture number entered in the standard composition data

NOTE: Unit cell data are necessary for INFHOMMEDIUM only if a mixture number other than the smallest mixture number is to be used in the cell and if a control sequence that executes XSDRNPM has been specified. If mixtures 1, 2, and 3 are specified and if mixture 3 is to be used in the cell, enter CELLMIX 3.

Table C4.4.4 (continued)

Unit cell specification for LATTICECELL problems (see Sect. C4.4.6 for details)

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration
				SQUAREPITCH	Use for cylindrical rods in a square pitch
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch
				ASQP	Use for annular cylindrical rods in a square pitch
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch
				ATRP	Use for annular cylindrical rods in a triangular pitch
				SPHSQUAREP	Use for spherical pellets in a cubic lattice
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice
				ASSP	Use for annular spherical pellets in a cubic lattice
				SPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASTP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				SYMMSLABCELL	Use for a symmetric array of slabs
				ASYMSLABCELL	Use for a periodic but asymmetric array of slabs
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps. For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm)
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	Annular cell	Mixture number	Mixture number representing the second moderator
7	TKMOD2	2nd moderator thickness	ASYMSLABCELL	Thickness	Thickness of the second moderator (cm) for ASYMSLABCELL
		or	or	or	or
		2nd moderator diameter (cm)	annular cell	diameter	diameter of inner moderator (cm) for other annular cells
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thickness of the fuel, gap, and clad
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad. A mixture number of zero is often used
12	END	Terminate LATTICECELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry number 12

Table C4.4.4 (continued)

Unit cell specification for **MULTIREGION problems** (see Sect. C4.4.7 for details)

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are:
				SLAB	Use for slab geometry
				CYLINDRICAL	Use for cylindrical geometry
				SPHERICAL	Use for spherical geometry
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction
2	BR	Right boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL optional for other geometries		Default is VACUUM. Describes the right/outside boundary condition
				VACUUM	This provides a non-return condition at the boundary
				REFLECTED	Do not use for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	This provides isotopic return at the boundary
3	BL	Left boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL optional for other geometries		Default is REFLECTED. Describes the left boundary condition
				VACUUM	This provides a non-return condition at the boundary
				REFLECTED	Recommended for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	This provides isotropic return at the boundary
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB and BUCKLEDCYL optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry. A value must be entered if subsequent data are to be entered
5	DY	Buckling height (cm)	BUCKLEDSLAB and BUCKLEDCYL	Appropriate dimension	Omit for SLAB, CYLINDRICAL, and SPHERICAL. This corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	Omit unless BUCKLEDSLAB was specified. This is the buckling depth corresponding to the second transverse dimension of a 3-D slab assembly
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1. At least two blanks must separate entry 7 from the first entry 8
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined. Enter the mixture number for this zone
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8-10 until all zones are defined. Enter the outside dimension of the zone (cm)
10	XMOD	External moderator index	Optional		Repeat entry numbers 8-10 until all zones are defined. Entry 10 is optional and can be omitted. If it is omitted, repeat entry numbers 8 and 9 until all zones are defined
				NOEXTERMOD	No moderating materials in the adjacent zones
				ONEEXTERMOD	A moderating material is present in one adjacent zone
				TWOEXTERMOD	Moderating materials are present in two adjacent zones
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entry numbers 8 through 10 for each zone. At least two blanks must follow this entry

Table C4.4.4 (continued)

Summary of available optional parameter data (see Sect. C4.4.8)

Entry number	Keyword name	Type of data	Applicable module	Comments
1	MORE DATA	Input flag		This signals that optional parameter data will be entered. Enter only those parameters you wish to change
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. This allows using another value
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0. 0<SZF<1.0 gives a finer mesh. SZF>1.0 gives a coarser mesh
4	IIM=	Max. number of inner iterations	XSDRNPM	The default value is 20. This allows using another value
5	ICM=	Max. number of outer iterations	XSDRNPM	The default value is 25. This allows using another value
6	EPS=	Overall convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value
8	BKL=	Buckling factor	XSDRNPM	The default value is 1.420892. Use ONLY for a multiregion problem that specifies BUCKLEDSLAB or BUCKLEDCYL
9	IUS=	Upscatter scaling factor	XSDRNPM	The default value is zero. IUS=0 doesn't utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence
10	RES=	Resonance data	BONAMI NITAWL	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE), and the thickness of the slab or radius of the sphere or cylinder in cm
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL	Enter the mixture number, mm, to which the Dancoff factor applies inside the parentheses; enter the Dancoff factor after the equal sign **Repeat entry numbers 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description**

Table C4.4.4 (continued)

Summary of available optional parameter data (continued)

Entry number	Keyword name	Type of data	Applicable module	Comments
12	BAL=	Key to print balance tables	XSDRNPM	The default value is FINE. BAL=NONE suppresses printing the balance table. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables
13	DY=	First transverse dimension	XSDRNPM	The first transverse dimension, in cm, used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder)
14	DZ=	Second transverse dimension	XSDRNPM	The second transverse dimension, in cm, used for a buckling correction (i.e., the width of a slab)
15	COF=	Diffusion coefficient option for transverse leakage correction	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRNPM will be read
17	FWR=	Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRNPM will be written
18	DAB=	Number of direct access data blocks	MIP[a]	The default is 200. Number of blocks allocated for direct access unit 90
19	AXS=	Unit on which a mixed ANISN library will be written	ICE[a]	Enter the unit number where ICE is to write a mixed ANISN library
20	COLL	Key to activate collapse of thermal groups	MIP[a]	Enter COLL to collapse all thermal groups into one group for the shielding sequences
21	END	Terminus		Terminate the optional parameter data. Do not start in column 1. At least two blanks must follow entry number 21

[a]MIP is the Material Information Processor.

Table C4.4.4 (continued)

Outline of KENO data (see Table C4.4.5 and Sects. C4.4.9 and F11.4 for details)

Type of data	Starting flag	Comments	Termination flag
Title	None	80 columns, must be entered first	None
Parameters	READ PARM	Enter desired parameter data	END PARM
Biasing or weighting	READ BIAS	Enter desired biasing data	END BIAS
Geometry	READ GEOM	Enter desired geometry data	END GEOM
Array data or unit orientation	READ ARRAY	Enter desired array data	END ARRAY
Boundary conditions or albedoes	READ BNDS	Enter desired albedo data	END BNDS
Start data or initial source	READ START	Enter desired start data	END START
Mixing table data	READ MIXT	The Material Information Processor allows only NSCT= and PBXS=	END MIXT
Plot data	READ PLOT	Enter desired plot data	END PLOT
KENO V.a data terminus	END DATA	Enter to signal the end of all KENO V.a data	

Outline of SEARCH[a] data (see Table C4.4.6 and Sect. C4.4.10 for details)

READ SEARCH	Enter desired search data	END SEARCH

[a]Search data are required for CSAS4 and CSAS4X.

Table C4.4.5 Summary of KENO V.a input data (continued)

Summary of parameter data

TITLE: The title must be entered first (80 columns) See Sect. F11.4.3

PARAMETERS: Format: READ PARAM enter parameter data here END PARAM
If parameters are entered, they must follow the title. See Sects. F11.4.3, F11.5.2, and F11.5.3.

KEY	STD.	DEFINITION	KEY	STD.	DEFINITION	KEY	STD.	DEFINITION	KEY	STD.	DEFINITION
RND=	Given	Random number	RUN=	YES	Execute problem	MKH=	NO	Matrix by hole	XSC=	14	Mixed xsecs
TME=	30 min	Execution time (min)	FLX=	NO	Fluxes	CKH=	NO	Cofactor k by hole	ALB=	79	Albedo
TBA=	0.5 min	Batch time (min)	FDN=	NO	Fission densities	FMH=	NO	Fiss. prod. by hole	WTS=	80	Weights
WTA=	0.5	Average weight	ADJ=	NO	Adjoint calculation	HHL=	NO	MKH at highest level	LTB=	4	Working xsecs
WTH=	3.0	Wt. for splitting	AMX=	NO	All mixture xsecs	MKA=	NO	Matrix by array			from NITAWL
WTL=	1/WTH	Russian Roulette wt.	XAP=	NO	Xsec angles & probs.	CKA=	NO	Cofactor k by array			or XSDRN
GEN=	103	No. of generations	XS1=	NO	1-D xsecs	FMA=	NO	Fiss. prod. by array	SKT=	16	Scratch
NPG=	300	No. per generation	XS2=	NO	2-D xsecs	HAL=	NO	MKA at highest level	RST=	95	Read restart
NSK=	3	Generations skipped	PKI=	NO	Fission spectrum	PLT=	YES	Printer plots	WRS=	95	Write restart
RES=	0	Gens. between restart	P1D=	NO	Extra 1-D xsecs	BUG=	NO	Debug print	XSC=	14	Mixed xsecs
NBK=	NPG+25	Neutron bank positions	FAR=	NO	Fiss. & abs.	TRK=	NO	Print neutron tracks			
XNB=	0	Extra bank entries	MKP=	NO	Matrix by location	PWT=	NO	Print avg. weight			
NFB=	NPG	Fission bank positions	CKP=	NO	Cofactor k by loc.	PGM=	NO	Unprocessed geometry			
XFB=	0	Extra bank entries	FMP=	NO	Fiss. prod. by loc.	SMU=	NO	Self-multiplication			
X1D=	0	No. of extra 1-Ds	MKU=	NO	Matrix by unit	NUB=	NO	Neutrons per fission			
LNG=	1000000	Words of storage*	CKU=	NO	Cofactor k by unit	PAX=	NO	Albedo-xsec array			
BEG=	1	Restart at this gen.	FMU=	NO	Fiss. prod. by unit						
NG8=	200	Blocks for d.a. unit									
NL8=	512	Length of d.a. block									

*The words of storage in CSAS are defaulted to 100,000 and can be overridden by using the size= parameter on the analytical sequence specification which then becomes the default value of LNG in KENO V.a.
For example: =CSAS25 PARM=SIZE=200000
or =CSAS25 PARM=(CHECK,SIZE=200000)

Table C4.4.5 (continued)

Summary of array data

ARRAY Format: READ ARRAY array parameters data type orientation data END ARRAY See Sects. F11.4.5, F11.5.6, and F11.5.7.

Repeat the sequence ARRAY PARAMETERS DATA TYPE ORIENTATION DATA for each array used in the problem.

ARRAY PARAMETERS			DATA TYPE
KEYWORD	DEFAULT	DEFINITION	FILL LOOP
ARA=	1	No. defining the array	
NUX=	1	No. of units in X direction	
NUY=	1	No. of units in Y direction	
NUZ=	1	No. of units in Z direction	
GBL=	Maxara	Global, universe, or overall array number[a]	
COM=	none	Delim comment delim optional comment is a maximum of 132 characters	

[a]Can be defaulted by the code. If specified, it need be entered only once per problem.

ORIENTATION DATA FOR FILL

Enter unit numbers to define every position in the array. When entering data utilizing the options in this table, the count field and option field must be adjacent with no imbedded blanks. The operand field may be separated from the option field by one or more blanks. Orientation data for FILL is terminated by entering END FILL.

COUNT FIELD	OPTION FIELD	OPERAND FIELD	COMMENTS
		j	Stores j at the current position in the array
i	R	j	Stores j in the next i positions in the array
i	*	j	Stores j in the next i positions in the array
i	$	j	Stores j in the next i positions in the array
	F	j	Fills remainder of the array with unit no. j starting with the current array position
	A	j	Sets the current position in the array to j
i	S		increments; current position in the array by i allows skipping i positions. The value of i may be positive or negative
i	Q	j	Repeats the previous j entries i times. The default value of i is 1
i	N	j	Repeats the previous j entries i times, inverting the sequence each time. The default value of i is 1
i	B	j	Starting with the entry at -i from the current position, store entries in inverse order until position -(i+j) is reached. Default value of i=1
i	P	j	Alternately stores j and -j in the next i positions of the array
i	I	j k	Provides the end points, j and k, with i entries linearly interpolated between them (i.e., a total of i+2 points). At least one blank must separate j and k. When used for an integer array, the I option should only be used to generate integer steps [i.e., (k-j)/(i+1) should be a whole number].
	T		Terminates the data reading for the array

ORIENTATION DATA FOR LOOP

Enter the unit number and nine numbers that define the position(s) of that unit. Data for each of these ten entries are repeated until every position in the array has been defined. Orientation data for LOOP is terminated by entering END LOOP.

ENTER DATA IN THE FORM:

DATA ENTRY	COMMENTS
LTYPE	The unit or box type. LTYPE must be greater than 1
IX1	Starting position in the X direction. IX1 must be at least 1 and no larger than the value entered for NUX
IX2	Ending position in the X direction. IX2 must be at least 1 and no larger than the value of NUX
INCX	The number of units by which increments are made in the X direction
IY1	The starting position in the Y direction. IY1 must be at least 1 and less than the value entered for NUY
IY2	Ending position int he Y direction. IY2 must be at least 1 and no larger than the value of NUY
INCY	The number of units by which increments are made in the positive Y direction
IZ1	Starting position in the Z direction. IZ1 must be at least 1 and no larger than NUZ
IZ2	Ending position in the Z direction. IZ2 must be at least 1 and no larger than NUZ
INCZ	The number of units by which increments are made in the positive Z direction

Table C4.4.5 (continued)

Summary of biasing data

BIAS (weighting)

Format: READ BIAS keyword correlation data auxiliary END BIAS
See Sects. F11.4.7 and F11.5.8

KEYWORD	DESCRIPTION	
ID=	CORRELATION DATA will be read next.	
	id	Material ID. Enter from table at right to use weighting data from the library
	ibgn	Beginning bias ID
	iend	Ending bias ID
WT=	AUXILIARY DATA will be read next.	
WTS=	AUXILIARY DATA will be read next.	
	wttitl	Material title (12-character maximum)
	id	Material ID
	nsets	Number of sets of group structures
	REPEAT	(thkinc, numinc, ngpwt, wtavg) nsets times
	thkinc	Thickness per increment
	numinc	Number of increments
	ngpwt	Number of energy groups for this set of wts
	wtavg	Enter numinc x ngpwt values of wtavg

MATERIAL	ID	ENERGY GROUPS	THICKNESS/ INCREMENT
Concrete	301	16,27,123	5 cm
Paraffin	400	16,27,123	3 cm
Water	500	16,27,123,218	3 cm
Graphite	6100	16,27,123	20 cm

For CORRELATION DATA, the material ID is chosen from material ID column above (the keyword is ID=).
For AUXILIARY DATA, the material ID is chosen by the user and the keyword is WT= or WTS=.
When AUXILIARY DATA are entered, CORRELATION DATA must also be entered to use the data.
Beginning and ending bias IDs are defined by the user. The geometry specificaiton that has the bias ID equal to the beginning bias ID utilizes the wtavg's from the first interval of material ID.

Table C4.4.5 (continued)

Summary of boundary condition data

BNDS (albedo or boundary conditions)

Format: READ BNDS face code albedo name END BNDS
See Sect. F11.4.7

The sequence FACE CODE ALBEDO NAME is entered as many times as necessary to define the appropriate albedo boundary conditions. The default for all faces is vacuum.

FACE CODES FOR ENTERING BOUNDARY (ALBEDO) CONDITIONS

FACE CODE	DEFINITION	FACE CODE	DEFINITION	FACE CODE	DEFINITION	FACE CODE	DEFINITION
+XB=	Positive X face	XFC=	Both X faces	+YX=	Positive X and Y faces	&ZY=	Positive Y and Z faces
&XB=	Positive X face	YFC=	Both Y faces	&XY=	Positive X and Y faces	-XY=	Negative X and Y faces
-XB=	Negative X face	ZFC=	Both Z faces	&YX=	Positive X and Y faces	=XZ=	Negative X and Z faces
+YB=	Positive Y face	+FC=	All positive faces	+XZ=	Positive X and Z faces	=YZ=	Negative Y and Z faces
&YB=	Positive Y face	&FC=	All positive faces	+ZX=	Positive X and Z faces	YXF=	All X and Y faces
-YB=	Negative Y face	-FC=	All negative faces	&XZ=	Positive X and Z faces	ZXF=	All X and Z faces
+ZB=	Positive Z face	XYF=	All X and Y faces	&ZX=	Positive X and Z faces	ZYF=	All Y and Z faces
&ZB=	Positive Z face	XZF=	All X and Z faces	+YZ=	Positive Y and Z faces	-YX=	Negative X and Y faces
-ZB=	Negative Z face	YZF=	All Y and Z faces	+ZY=	Positive Y and Z faces	-ZX=	Negative X and Z faces
ALL=	All 6 faces	+XY=	Positive X and Y faces	&YZ=	Positive Y and Z faces	-ZY=	Negative Y and Z faces

ALBEDO NAMES AVAILABLE ON THE KENO V ALBEDO LIBRARY, FOR USE WITH THE FACE CODES

ALBEDO NAME	DESCRIPTION	ALBEDO NAME	DESCRIPTION	ALBEDO NAME	DESCRIPTION
DPOH20 DPOH20 DPO DPO	12-in. double PO water differential albedo with 4 incident angles	CONC-4 CON4 CONC4	4-in. concrete differential albedo with 4 incident angles	VACUUM VOID VACU VAC	Vacuum condition
H20 WATER	12-in. water differential albedo with 4 incident angles	CONC-8 CON8 CONC8	8-in. concrete differential albedo with 4 incident angles	SPECULAR MIRROR MIRR	Mirror image reflection
PARAFFIN PARA WAX	12-in. paraffin differential albedo with 4 incident angles	CONC-12 CON12 CONC12	12-in. concrete differential albedo with 4 incident angles	SPEC SPE MIR	
CARBON GRAPHITE C	200-cm carbon differential albedo with 4 incident angles	CONC-16 CON16 CONC16	16-in. concrete differential albedo with 4 incident angles	PERIODIC PERI PER	Periodic boundary condition
ETHYLENE POLY CH2	12-in. polyethylene differential albedo with 4 incident angles	CONC-24 CON24 CONC24	24-in. concrete differential albedo with 4 incident angles		

Table C4.4.5 (continued)

Summary of geometry data

GEOMETRY (region)

Format: READ GEOM enter geometry region data here END GEOM
See Sects. F11.4.4, F11.5.1.2, F11.5.6, and F11.5.7.

GEOMETRY REGION DATA consists of SIMPLE GEOMETRY REGION DATA and EXTENDED GEOMETRY REGION DATA.

ENTER GEOMETRY REGION DATA IN THE FOLLOWING FORM:

OPTIONAL GLOBAL SPECIFICATION
UNIT n
OPTIONAL GEOMETRY COMMENT
SIMPLE GEOMETRY REGION DATA
and/or
EXTENDED GEOMETRY REGION DATA

* * * \

Table C4.4.5 (continued)

Summary of geometry data (cont.)

GEOMETRY (region) (cont.)

ENTER EXTENDED GEOMETRY DATA IN THE FOLLOWING FORM:

fgeom ref. ID bias ID thickness per region origin coordinates nreg

EXTENDED GEOMETRY REGION INPUT DATA REQUIREMENTS

TYPE OF DATA	TYPE 1 DATA	TYPE 2 DATA	TYPE 3 DATA
fgeom	ARRAY CORE COREBDY COREBNDS COREBOUN	HOLE	REPLICATE REFLECTOR
Ref. ID	Array no.	Emplaced unit No.	Mixture No. in generated regions
Bias ID	Omit for ARRAY	Omit	First bias ID
Thick./reg.	Omit	Omit	Variable*
Origin coord.	Enter the X Y Z coord. of most neg. pt. of array	Enter the X Y Z coord. of origin	Omit
nreg	Omit	Omit	No. of regions to be generated

*The number of dimensions to be entered is the same as the region preceding the replicate or reflector specification because the generated regions have that shape. The value of the dimensions is the thickness of each generated region of material on that surface.

Table C4.4.5 (continued)

Summary of mixing table data

MIXTURES Format: READ MIXT xsec parameters END MIXT

Note: In CSAS, only xsec parameters should be entered.
KENO V.a mixing table data consists of "xsec parameters" and a "mixing table." The "mixing" table" is used to define the materials used in the KENO V.a problem. This data is automatically created by CSAS and provided to KENO V.a. It cannot be overridden.
See Sects. F11.4.10 and F11.5.5.

XSEC PARAMETERS consists of keywords and associated values.
These parameters, if entered, need be entered only once.

KEYWORD	DEFAULT	DEFINITION
SCT=	1	No. of discrete scattering angles 0 is isotropic 1 is P1 2 is P3 3 is P5
EPS=	0.00003	Cross-section message cutoff value; use to suppress message No. K5-60

Table C4.4.5 (continued)

Summary of plot data

PLOT — Format: READ PLOT plot parameters END PLOT plot parameters must be entered for each plot that is to be made.
See Sects. F11.4.1 and F11.5.9

KEYWORD	DEFAULT	DEFINITION
TTL=	Prob. title	delim ptitl delim delim is a one-character delimiter that signals the beginning and end of the title. ptitl is the plot title (max. 132 char.)
PIC=	MAT	Type of picture: MIXTURE, UNIT NO. or BIAS ID NO.
		MIXTURE ---------- MAT
		MIX
		MIXT
		MIXTURE
		MEDI
		MEDIA
		UNIT NO. ---------- BOX
		BOXT
		BOXTYPE
		UNT
		UNIT
		UNITTYPE
		BIAS ID NO. ------- IMP
		BIAS
		BIASID
		WTS
		WEIG
		WEIGHTS
		WGT
		WGTS
XUL=	Prev. plot	X coord. of upper left corner of plot
YUL=	Prev. plot	Y coord. of upper left corner of plot
ZUL=	Prev. plot	Z coord. of upper left corner of plot
XLR=	Prev. plot	X coord. of lower right corner of plot
YLR=	Prev. plot	Y coord. of lower right corner of plot
ZLR=	Prev. plot	Z coord. of lower right corner of plot

KEYWORD	DEFAULT	DEFINITION
UAX=	Prev. plot 0 IF VAX OR WAX is read	X component of direction cosine for the AX axis of the plot (across)
VAX=	Prev. plot 0 IF UAX OR WAX is read	Y component of direction cosine for the AX axis of the plot (across)
WAX=	Prev. plot 0 IF UAX OR VAX is read	Z component of direction cosine for the AX axis of the plot (across)
UDN=	Prev. plot 0 IF VDN OR WDN is read	X component of direction cosine for the DN axis of the plot (down)
VDN=	Prev. plot 0 IF UDN OR WDN is read	Y component of direction cosine.for the DN axis of the plot (down)
WDN	Prev. plot 0 IF UDN OR VDN is read	Z component of direction cosine for the DN axis of the plot (down)
DLX=		Horizontal spacing between points on plot
DLD=		Vertical spacing between points on plot
NAX=		No. of intervals to be printed across page
NDN=		No. of intervals to be printed down page
LPI=	8	Lines per inch printed down the page
NCH=	CHRS[4]	Delim CHRS delim a one-character delimiter signals the beginning and end of the character string
RUN=	YES	YES allows the problem to execute NO terminates problem after data checking
PLT=	YES	YES allows the plot(s) to be made NO allows reading the plot data without making a plot

PLOT ORIGIN:

(1) SINGLE UNIT - coincides with origin of geometry description.

(2) BASE ARRAY - at the most negative point of the array (lower left-hand back corner of the global array).

(3) REFLECTED ARRAY - coincides with the origin of the CORE or ARRAY description of the global array.

[4]Default values of CHRS are given below:

MEDIA	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
CHRS		1	2	3	4	5	6	7	8	9	A	B	C	D	E	F	G	H	I	J	K	L	M

MEDIA	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	
CHRS	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	#	,	$	-	+	)	|	

MEDIA	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58					
CHRS	£	>	:	;	.	-	%	*	"	=	!	(	@	<	/	0					

Table C4.4.5 (continued)

Summary of starting data

START Format: READ START enter start data here END START
The default value of start type is zero. See Sect. F11.4.8.

START TYPE	REQUIRED DATA	OPTIONAL DATA	STARTING DISTRIBUTION
0	None	NST XSM XSP YSM YSP ZSM ZSP RFL PSP	Uniform
1	NST	XSM XSP YSM YSPO ZSM ZSP RFL PSP	Cosine
2	NST NXS NYS NZS FCT	XSM XSP YSM YSP ZSM ZSP RFL PSP	Cosine with fraction in specified unit
3	NST TFX TFY TFZ NXS NYS NZS	KFS PSP	Spike
4	NST TFX TFY TFZ NBX	KFS PSP	Multiple spikes
5	NST NBX	PSP	In specified units
6	NST TFX TFY TFZ LNU*	NXS NYS NZS KFS PS6 PSP	Arbitrary points

KEYWORD	DEFAULT	DEFINITION
NST=	0	Start type
TFX=	0.0	X coordinate
TFY=	0.0	Y coordinate
TFZ=	0.0	Z coordinate
NXS=	0	X index of unit pos.
NYS=	0	Y index of unit pos.
NZS=	0	Z index of unit pos.
KFS=		Fission spectra
LNU=	0	Number of last neutron
NBX=	0	Source unit number
FCT=	0	Fraction
XSM=	-X	-X of source cuboid
XSP=	+X	+X of source cuboid
YSM=	-Y	-Y of source cuboid
YSP=	+Y	+Y of source cuboid
ZSM=	-Z	-Z of source cuboid
ZSP=	+Z	+Z of source cuboid
RFL=	NO	Start in reflector
PS6=	NO	Print start 6 input
PSP=	NO	Print starting points

*LNU must be the last entry for each set of start 6 data. The LNU of each successive set of data must be larger than the last.

Table C4.4.6 Summary of SEARCH input data

Outline of search type specification (see Sect. C4.4.10.1 for details)

Entry number	Type of data	Data entry	Comments
1	Search descriptor	OPTIMUM OPT OPTM	Initiates a search for the maximum value of k-effective
		CRITICAL CRTL	Initiates a search for a specified value of k-effective. Initiates a search for the minimum value of k-effective
		MINIMUM MINM MIN	
2	Search type	PITCH PIT PTCH	Vary the pitch
		DIMENSION DIM DMSN	Vary one or more dimensions in one or more regions
		CONCENTRATION CON	NOT IMPLEMENTED
3	Optional search parameters		Optional search parameters allow changing default values. Any or all may be entered in any order
3a	No. of search passes	PAS=	Enter the keyword PAS= followed by the desired number of search passes. default=10
3b	No. of search parameters	NPM=	Enter the keyword NPM= followed by the number of search parameters. Present capability is limited to 1. default=1
3c	Search convergence tolerance	EPS=	Enter the keyword EPS= followed by the desired convergence tolerance Default=0.005
3d	Desired value of k-effective	KEF=	Enter the keyword KEF= followed by the desired value of k-effective. The default value is 1.000. DO NOT ENTER FOR OPTIMUM OR MINIMUM SEARCHES
3e	Maximum allowed pitch	MAXPITCH=	Enter the keyword MAXPITCH= followed by the maximum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the pitch corresponding to -5.0 times the parameter at the minimum possible pitch
3f	Minimum allowed pitch	MINPITCH=	Enter the keyword MINPITCH= followed by the minimum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the minimum possible pitch (i.e., the pitch at which the shapes in the array touch)
4	Additional search data	MORE	Enter the delimiter MORE. This delimiter ends the optional search commands and initiates the auxiliary search commands found in Table C4.4.17.

Table C4.4.6 (continued)

Outline of auxiliary search commands and constraints (see Sect. C4.4.10.2 for details)

Entry number	Keyword name	Type of data	Entry requirements	Comments
1a	ALTER ALTR ALT CHANGE CHNG MODIFY MOD MDFY	Begin a new search command	DIMENSION PITCH	These words are used to specify that modifications will be made to the geometry according to subsequent commands (entries 3 through 6 as required to specify the desired changes)
1b	MAINTAIN MNTN	Begin a new search command	DIMENSION PITCH	The spacing (thickness) of the specified geometry regions will be maintained when the interior regions grow or shrink
1c	KEEP HOLD	Begin a new search command	DIMENSION PITCH	This command resets the specified geometry to the original input specifications
2	PAR=	Parameter number	DIMENSION PITCH	Enter the parameter number that the current command (ALTER, MAINTAIN, KEEP) applies to. The present capability is limited. Default=1 and should not be overridden
3	UNIT=	Unit the current command applies to	DIMENSION PITCH	Enter the unit in which regions are to be altered
4	REG=	First region to be altered in the unit	DIMENSION PITCH	Enter the first or only region in the unit that the search constants (entry 6a, b, c and/or d) apply to. Default is the first region
5	TO	Last region to be altered in the unit	DIMENSION PITCH	Enter the last region in the unit that the search constants (entry 6a, b, c and/or d) apply to. Default is the first region NOTE: Entry 4 must be entered in order to alter a single region in a unit. Entries 4 and 5 must both be entered in order to alter more than one region in a unit
6a	ALL=	Search constant for all surfaces (faces) of the region(s)	DIMENSION PITCH	Enter a value for the search constants for the specified regions. This value will be applied to all surfaces of the region(s)
6b	+X=	Search constant for +X face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +X face of a cuboid
	-X=	Search constant for -X face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -X face of a cuboid
	+Y=	Search constant for +Y face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +Y face of a cuboid
	-Y=	Search constant for -Y face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -Y face of a cuboid
	+Z=	Search constant for +Z face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +Z face of a cuboid
	-Z=	Search constant for -Z face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -Z face of a cuboid
6c	+R=	Search constant for radius	DIMENSION PITCH	Enter a value for the search constant for the radius of a sphere or a cylinder
	+H=	Search constant for + height	DIMENSION PITCH	Enter a value for the search constant for the + height of a cylinder
	-H=	Search constant for - height	DIMENSION PITCH	Enter a value for the search constant for the - height of a cylinder
6d	CH=	Search constant for chord	DIMENSION PITCH	Enter a value for the search constant for the chord face of a hemisphere or hemicylinder.
7	+CON=	Maximum constraint	DIMENSION PITCH	Enter the maximum constraint for the current parameter. default=+10E10
8	-CON=	Minimum constraint	DIMENSION PITCH	Enter the minimum constraint for the current parameter. default=-10E10

C4.4.2 INPUT DATA REQUIREMENTS AND DATA CHECKING

Table C4.4.7 summarizes the input data required by Criticality Safety Analysis Sequence No. 4. The types of data needed are:

Table C4.4.7 Summary of data input requirements

Type of data	Analytical sequence							
1 Analytical sequence specification	=CSASN	=CSAS1X	=CSASI	=CSASIX	=CSAS25	=CSAS2X	=CSAS4	=CSAS4X
2 Material Information Processor data	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes
3 KENO V.a data	No	No	No	No	Yes	Yes	Yes	Yes
4 Search data	No	No	No	No	No	No	Yes	Yes
5 END for the analytical sequence	Yes	Yes	Yes	Yes	Yes	Yes	Yes	Yes

1. Analytical sequence specification. Enter the desired sequence name, starting in column 1. The available options are =CSAS4, =CSAS4X, =CSAS25, =CSAS2X, =CSAS1X, =CSASI, =CSASIX, and =CSASN. Enter PARM=CHK in column 11 to check the data.

2. Material Information Processor data. These data are required for processing the cross sections for use in the problem. These data are described in detail in Sects. M7.4 and C4.4.3 through C4.4.8.

3. KENO V.a data. These data are described briefly in Sect. C4.4.9. A detailed description is found in Sect. F11.4 with additional information in Sect. F11.5.

4. Search data. These data are required for CSAS4 and CSAS4X. A detailed description is given in Sect. C4.4.10. The data required for a simple optimum pitch search are

READ SEARCH OPTIMUM PITCH END SEARCH

5. END for analytical sequence—Enter END, starting in column 1.

To check the input data, specify the desired analytical sequence and specify PARM=CHECK or PARM=CHK starting beyond column 10. For example, to check CSAS data, the analytical sequence specification would be:

=CSAS4 PARM=CHECK

Note that =CSAS4 starts in column 1 and PARM=CHECK starts beyond column 10. This causes the input data to be checked, the problem description to be printed, appropriate warning and error messages to be printed, and if KENO V.a data are entered, the data and printer plots are printed.

This feature allows checking the input data without executing any of the functional modules. Simply remove the PARM=CHECK to actually execute the problems.

C4.4.3 MATERIAL INFORMATION PROCESSOR DATA

The Material Information Processor reads the standard compositions specification data and the unit cell geometry specifications. It then produces the mixing table and unit cell information necessary for processing the cross sections. Table C4.4.8 outlines the input data for the Material Information Processor.

The input data for the Material Information Processor are identical to the input for CSAS1 of SCALE 3.1 with the following exceptions:

- The analytical sequence card is considered to be part of the overall data input.
- Items 2, 3, 4, 6, and 7 from Sect. C1.6 are omitted from the parameter card.
- The words END COMP are entered to signal the completion of the standard compositions specification data.
- The MULTIREGION zone description data are terminated by the words END ZONE.
- If optional control parameters are entered, the words MORE DATA must precede the first optional parameter data entry.

Note that CSAS1 is not included in this SCALE release.

The Material Information Processor allows terse data input for all data except the standard composition names and the keyword entries in the optional parameter data (MORE DATA). Terse data entry requires the user to enter only as many characters as are necessary to uniquely define the data entry. However, as many characters as are specified by the user must match the name allowed by the code. For example, refer to Table C4.4.8, **Outline of Material Information Processor data**, data position 3. The available choices for the type of calculation are INFHOMMEDIUM, LATTICECELL, and MULTIREGION. Therefore, it would be sufficient to specify I for an infinite homogeneous medium, L for lattice cell, and M for multiregion. If it is desirable to use more characters, the user is free to do so. However, as many characters as are entered must match the name allowed by the code. For example, if INFHOMMEDIUM is to be specified, INFH is correct, but INFI is not.

WARNING: If several choices begin with the same letters, sufficient characters should be entered to uniquely define the name. For example, ASPHSQUAREP and ASPHTRIANGP are identical through the first four characters. If only ASPH is entered, the code will accept the first name whose first four characters are ASPH. This may not be the one the user intended to use.

The types of data required for the Material Information Processor are given in Table C4.4.8. The individual entries are explained in detail in the text following the table.

Table C4.4.8 Outline of Material Information Processor data

Data position	Type of data	Data entry	Comments
1	Title	Enter a title	80 characters
2	Cross-Section Library Name	HANSEN-ROACH 27GROUPNDF4 123GROUPGMTH 218GROUPNDF4 27BURNUPLIB etc.	The currently available libraries are listed in Tables C4.4.4 and C4.4.8.
3	Type of Calculation	INFHOMMEDIUM LATTICECELL MULTIREGION	These are the available options. See the explanation in Sect. C4.4.3
4	Standard Composition Specification Data	Enter the appropriate data	Terminate this data block with END COMP. See Sect. C4.4.4
5	Unit Cell Geometry Specification	Enter the appropriate data (optional for INFHOMMEDIUM)	Optional for INFHOMMEDIUM See Sect. C4.4.5 for INFHOMMEDIUM See Sect. C4.4.6 for LATTICECELL See Sect. C4.4.7 for MULTIREGION
6	Optional Parameter Data	Enter the desired data	Precede this data block by MORE DATA if more parameter data are to be entered. Otherwise, omit these data entirely. See Sect. C4.4.8

1. Title. An 80-character title is required. The title is the first 80 characters of the Material Information Processor data.

2. Cross-Section Library Name. This item specifies the cross-section library that is to be used in the calculation. See Sect. C4.3, Table C4.4.8, or Sect. M8, Table M8.2.2, for a list of the available libraries.

3. Type of Calculation. The options are INFHOMMEDIUM, LATTICECELL, and MULTIREGION.

   INFHOMMEDIUM is used for an infinite homogeneous medium. It provides cross sections to represent large homogeneous pieces. The cross sections are treated as if each mixture is infinite. Thus, the self-shielding calculations will not account for any geometrical effects. By default, the smallest mixture number will be used in the cell. A different mixture can be used as described in Sect. C4.4.5 and Table C4.4.10.

   LATTICECELL is used when the geometry can be described as a lattice. It is especially suited for arrays of cylindrical rods or spherical pellets. The use of LATTICECELL requires the entry of additional geometry information (unit cell specification), which is described in Sect. C4.4.6 and Table C4.4.11. When the problem consists of an array of fuel bundles or similar geometry, the cross sections are corrected for resonance self-shielding, including geometry effects. If cell-weighted cross sections are desired, CSAS2X, CSAS1X, CSASIX, or CSAS4X must be used. A flux disadvantage factor is then applied to the cross sections of the materials that are used in the unit cell. The KENO V.a geometry description may represent a fuel bundle discretely or as a homogeneous region.

By using CSAS2X or CSAS4X, a fuel bundle can be represented as a single homogeneous region by specifying a mixture number of 500 on the KENO V.a geometry card that defines the overall size and shape of the bundle. This utilizes the cell-weighted cross sections that represent the spatial behavior of the unit cell. The use of CSAS2X or CSAS4X precludes using individual mixtures from the unit cell in the KENO V.a geometry.

MULTIREGION may be used to define a geometric configuration that is more complicated than that allowed by LATTICECELL. It can also be used for a system involving large geometric regions where geometry effects may be minimal. The cross sections utilized in the unit cell are corrected for resonance self-shielding, and an appropriate Dancoff factor is applied (see Sect. M7.2.4.3). If a cell-weighted mixture is generated, it is derived from homogenizing the entire MULTIREGION unit cell. The additional geometry information (unit cell specification) required for a MULTIREGION problem is described in Sect. C4.4.7 and Table C4.4.12.

4. Standard Compositions. These data are used to define the mixtures that will be used in the problem. See Sect. C4.4.4, and Table C4.4.9, for a description of the standard compositions specification data. These data are required for every problem.

5. Cell Geometry Specificaiton. See Sect. C4.4.5 and Table C4.4.10 for an explanation of the optional unit cell data associated with an INFHOMMEDIUM problem. See Sect. C4.4.6 and Table C4.4.11 for an explanation of the data associated with LATTICECELL problems. Section C4.4.7 and Table C4.4.12 explain the data required for a MULTIREGION problem.

6. Optional Parameter Data. This option allows certain defaulted parameters to be respecified by the user. Omit these data unless they are needed. If data are to be entered, see Sect. C4.4.8 and Table C4.4.13 for assistance.

C4.4.4 STANDARD COMPOSITIONS SPECIFICATION DATA

The standard compositions specification data are used to define mixtures that are to be utilized in the problem. These data can be considered to be a mixing table that defines mixtures in terms of standard compositions specification data (available from Sect. M8.2, Table M8.2.1). The required input for the standard compositions specification data varies, depending on the standard composition component name. However, every standard composition specification must include the following:

1. a standard composition component name (SC),

2. the mixture that contains this component (MX),

3. a terminator for the standard compositions specification data (enter the word END).

Enter as many standard composition specifications as necessary to define all the mixtures needed for the problem. When all the necessary mixtures have been described, enter the words END COMP to signal the completion of this type of data.

The data required to define a standard composition specification are contained in Table C4.4.9. In the column entitled "Entry requirement," "ARBM" is used to denote entries required only for arbitrary materials, and "SOLN" is used for entries required only for solutions.

The input data for standard composition specifications are arranged with entry numbers 1 through 7 that apply to all standard composition data. Entries A1 through A7 apply only to arbitrary materials. Entries S1 and S2 apply only to solutions. Entry O1 is optional data that applies to both basic standard compositions and solutions. The individual entries specified in Table C4.4.9 are explained in detail in the text accompanying the table.

Table C4.4.9 Outline of standard composition specification data

Entry number	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Table M8.2.1. Additional allowed names include those beginning with **ARBM** for arbitrary materials and **SOLN** for solutions
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each standard composition component that is an arbitrary material
A2	NEL	Number of elements in the material	ARBM	Enter once for each standard composition component that is an arbitrary material
A3	IVIS	Multiple isotope indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 for a material that does not contain multiple isotope elements. Enter 1 if the material contains a multiple isotope element. An arbitrary material cannot have more than one multiple isotope element. If necessary, several arbitrary materials may be used in a single mixture
A4	ICP	Compound indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 1 for a compound, 0 for alloys, mixtures, etc.
A5	IRS	Resonance indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 if all the nuclides in the material are nonresonance nuclides; enter 1 if one or more have resonance data. See Sect. M8.2, Table M8.2.1
A6	NCZA	ID number (from far right column of Table M8.2.1)	ARBM	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry 2. Enter the number from the far right column of Table M8.2.1. (Premixed standard compositions cannot be used in an arbitrary material definition)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material or weight percent of this element in this arbitrary material	ARBM and ICP=1 or ARBM and ICP=0	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry 2. Do not enter a value unless ICP=1 or repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry 2. Do not enter a value unless ICP=0

Table C4.4.9 (continued)

Entry number	Variable name	Type of data	Entry requirement	Comments
2	MX	Mixture ID number	Always	Enter once for each standard composition component
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML=0 if there is no acid in the solution
O1	SPGR or ROTH	Specific gravity of the solution or density of the basic standard composition	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR or if the density of a basic standard composition (ROTH) is to be entered, use DEN=ROTH
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF=0 is not allowed for SOLN or ARBM
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF=0	Enter only if VF=0.0
5	TEMP	Temperature, in K	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted
6a	IZA	Isotope's ZA number	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
6b	WTP	Weight percent of the isotope	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
7*	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP

*NOTE: Entry 7 should not begin in column 1 unless a name is associated with it. At least two blanks should separate the last entry 7 from the END COMP.

1. SC Standard Composition Component Name. The names of the standard composition components (the alphanumeric identifiers) may be (1) chosen from Table M8.2.1 of Sect. M8.2, which contains the list of elements, compounds, and alloys found in the Standard Composition Library, (2) they may be chosen from the table of available solutions, Sect. M8.3, or (3) they may be designated as an arbitrary material (ARBM). An error message will be printed if the user enters an invalid standard composition component name.

For standard compositions taken from Table M8.2.1 of the Standard Composition Library (basic standard compositions), certain data such as the volume fraction or theoretical density and other engineering type data may need to be entered. For standard compositions containing more than one isotope of an element (such as UO_2), the user is free to specify the weight percent for each isotope such that they total 100%. See Sect. M7.5.5.1 for examples of basic standard compositions.

Solutions require the specification of the density of the heavy metal in the solution and the acid molarity of the solution. The alphanumeric specification of a solution starts with the four characters "SOLN." Some common fissile solutions are SOLNUO2(NO3)2, SOLNPU(NO3)4, and SOLNUO2F2. See Sect. M8.3 for a complete listing of the available solutions. Sections M7.5.5.3 and M7.5.9 contain examples of the input data for solutions.

Arbitrary materials require the user to provide all the information normally found in the Standard Composition Library. The arbitrary material option allows specifying a compound or alloy not available in the Standard Composition Library by utilizing the standard compositions available in the library. Table M8.2.1 indicates which nuclides require a resonance self-shielding calculation.

An arbitrary material name must start with the four characters "ARBM." A maximum of twelve characters is allowed for the standard composition component name. Imbedded blanks are not allowed in a standard composition component name. Section M7.5.5.2 contains examples of input data for arbitrary materials.

An additional example of an arbitrary material specification is as follows:

Consider a mixture of boral having 35 wt % B_4C, 65 wt % aluminum and an overall density of 2.64 g/cc. If neither BORAL nor B4C were available in the Standard Composition Library, the components BORON, C, and AL could be used as basic standard compositions to describe the boral. The necessary volume fractions would have to be determined as shown in Sect. M7.5.5.4, examples 3 and 4. By utilizing the arbitrary material option, both B_4C and aluminum can be described as a component of the same mixture (assume it is desired to be mixture 3), both have a density of 2.64 g/cc, and the volume fractions are 0.35 for the B_4C and 0.65 for the aluminum. The resulting standard compositions specification data do not require any calculations (see example 1, Sect. M7.5.5.5 for a similar situation) and could be entered as

```
ARBMTL-B4C  2.64 2 1 1 0 5000 4 6012 1 3 0.35 END
ARBMTL-AL   2.64 1 0 0 0 13027 100.0 3 0.65 END
```

A1. ROTH Theoretical density of material. Enter ONLY for arbitrary materials. The density of the arbitrary material is entered in units of grams per cubic centimeter.
NOTE: ROTH can be entered for a basic standard composition as shown by entry O1.

A2. NEL Number of elements in the material. Enter ONLY for arbitrary materials. Enter the number of components from the Standard Composition Library that are to be used to define this arbitrary material. In the above example, the ARBMTL-B4C contains two components, the B and the C. Therefore, NEL is 2 for the B_4C arbitrary material. The ARBMTL-AL contains only one component; so NEL is 1 for it.

A3. IVIS Multiple isotope indicator. Enter ONLY for an arbitrary material. An arbitrary material cannot have more than one multiple isotope element. If more than one is needed, define additional arbitrary materials. Enter a zero if none of the elements in the arbitrary material have multiple isotopes. In the above example, the boron is a multiple-isotope element, so IVIS is 1 for the B_4C arbitrary material. The arbitrary material describing the aluminum contains no multiple-isotope elements, so IVIS is zero for it.

A4. ICP Compound indicator. Enter ONLY for arbitrary materials. A compound is a substance containing more than one constituent element and having properties different from those which their constituents had as elementary substances. The composition of a pure compound is perfectly definite and is always the same, regardless of the method of formation. Examples of compounds are H_2O, B_4C, CO_2, $Ca(OH)_2$, C_2H_6, Fe_2S_3, Cr_2O_3, etc. ICP is 1 for a compound. ICP is 0 for alloys (stainless steel, monel, etc.) and conglomerates or mixtures such as concrete.

In the B_4C arbitrary material example, ICP is 1; in the aluminum arbitrary material example, ICP is 0. These examples are given in the explanation of entry number 1, SC.

A5. IRS Resonance indicator. Enter ONLY for arbitrary materials. If any of the nuclides in the arbitrary material have resonance data associated with them, set IRS to 1. If all the nuclides are nonresonance nuclides, set IRS to zero. Table M8.2.1 lists the nuclides that have resonance data associated with them.

IRS is zero for both the B_4C and aluminum arbitrary material examples given in the explanation of entry number 1.

A6. NCZA ID number. Enter ONLY for arbitrary materials. This is the "ZA" ID number for the element or isotope. Usually, NCZA=A+1000*Z, where A is the atomic mass or weight of the nuclide, and Z is the atomic number. For example, NCZA is 1001 for hydrogen, 8016 for oxygen, and 92235 for ^{235}U. For elements for which the natural abundance is acceptable, NCZA can be entered as 1000*Z. For example, 92000 is used for uranium and 5000 is used for boron.

If the arbitrary material contains an element that has multiple isotopes, that element MUST be the first element specified in the arbitrary material. Furthermore, that element MUST be listed in the Isotope Distribution Table, Table M8.4.1. Uranium (92000), plutonium (94000), and boron (5000) are multiple isotope elements.

For example:
ARBMTL-B4C 2.64 2 1 1 0 5000 4 6012 1 3 0.35 END is correct;
ARBMTL-B4C 2.64 2 1 1 0 6012 1 5000 4 3 0.35 END is incorrect because the multiple isotope element is not listed first.

REPEAT THE SEQUENCE NCZA and ATPM (A6 and A7) FOR EVERY ELEMENT IN THE ARBITRARY MATERIAL.

A7. ATPM Enter ONLY for arbitrary materials. Repeat the sequence A6 and A7 for every element in the arbitrary material before going on to entry 2.

If ICP is 1 (entry A4), enter the NUMBER OF ATOMS PER MOLECULE.
If the arbitrary material is a compound (entry A4, ICP is 1), enter the number of atoms of this element per molecule of arbitrary material.

If ICP is 0 (entry A4), enter the WEIGHT PERCENT OF THIS ELEMENT IN THE ARBITRARY MATERIAL. If the arbitrary material is a mixture, alloy, or conglomerate rather than a compound (entry A4, ICP is 0), enter the weight percent of this element in the arbitrary material. If ICP is 0, the sum of all the weight percents for the arbitrary material MUST be 100.0.

2. MX Mixture ID number. A mixture number is required on every standard composition specification. It defines the mixture that contains the material defined by the standard composition specifications data. The mixture numbers are utilized in the unit cell specification for INFHOMMEDIUM, LATTICECELL, or MULTIREGION problems and the KENO V.a geometry data. NOTE: The maximum allowable MIXTURE ID NUMBER that can be used for a mixture containing one or more resonance nuclides is 167 on an IBM computer.

S1. FD Fuel density. Enter ONLY for a solution. The standard composition component name for a solution starts with the four characters "SOLN." The available solution names are listed in Sect. M8.3. Enter the fuel density in units of grams of heavy metal (fissile material) per liter of solution.

S2. AML Acid molarity. Enter ONLY for a solution. If there is no acid in the solution, enter zero. If acid is present in the solution, enter the molarity of the solution.

O1. SPGR or ROTH Optional data. Does NOT apply to ARBITRARY MATERIALS. These optional data can be entered for a solution or for a basic standard composition using a keyword in the form SPG=SPGR, DEN=SPGR, DEN=ROTH, or SPG=ROTH. The keywords SPG= and DEN= are interchangeable. SPGR is the specific gravity of the fuel solution. If the standard composition name begins with SOLN and if the specific gravity of the solution is known, it should be entered. Otherwise the code has to interpolate in a table to obtain a specific gravity to use in the calculation. ROTH is the specified density of the standard composition in grams per cubic centimeter and can be entered if desired. The interaction between ROTH, the density of the standard composition, and VF (entry 3) is demonstrated in Sect. M7.5.5.

3. VF Volume fraction. The default value of the volume fraction is 1.0. It can be omitted if items 4, 5, 6a, and 6b are also omitted. The volume fraction can be interpreted as:

a. the volume fraction of this standard composition component in the mixture,

b. the density of the standard composition component in this application divided by the theoretical density listed in the Standard Composition Library (Sect. M8.2, Table M8.2.1), or a product of (a) and (b).

Section M7.5.5 discusses the interaction between ROTH and VF. For example, assume a homogenized mixture representing the water moderator and zircalloy cladding around a fuel pin is to be described. If the volume of the clad is 5.32 cc and if the volume of the water moderator

is 44.68 cc, the mixture can be described using H_2O with a volume fraction of 0.8936 [i.e., 44.68/(44.68+5.32)] and ZIRCALLOY with a volume fraction of 0.1064 [i.e., 5.32/(44.68+5.32)].

For UO_2 fuel at 95% theoretical density, the volume fraction is 0.95. For the coolant water in an operating pressurized water reactor, the volume fraction might typically be 0.71.

To describe a mixed-oxide fuel pin with a density of 10.5 g/cc, that is 17.8 wt % PuO_2 and 82.2 wt % UO_2, two standard compositions specifications must be entered: one for the PuO_2 component and one for the UO_2 component. From the Standard Composition Library, Table M8.2.1, the theoretical density of the PuO_2 is 11.46 g/cc, and that of the UO_2 is 10.96 g/cc. Therefore, the volume fraction for the PuO_2 is 0.1631 (i.e., 0.178*10.50/11.46), and the volume fraction for the UO_2 is 0.7875 (i.e., 0.822*10.50/10.96).

Occasionally, a special mixture will be desired for which the determination of the component volume fractions will not be so straightforward. Consider a mixture of boral having 35 wt % B_4C, 65 wt % aluminum, and an overall density of 2.64 g/cc. Assume that neither boral nor B_4C are in the Standard Composition Library. The volume fractions corresponding to boron, carbon, and aluminum may be computed as illustrated in Sect. M7.5.5.4, examples 3 and 4. Note that the calculation is complicated by the fact that B_4C is a compound and boron has two isotopes. It might be simpler to enter B_4C and aluminum as arbitrary materials as illustrated in example 1 of Sect. M7.5.5.5. Examples 1 and 2 of Sect. M7.5.5.4 illustrate the use of B_4C and aluminum to describe a boral mixture. **If the volume fraction is set to 0.0, the user can enter the number density for the nuclide (in atoms per barn-cm) for item 4. Number densities cannot be entered for standard compositions that represent multiple nuclides.**

4. ADEN Number density. Enter a value for the number density ONLY if the volume fraction (VF, entry 3) was entered as zero. The number density is entered in units of atoms per barn-cm.

5. TEMP Temperature. The default value of the temperature is 293 K. The temperature can be omitted if items 6a and 6b are also omitted.

   The temperature is used for Doppler broadening and/or the selection of the proper set of thermal scattering data.

   The resonance self-shielding calculation performed by NITAWL-II uses the Nordheim integral method and can account for Doppler broadening of the resonances at any specified temperature. If this material is known to contain a resonance nuclide, the user should enter a rough estimate of the temperature of the material. To determine whether resonance data are available for any of the nuclides in a material,

   a. check Table M8.2.1 if entry number 1 is not a solution, SOLN;

   b. check Table M8.3.1 if entry number 1 denotes a solution, SOLN.

   For each of the light nuclides ($A \leq 20$ a.m.u.), the master cross-section library may contain one or more sets of thermal scattering data, each set corresponding to a different temperature. Scattering matrices for nuclides in media at elevated temperatures are generally fuller than those at lower temperatures. Tables M8.2.1 and M8.3.1 indicate the isotopes, elements, compounds, solutions, and alloys for which multiple sets of thermal scattering data are currently available. If multiple sets of thermal scattering data are available, the user should enter a rough estimate

of the temperature of the material. The code will then use the set of cross-section data that is most appropriate.

6a. IZA Isotope ZA number. Enter a value for each isotope in the standard composition component, item 1. Do not enter a value if the volume fraction, VF, is zero (entry 3).

The ZA number of the isotope is entered if the user wishes to specify the isotopic distribution. This is done by entering 6a and 6b for each isotope until all the desired isotopes have been described. The "ZA" ID number is (A+1000*Z), where A is the atomic mass or weight of the isotope, and Z is the atomic number.

Entries 6a and 6b can be skipped if the default values listed in the Isotope Distribution Table, Table M8.4.1, are acceptable.

6b. WTP Weight percent of the isotope. Do not enter a value if the volume fraction, VF, item 3 is zero. If entry 6a is entered, a value must also be entered for 6b. The weight percent of the isotope is the percent of this isotope in the element.

The user need not enter entries 6a and 6b for each isotope listed for the element in Table M8.4.1. The only requirement is that the sum of entries 6b for the element must sum to 100.0. Thus, uranium could be specified as 92235 3.2 92238 96.8 to represent 3.2% enriched uranium and ignore the 234 and 236 isotopes. However, 92235 3.0 and 92238 96.8 would not be correct because the 3.0 and 96.8 do not sum to 100.0. But 92235 3.0, 92234 0.2, and 92238 96.8 would be correct.

REPEAT THE SEQUENCE 6a and 6b until all the isotopes of the element have been defined as desired.

7. END The word END is entered to terminate the input data for a standard composition component. This END can have a label associated with it that can be as long as 12 characters. The label is optional and, if entered, is separated from the END by a single blank. At least two blanks must separate item 7 from the next data entry.

END COMP The words END COMP are entered only once for a problem. Their purpose is to signal the end of all the standard composition specification data that will be used in the problem. At least two blanks should separate entry 7 from the END COMP. Note that COMP is a label associated with this END. This label can be as long as 12 characters, but the first four characters must be COMP.

C4.4.5 OPTIONAL UNIT CELL SPECIFICATION FOR INFINITE HOMOGENEOUS PROBLEMS

This section describes the unit cell data that can be entered for an INFHOMMEDIUM problem (data position 3 of Table C4.4.8). By default, the smallest mixture number is the mixture that will be used for the cell in XSDRNPM. In order to calculate the eigenvalue of the system, the mixture should contain fissionable material. Unit cell data are required for an infinite homogeneous medium problem ONLY if XSDRNPM is utilized by the control sequence and a mixture number other than the smallest mixture number is to be used in the cell. Control sequences that end in X (CSAS1X, etc.) utilize XSDRNPM. Additional information is available in Sect. M7.5.12 (see also Sect. M7.5.4.1 and M7.5.6.1).

The data required to specify the unit cell for an INFHOMMEDIUM problem are given in Table C4.4.10. The individual entries are explained in the text following the table.

Table C4.4.10 Optional unit cell specification for INFHOMMEDIUM problems

Entry number	Variable name	Type of data	Data entry	Comments
1	NAME	Keyword	CELLMIX	Initiates reading cell data for INFHOMMEDIUM
2	MFUEL	Mixture number in the cell	Mixture number	Specifies the mixture number to be used in the cell. Defaults to the smallest mixture number entered in the standard composition data

NOTE: Unit cell data are necessary for INFHOMMEDIUM only if a mixture number other than the smallest mixture number is to be used in the cell and if a control sequence that executes XSDRN has been specified. If mixtures 1, 2, and 3 are specified and if mixture 3 is to be used in the cell, enter CELLMIX 3.

1. NAME Keyword. The keyword CELLMIX is entered to indicate that unit cell data will be entered. If this entry is entered, entry 2 must also be entered. These data can be entered ONLY if item 3, the "type of calculation" from Table C4.4.8, is entered as INFHOMMEDIUM.

2. MFUEL Mixture number. The mixture number that defines the mixture to be used in the cell. The default value is the smallest mixture number specified in the standard compositions specification data. If either entry 1 or 2 is entered, the other must also be entered.

To enter the above data, enter the keyword CELLMIX, one or more blanks, and the desired mixture number, MFUEL, as shown below:

CELLMIX MFUEL

To specify mixture 5 to be used in the cell, enter the following data:

CELLMIX 5

WARNING: If unit cell data are to be entered as in example 3 below, the word CELLMIX must be spelled correctly. If it is misspelled, the code will not give an error message and will attempt to use the smallest mixture number. The input data will get out of phase for CSAS and SAS sequences that expect to read data after the unit cell specification. For example, CSAS25 expects to read KENO V.a data after the unit cell specification. If CELLMIX is misspelled, the code assumes that it is reading the KENO V.a title card and the data reading gets out of phase.

C4.4.6 UNIT CELL SPECIFICATION FOR LATTICECELL PROBLEMS

This section describes the unit cell data that must be entered for a LATTICECELL problem (data position 3 of Table C4.4.8). Additional information is available in Sects. M7.5.4, M7.5.4.2, M7.5.6.2, and M7.5.8.2. The lattice cell description is especially suited to large arrays of identical cells. The code is limited to a single unit cell description for each problem. The unit cell data are used to provide the lump shape and dimensions for resonance cross-section processing, to provide lattice corrections for cross-section processing, and to provide data used by XSDRNPM to create cell-weighted cross sections. Thus the unit cell specification plays a major role in providing problem-dependent cross sections. The configuration of the unit cell is

determined by the specified "type of lattice." The unit cells are limited to infinitely long cylindrical rods in a square or triangular lattice, spheres in a cubic or triangular lattice, a symmetric array of slabs, or an asymmetric array of slabs. Two distinct types of cells ("Regular" and "Annular") are available to be used in a lattice cell problem. "Regular" cells allow a concentric spherical, cylindrical, or symmetric slab configuration constrained to a central fuel region surrounded by an optional gap, an optional clad, and an external moderator. The outer boundary of the cell is limited to provide an array having a square or triangular pitch. "Annular" cells allow a concentric spherical, cylindrical, or asymmetric slab configuration constrained to a central (second) moderator region surrounded by a fuel region having an optional gap and optional clad on each side of the fuel. The gap, if present, is identical on both sides of the fuel. The clad, if present, is identical in dimension and composition on both sides of the fuel. The outer region of the cell is filled with an external (first) moderator. The outer boundary of the cell is limited to provide an array having a square or triangular pitch.

Regular cells are: SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, and SYMMSLABCELL.

Annular cells are: ASQUAREPITCH, ASQP, ATRIANGPITCH, ATRP, ASPHSQUAREP, ASSP, ASPHTRIANGP, ASTP, and ASYMSLABCELL.

The unit cell data are utilized by the code to define the geometric and resonance self-shielding corrections that will be applied to the cross sections. Cell-weighted cross sections are created only if XSDRNPM is invoked by executing a control sequence ending in X, (CSAS1X, CSAS2X, etc.). The cell-weighted cross sections have a flux disadvantage factor applied to them. Because this weighting is applied to each mixture used in the cell, these cell-weighted mixtures should not be used in the geometry description of a subsequent code. However, the cell-weighted mixture that is created is always assigned a mixture number of 500 and can be used in a subsequent code. KENO V.a is the subsequent code in CSAS2X and CSAS4X. Note that cell-weighted cross sections are not generated if CSAS25 or CSAS4 are used.

The unit cell geometry data required to specify a LATTICECELL problem are given in Table C4.4.11. The individual entries are explained in the text accompanying the table.

Table C4.4.11 Unit cell specification for latticecell problems

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration
				SQUAREPITCH	Use for cylindrical rods in a square pitch
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch
				ASQP	Use for annular cylindrical rods in a square pitch
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch
				ATRP	Use for annular cylindrical rods in a triangular pitch
				SPHSQUAREP	Use for spherical pellets in a cubic lattice
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice
				ASSP	Use for annular spherical pellets in a cubic lattice
				SPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASPHTRIANGP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				ASTP	Use for spherical pellets in a bi-centered or face centered hexagonal close-packed lattice
				SYMMSLAECELL	Use for a symmetric array of slabs
				ASYMSLABCEL	Use for a periodic, but asymmetric array of slabs
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm)
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	ASYMSLABCELL annular cells	Mixture number	Mixture number representing the second moderator
7	TKMOD2	2nd moderator thickness or 2nd moderator diameter (cm)	ASYMSLABCELL or annular cells	Thickness or diameter	Thickness of the second moderator (cm) for ASYMSLABCELL or diameter of inner moderator (cm) for other annular cells
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thicknesses of the fuel, gap, and clad
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad. A mixture number of zero is often used
12	END	Terminate LATTICECELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry 12

1. CTP Type of lattice. This defines the type of lattice or array configuration. Any one of the following alphanumeric descriptions may be used. Note that the alphanumeric description must be separated from subsequent data entries by one or more blanks. Figures C4.4.2 through C4.4.7 are used to illustrate the type of lattice configurations available in a LATTICECELL problem. The fuel region is labeled F; the gap, G; the clad, C; and the moderator, M. If two moderators are present, M1 is the first moderator, and M2 is the second moderator. Both "regular" and "annular" unit cells are available. The arrangement of the materials in the unit cell is strictly constrained. Regular cells are limited to a minimum of two regions and a maximum of four regions. The innermost regions must be fuel, which is surrounded by an optional gap and/or optional clad. The outer region is moderator. Annular cells are limited to a minimum of three regions. The innermost region must be the second moderator. The annular fuel region is outside the second moderator. If a clad is present, it must be identical in thickness and composition on both sides of the fuel. If a gap is present, it is the same thickness on both sides of the fuel. If the first and second moderators are the same material at the same density and temperature and do not contain resonance nuclides, the same mixture number can be used for both moderators. Otherwise, different mixture numbers must be used for the two moderators.

Regular and annular cell configurations are specified as shown below.

Regular Cells

SQUAREPITCH is used for an array of cylinders arranged in a square lattice as shown in Fig. C4.4.2. The clad and/or gap can be omitted.

TRIANGPITCH is used for an array of cylinders arranged in a triangular pitch lattice as shown in Fig. C4.4.3. The clad and/or gap can be omitted.

SPHSQUAREP is used for an array of spheres arranged in a square pitch lattice. A cross-section view through a cell is represented by Fig. C4.4.2. The clad and/or gap can be omitted.

SPHTRIANGP is used for an array of spheres arranged in a triangular pitch (dodecahedral) lattice. A cross-section view through a cell is represented by Fig. C4.4.3. The clad and/or gap can be omitted.

SYMMSLABCELL is used for an infinite array of symmetric slab cells as shown in Fig. C4.4.4. The clad and/or gap can be omitted.

Annular Cells

ASQUAREPITCH or ASQP is used for annular cylindrical rods in a square pitch lattice as shown in Fig. C4.4.5. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ATRIANGPITCH or ATRP is used for annular cylindrical rods in a triangular pitch lattice as shown in Fig. C4.4.6. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ASPHSQUAREP or ASSP is used for spherical shells in a square pitch lattice as shown in Fig. C4.4.5. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

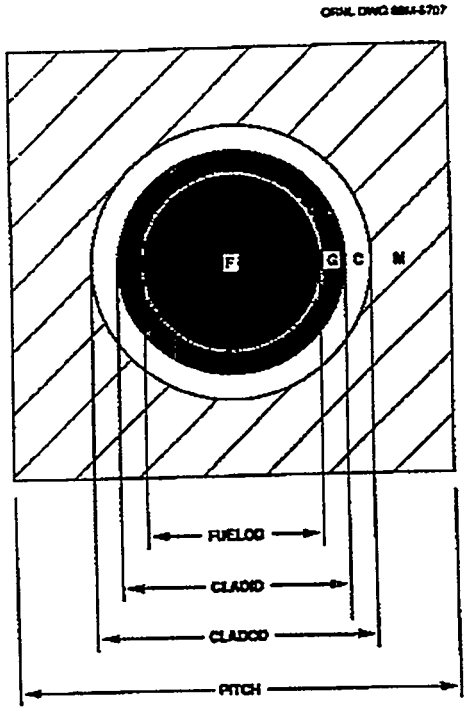


Figure C4.4.2 Arrangement of materials in a SQUAREPITCH and SPHSQUAREP unit cell

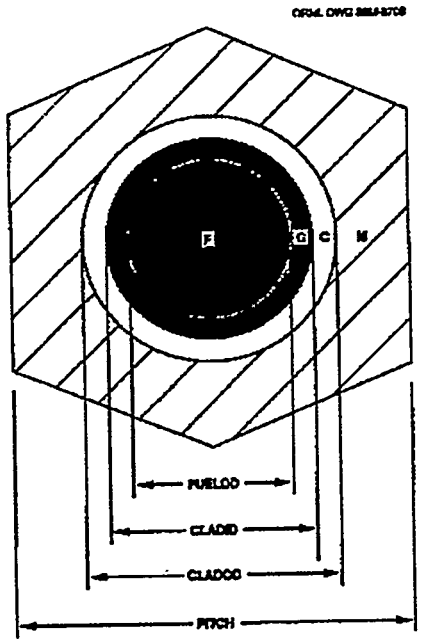


Figure C4.4.3 Arrangement of materials in a TRIANGPITCH and SPHTRIANGP unit cell

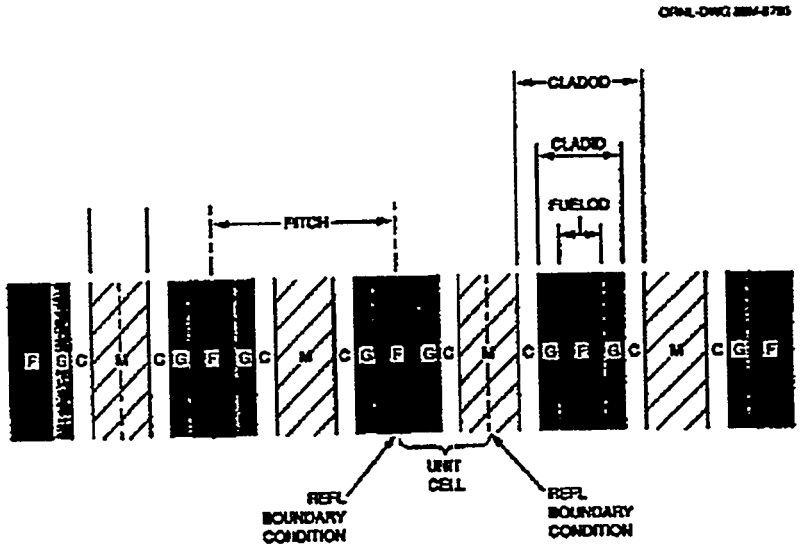


Figure C4.4.4 Arrangement of materials in a SYMMSLABCELL unit cell having reflected left and right boundary conditions

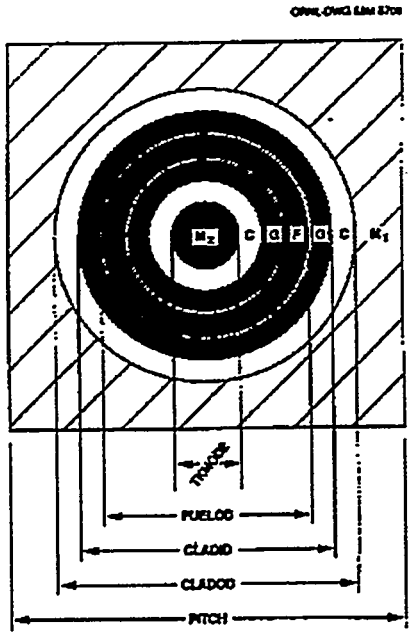


Figure C4.4.5 Arrangement of materials in an ASQUAREPITCH or ASPHSQUAREP unit cell

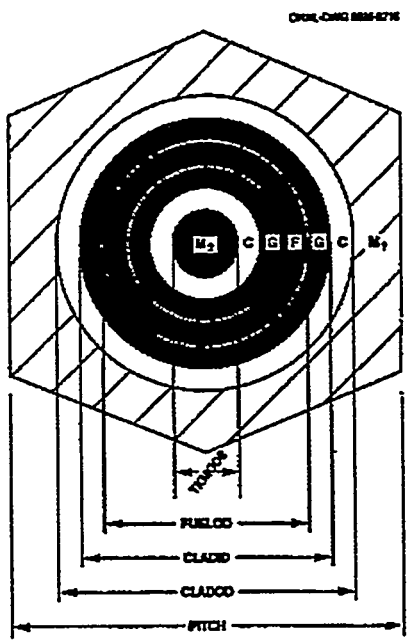


Figure C4.4.6 Arrangement of materials in an ATRIANGPITCH or ASPHTRIANGP unit cell

ASPHTRIANGP or ASTP is used for spherical shells in a triangular pitch (dodecahedral) lattice as shown in Fig. C4.4.6. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

ASYMSLABCELL s used for a periodic, but asymmetric, array of slabs as shown in Fig. C4.4.7. The gap on both sides of the fuel must be identical, as must the clad. The clad and/or gap can be omitted.

2. PITCH Array pitch. This is the center-to-center spacing between the fuel lumps (rods, pellets, or slabs) in centimeters shown in Figs. C4.4.2 through C4.4.7. For an ASYMSLABCELL, enter the distance from the center of one moderator to the center of the other moderator. See Fig. C4.4.7.

3. FUELOD Outside dimension of fuel. This is the outside diameter of the fuel in centimeters as shown in Figs. C4.4.2 through C4.4.7. In slab geometry, enter the thickness of the fuel (see Figs. C4.4.2 through C4.4.7).

4. MFUEL Fuel mixture number. This is the mixture number representing the fuel (F in Figs. C4.4.2 through C4.4.7).

5. MMOD Moderator mixture number. This is the mixture number representing the moderator (M or M1 in Figs. C4.4.2 through C4.4.7).

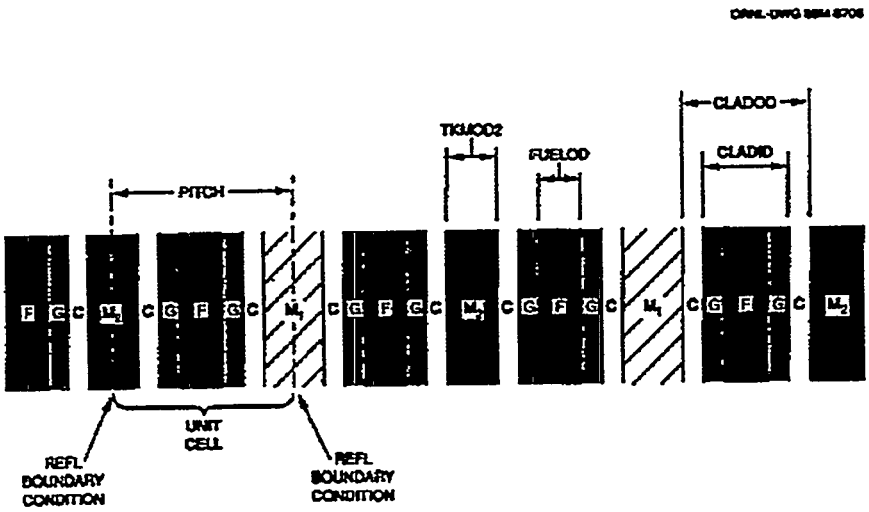


Figure C4.4.7 Arrangement of materials in an ASYMSLABCELL unit cell

6. MMOD2 Second moderator mixture number. Enter ONLY for annular cells. This is the mixture number representing the second moderator (M2 in Figs. C4.4.5 through C4.4.7).

7. TKMOD2 Second moderator thickness. Enter ONLY for annular cells. This is the thickness or diameter of the second moderator in centimeters. See Figs. C4.4.5 through C4.4.7.

8. CLADOD Outside diameter of clad. Enter ONLY if a clad is present. Enter the thickness of the clad in centimeters. For a slab, CLADOD is the sum of the fuel thickness, twice the gap thickness, and twice the clad thickness. See Figs. C4.4.2 through C4.4.7.

9. MCLAD Clad mixture number. Enter ONLY if a clad is present. Enter the mixture number that represents the clad (C in Figs. C4.4.2 through C4.4.7).

10. CLADID Inside diameter of clad. Enter ONLY if a gap is present between the fuel and the clad. Omit if there is no gap. If a gap is present, enter the inside diameter of the clad in centimeters. This corresponds to the outside diameter of the gap. In slab geometry, CLADID is the sum of the fuel thickness and twice the gap thickness. See Figs. C4.4.2 through C4.4.7.

11. MGAP Gap mixture number. Enter ONLY if a gap is present between the fuel and the clad. Omit if there is no gap. Enter the mixture number representing the gap (G in Figs. C4.4.2 through C4.4.7). Zero is often used to represent a void.

12. END The word END is entered to terminate the LATTICECELL data. An optional label can be associated with this END. The label can be as many as 12 characters long and is separated from the END by a single blank. At least two blanks must follow entry 12.

C4.4.7 UNIT CELL SPECIFICATION FOR MULTIREGION PROBLEMS

These data are entered only if the problem is defined as a MULTIREGION problem. They describe the additional geometry data that are required for a MULTIREGION problem (data position 3 of Table C4.4.8). A MULTIREGION problem can be used to define a geometric arrangement that is more complicated than is allowed by a lattice cell. It can also be used for large geometric regions where the geometry effects for the cross sections are minimal. Additional information is available in Sects. M7.5.4, M7.5.4.3, M7.5.6.3, and M7.5.8.3. BE FULLY AWARE THAT CROSS SECTIONS GENERATED USING MULTIREGION IGNORE THE LATTICE GEOMETRY EFFECTS IN DOING THE RESONANCE CORRECTIONS.

The additional data required for a MULTIREGION problem are given in Table C4.4.12; individual entries are explained in the text accompanying the table.

1. CS Type of geometry. The type of geometry must always be specified for a MULTIREGION problem. The cross-section corrections do not account for lattice effects. The available geometry options are listed below.

   SLAB. This is used to describe a slab geometry.

   CYLINDRICAL. This is used to describe cylindrical geometry.

   SPHERICAL. This is used to describe spherical geometry.

   BUCKLEDSLAB. This is used for slab geometry with a buckling correction for the two transverse directions.

   BUCKLEDCYL. This is used for cylindrical geometry with a buckling correction in the axial direction.

2. BR Right boundary condition. This is defaulted to vacuum. A value for BR **MUST** be entered for BUCKLEDSLAB and BUCKLEDCYL but is optional for SLAB, CYLINDRICAL, or SPHERICAL. The available options and their qualifications are listed below:

   VACUUM. This imposes a vacuum at the boundary of the system.

   REFLECTED. This imposes mirror image reflection at the boundary. Do not use for CYLINDRICAL or SPHERICAL.

   PERIODIC. This imposes periodic reflection at the boundary. Do not use for CYLINDRICAL or SPHERICAL.

   WHITE. This imposes isotropic return at the boundary.

3. BL Left boundary condition. This is defaulted to reflected. A value for BL **MUST** be entered for BUCKLEDSLAB but is optional for SLAB, CYLINDRICAL, or SPHERICAL. The available options and their qualifications are listed below:

   VACUUM. This imposes a vacuum at the boundary of the system.

Table C4.4.12 Geometry specification for MULTIREGION problems

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are listed below
				SLAB	Use for slab geometry
				CYLINDRICAL	Use for cylindrical geometry
				SPHERICAL	Use for spherical geometry
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction
2	BR	Right boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL; optional for other geometries		Default is VACUUM. Describes the right/outside boundary condition
				VACUUM	This provides a non-return condition at the boundary
				REFLECTED	Do not use for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	This provides isotopic return at the boundary
3	BL	Left boundary condition	Required for BUCKLEDSLAB and BUCKLEDCYL; optional for other geometries		Default is REFLECTED. Describes the left boundary condition
				VACUUM	This provides a non-return condition at the boundary
				REFLECTED	Recommended for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	This provides isotropic return at the boundary
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB and BUCKLEDCYL; optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry. A value must be entered if subsequent data are to be entered
5	DY	Buckling height (cm)	BUCKLEDSLAB and BUCKLEDCYL	Appropriate dimension	Omit for SLAB, CYLINDRICAL, and SPHERICAL. This corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	Omit unless BUCKLEDSLAB was specified. This is the buckling depth corresponding to the second transverse dimension of a 3-D slab assembly
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined. Enter the mixture number for this zone
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8-10 until all zones are defined. Enter the outside dimension of the zone (cm)
10	XMOD	External moderator index	Optional		Repeat entry numbers 8-10 until all zones are defined. Entry 10 is optional and can be omitted. If it is omitted, repeat entries 8 and 9 until all zones are defined
				NOEXTERMOD	No moderating materials in the adjacent zones
				ONEEXTERMOD	A moderating material is present in one adjacent zone
				TWOEXTERMOD	Moderating materials are present in two adjacent zones
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entries 8 through 10 for each zone

REFLECTED. This imposes mirror image reflection at the boundary. For CYLINDRICAL or SPHERICAL, this is the only valid boundary condition because the left boundary corresponds to the centerline.

PERIODIC. This imposes periodic reflection at the boundary.

WHITE. This causes isotropic return at the boundary.

4. ORGN Location of left boundary on the origin. The default value of ORGN is 0.0. This is the only value allowed for CYLINDRICAL or SPHERICAL geometry. Enter the location of the left boundary on the axis perpendicular to the slab (in cm).

5. DY Buckling height. Enter *ONLY* for BUCKLEDSLAB or BUCKLEDCYL. This is the buckling height in centimeters. It corresponds to one of the transverse dimensions of an actual 3-D slab assembly or the length of a finite cylinder.

6. DZ Buckling depth. Enter *ONLY* for BUCKLEDSLAB. This is the buckling depth in centimeters. It corresponds to the second transverse dimension of an actual 3-D slab assembly.

7. END The word END is entered to terminate these data before entering the zone description data. It must not be entered in columns 1 through 3. At least two blanks are required between items 1 and 7 if they are the only entries. A label can be associated with this END. The label can be a maximum of 12 characters and is separated from the END by a single blank. At least two blanks must follow entry 7.

The zone description data are entered at this point. Entries 8, 9, and 10 are entered for each zone, and the sequence is repeated until all the desired zones have been described. To terminate the data, enter the words END ZONE.

8. MXZ Mixture number in the zone. Enter the mixture number of the material that is present in the zone. Enter a zero for a void. Repeat the sequence of entries 8 through 10 for each zone.

9. RZ Outside radius of the zone. Enter the outside dimension of the zone in centimeters. In slab geometry, RZ is the location of the zone's right boundary on the x-axis. Repeat the sequence of entries 8 through 10 for each zone.

10. XMOD Optional external moderator index. This optional entry describes the conditions existing in the zones adjacent to the present zone. Appropriate conditions are provided by default. The available options are listed below.

NOEXTERMOD. This means there are no moderating materials between this zone and either boundary.

ONEEXTERMOD. This means one of the zones between this zone and one of the boundaries contains a material.

TWOEXTERMOD. This indicates that at least one zone on either side of this zone contains a material.

CAUTION: User-provided entries do not always supersede the default values: (1) For SLAB geometry, user-supplied values will be used everywhere except zone 1. If the left boundary is reflected, the default value of ONEEXTERMOD will be used unless NOEXTERMOD is specified. (2) For SPHERICAL and CYLINDRICAL geometry, default values will be used for all zones unless NOEXTERMOD is specified. NOEXTERMOD allows the user to "turn off" geometric corrections.

Repeat the sequence of entries 8 and 9 or 8 through 10 for each zone. When all the zones have been described, enter the words END ZONE.

END ZONE This is used to terminate the MULTIREGION zone data. Enter the words END ZONE when all the zones have been described. Note that ZONE is a label associated with this END. This label can be as long as 12 characters, but the first four characters must be ZONE. At least two blanks must follow this entry.

C4.4.8 OPTIONAL PARAMETER DATA

Most of the parameter data for Criticality Safety Analysis Sequence No. 4 are determined by the control module and cannot be adjusted. However, certain parameters can be altered. If the default parameters are acceptable, this section of input data should be omitted in its entirety. Nondefault values for one or more of the parameters can be specified by entering the words MORE DATA followed by the desired keyworded parameters and their associated values. One or more of the parameters can be entered in any order. Default values are used for parameters that are not entered. Each parameter is entered by spelling its name, followed immediately by an equal sign and the value to be entered. There should not be a blank between the parameter name and the equal sign. Each parameter specification must be separated from the rest by at least one blank. For example

MORE DATA ISN=16 EPS=0.00008 END

would result in using an S16 angular quadrature set and tightening the convergence criteria to 0.00008 in the XSDRNPM calculation. Note that the END is not the end for the analytical sequence, entry 5 of Table C4.4.7.

Table C4.4.13 describes the optional parameters that can be entered as data and the code or codes the parameters apply to. A description of each entry is contained in the text accompanying the table.

Table C4.4.13 Optional parameter data

Entry number	Keyword name	Type of data	Applicable module	Comments
1	MORE DATA	Input flag		This signals that optional parameter data will be entered. Enter only those parameters you wish to change
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. This allows using another value
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0. 0<SZF<1.0 gives a finer mesh. SZF>1.0 gives a coarser mesh
4	IIM=	Max. number of inner iterations	XSDRNPM	The default value is 20. This allows using another value
5	ICM=	Max. number of outer iterations	XSDRNPM	The default value is 25. This allows using another value
6	EPS=	Overall convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value
8	BKL=	Buckling factor	XSDRNPM	The default value is 1.420892. Use ONLY for a multiregion problem that specifies BUCKLEDSLAB or BUCKLEDCYL
9	IUS=	Upscatter scaling factor	XSDRNPM	The default value is zero. IUS=0 doesn't utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence
10	RES=	Resonance data	BONAMI NITAWL-II	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE), and the thickness of the slab or radius of the sphere or cylinder, in centimeters
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL-II	Enter the mixture number, mm, to which the Dancoff factor applies inside the parentheses; enter the Dancoff factor after the equal sign Repeat entries 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description

Table C4.4.13 (continued)

Entry number	Keyword name	Type of data	Applicable module	Comments
12	BAL=	Key to print balance tables	XSDRNPM	The default value is FINE. BAL=NONE suppresses printing the balance table. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables
13	DY=	First transverse dimension	XSDRNPM	The first transverse dimension, in centimeters, used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder)
14	DZ=	Second transverse dimension	XSDRNPM	The second transverse dimension, in centimeters, used for a buckling correction (i.e., the width of a slab)
15	COF=	Diffusion coefficient option for transverse leakage correction	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRNPM will be read
17	FWR=	Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRNPM will be written
18	DAB=	Number of direct access data blocks	MIP[a]	The default is 200. Number of blocks allocated for direct-access unit 90
19	AXS=	Unit on which a mixed ANISN library will be written	ICE	Enter the unit number where ICE is to write a mixed ANISN library
20	COLL	Key to activate collapse of thermal groups	MIP[a]	Enter COLL to collapse all thermal groups into one group for the shielding sequences
21	END	Terminus		Terminate the optional parameter data. Do not start in column 1. At least two blanks must follow entry number 21

[a]MIP is the Material Information Processor.

1. MORE DATA...These words, followed by one or more blanks, are entered ONLY if optional parameter data are to be entered. They must precede all other optional parameter data. Entries 2 through 19 can be entered in any order.

2. ISN Order of angular quadrature for XSDRNPM. Quadrature sets are geometry-dependent quantities that are defaulted to order 8 by the Material Information Processor. See Sects. M7.2.5.7 and M7.5.7 for a more detailed explanation.

3. SZF Spatial mesh size factor for XSDRNPM. The size of the largest mesh interval can be adjusted by entering a value for SZF. The default value is 1.0. A value between zero and 1.0 yields a finer mesh; a value greater than 1.0 yields a coarser mesh. See Sects. M7.2.5.6 and M7.5.7 for more details.

4. IIM Maximum number of inner iterations for XSDRNPM. This is the maximum number of inner iterations to be used in the XSDRNPM calculation. The default value is 20. See Sect. M7.5.7 for a more detailed explanation.

5. ICM Maximum number of outer iterations for XSDRNPM. This is the maximum number of outer iterations to be used in the XSDRNPM calculation. The default value is 25. If the calculation reaches the outer iteration limit, a larger value should be used. See Sect. M7.5.7 for a more detailed explanation.

6. EPS Overall convergence criteria for XSDRNPM. This is used by XSDRNPM after each outer iteration to determine if the problem has converged. The default value of EPS is 0.0001. A value less than 0.0001 tightens the convergence criteria; a larger value loosens the convergence criteria. See Sects. M7.2.5.8 and M7.5.7 for additional information.

7. PTC Pointwise convergence criteria for XSDRNPM. This is the point flux convergence criteria used by XSDRNPM to determine if convergence has been achieved after an inner iteration. The default value is 0.0001. A smaller value tightens convergence; a larger value loosens it. See Sects. M7.2.5.8 and M7.5.7 for more details.

8. BKL Buckling factor for XSDRNPM. A buckling factor should be used ONLY for a MULTIREGION BUCKLEDSLAB or BUCKLEDCYL problem. Because cylinders are assumed to be infinitely long and slabs are assumed to be infinite in both transverse directions, the analytic sequence may tend to overestimate the total flux for a finite system. A buckling correction can be used to approximate the leakage from the system in the transverse direction(s). The extrapolation distance factor, BKL, is defaulted to 1.420892. See Sects. M7.2.5.4 and M7.5.7 for additional details.

9. IUS Upscatter scaling flag for XSDRNPM. This option allows the use of upscatter scaling to accelerate the solution or force convergence. The default value is zero, in which case upscatter scaling is not used. IUS=1 facilitates upscatter scaling. Guidelines are not available to indicate when upscatter scaling is needed. Some problems will not converge with it, and some will not converge without it. See Sect. M7.5.7 for a more detailed explanation.

10. RES Resonance data for BONAMI and NITAWL-II. This parameter allows overriding the default resonance data for materials that are not used in the unit cell. The default resonance data are infinite homogeneous media that may not accurately represent the geometry (for example, a thin clad or container region). The resonance data are entered in the form:

RES= mixture number geometry type thickness.

The mixture number is the material for which the resonance data apply. The geometry type can be a sphere, slab, or cylinder and defines the third entry of the 3* array in NITAWL-II. The thickness is the thickness of a slab or the radius of a sphere or cylinder in centimeters and defines the fourth entry of the 3* array in NITAWL-II. This entire data sequence should be entered for each material for which the default data are inadequate. See Sect. M7.5.7 for additional details. WARNING: If this parameter is used to enter resonance data for a mixture that is used in the unit cell specification, it will NOT be used. Information provided in the unit cell data will be used instead.

11. DAN(mm)= Dancoff factor for the specified mixtures. This allows entering a Dancoff factor to be used in the resonance correction for the specified mixture. The Dancoff data are entered in the form:

    DAN(mm) = Dancoff factor.

    Note that the parentheses must be entered as part of the data. The mixture number, mm, to which the Dancoff factor applies, must be enclosed in the parentheses. The Dancoff factor to be used is entered after the equal sign. See Sect. M7.5.7 for additional details.

    Items 10 and 11 should be entered for each resonance mixture that is not specified in the LATTICECELL or MULTIREGION unit cell specification data. See Sects. M7.5.10 and C4.5.1 for additional information.

12. BAL Balance table print flag for XSDRNPM. This allows control of the balance table print from XSDRNPM. The default value is FINE. BAL=NONE suppresses the balance table print. BAL=ALL prints all of the balance tables. BAL=FINE prints only the fine-group balance tables. See Sect. M7.5.7 for additional details.

13. DY= First transverse dimension for XSDRNPM. This is the first transverse dimension, in centimeters, used in a buckling correction to calculate the leakage normal to the principal calculation direction (the height of a slab or cylinder). It should only be entered if XSDRNPM is to create cell-weighted cross sections and/or calculate the eigenvalue of a cylinder or slab system of finite height for a LATTICECELL problem. DY= is defaulted to an infinite height, or is set to DY for a buckled MULTIREGION cell description. See Sects. M7.2.5.4 and M7.5.7 for additional details.

14. DZ= Second transverse dimension for XSDRNPM. This is the second transverse dimension, in centimeters, used for a buckling correction for a slab of finite width. It should only be entered if XSDRNPM is to create cell-weighted cross sections and/or calculate the eigenvalue of a LATTICECELL slab of finite width. DZ= is defaulted to an infinite width, or is set to DZ for a buckled MULTIREGION slab cell of finite width. See Sects. M7.2.5.4 and M7.5.7 for additional details.

15. COF= Diffusion coefficient for transverse leakage corrections in XSDRNPM. The default value is 0. The available options are

    COF=0 sets a transport-corrected cross section for each zone.

    COF=1 use a spatially averaged diffusion coefficent for each zone.

COF=2 use a diffusion coefficient for all zones that is one-third the diffusion coefficient determined from the spatially averaged transport cross section for all zones.

COF=3 use a flux and volume weighting across all zones.

See Sect. M7.5.7 or Sect. F3.5, 3$ array, variable IPN for more details.

16. FRD= Unit from which fluxes are read for XSDRNPM. If fluxes are to be used for the initial flux guess, enter the unit number from which they are to be read. The user is responsible for supplying job control language data that is necessary for reading the flux dataset. See Sect. M7.5.7 for more details.

17. FWR= Unit on which fluxes will be written for XSDRNPM. If binary fluxes are to be saved from this XSDRNPM calculation, enter the unit number where they will be written. The user is responsible for supplying job control language data that is necessary for creating and saving the flux dataset. See Sect. M7.5.7 for more details.

18. DAB= Number of direct-access data blocks for the Material Information Processor. This is the number of blocks allocated for direct access on unit 90. The default is 200. See Sect. M7.5.7 for additional details. If the job fails in the Material Information Processor with an LMP005 DA ERROR, then DAB must be used to enter a larger value. See Sect. C4.7.4 for additional details.

19. AXS= Logical unit number for ICE. Write a mixed ANISN library on this unit. The default is zero (no library). If the unit number is input as 7, the ANISN library will be in free-form card image. For any other unit number, the library will be binary. The user is responsible for supplying job control language data that is necessary for creating and saving the ANISN cross-section library. An ANISN cross section can only be created by the control sequences CSASI, CSASIX, and SAS3. See Sect. M7.5.7 for additional details.

20. COLL Activate collapse of thermal groups. This parameter should only be used with the shielding analysis sequences (SAS1, etc.). It causes the Material Information Processor to instruct XSDRN to collapse all thermal groups into one group.

21. END The word END is entered to terminate the optional parameter data. A label can be associated with this END. The label can be as long by a single blank. If this END is entered without a label, it must not begin in column 1. At least two blanks must follow this entry.

C4.4.9 SUMMARY OF KENO V.a DATA

KENO V.a data are required for CSAS25, CSAS2X, CSAS4, and CSAS4X. A brief outline of the KENO V.a data is given in Table C4.4.14. The input data are summarized in Table C4.4.15. The input data for KENO V.a are discussed in detail in Sects. F11.4 and F11.5. Data need not be supplied for entries whose default value is acceptable. KENO V.a mixing table data cannot be entered or used in CSAS because they are automatically supplied by the control module.

Table C4.4.14 Outline of KENO V.a data

Type of data	Starting flag	Comments	Termination flag
Title	None	80 columns, must be entered first	None
Parameters	READ PARM	Enter desired parameter data	END PARM
Biasing or weighting	READ BIAS	Enter desired biasing data	END BIAS
Geometry	READ GEOM	Enter desired geometry data	END GEOM
Array data or unit orientation	READ ARRAY	Enter desired array data	END ARRAY
Boundary conditions or albedoes	READ BNDS	Enter desired albedo data	END BNDS
Start data or initial source	READ START	Enter desired start data	END START
Mixing table data	READ MIXT	The CSAS4 modules allow only SCT= and EPS=	END MIXT
Plot data	READ PLOT	Enter desired plot data	END PLOT
KENO V.a data terminus	END DATA	Enter to signal the end of all KENO V.a data	

Table C4.4.15 Summary of KENO V.a data

Summary of parameter data

TITLE: The title must be entered first (80 columns) See Sect. F11.4.3

PARAMETERS: Format: READ PARAM enter parameter data here END PARAM
If parameters are entered, they must follow the title. See Sects. F11.4.3, F11.5.2, and F11.5.3.

KEY	STD.	DEFINITION	KEY	STD.	DEFINITION	KEY	STD.	DEFINITION	KEY	STD.	DEFINITION
RND=	given	Random number	RUN=	YES	Execute problem	MKH=	NO	Matrix by hole	XSC=	14	Mixed xsecs
TME=	30 min	Execution time (min)	FLX=	NO	Fluxes	CKH=	NO	Cofactor k by hole	ALB=	79	Albedo
TBA=	0.5 min	Batch time (min)	FDN=	NO	Fission densities	FMH=	NO	Fiss. prod. by hole	WTS=	80	Weights
WTA=	0.5	Average weight	ADJ=	NO	Adjoint calculation	HHL=	NO	MKH at highest level	LTB=	4	Working xsecs
WTH=	3.0	Wt. for splitting	AMX=	NO	All mixture xsecs	MKA=	NO	Matrix by array			from NITAWL
WTL=	1/WTH	Russian Roulette wt.	XAP=	NO	Xsec angles and probs.	CKA=	NO	Cofactor k by array			or XSDRN
GEN=	103	No. of generations	XS1=	NO	1-D xsecs	FMA=	NO	Fiss. prod. by array	SKT=	16	Scratch
NPG=	300	No. per generation	XS2=	NO	2-D xsecs	HAL=	NO	MKA at highest level	RST=	95	Read restart
NSK=	3	Generations skipped	PKI=	NO	Fission spectrum	PLT=	YES	Printer plots	WRS=	95	Write restart
RES=	0	Gens. between restart	P1D=	NO	Extra 1-D xsecs	BUG=	NO	Debug print	XSC=	14	Mixed xsecs
NBK=	NPG+25	Neutron bank positions	FAR=	NO	Fiss. and abs.	TRK=	NO	Print neutron tracks			
XNB=	0	Extra bank entries	MKP=	NO	Matrix by location	PWT=	NO	Print avg. weight			
NFB=	NPG	Fission bank positions	CKP=	NO	Cofactor k by loc.	PGM=	NO	Unprocessed geometry			
XFB=	0	Extra bank entries	FMP=	NO	Fiss. prod. by loc.	SMU=	NO	Self-multiplication			
X1D=	0	No. of extra 1-D's	MKU=	NO	Matrix by unit	NUB=	NO	Neutrons per fission			
LNG=	1000000	Words of storage*	CKU=	NO	Cofactor k by unit	PAX=	NO	Albedo-xsec array			
BEG=	1	Restart at this gen.	FMU=	NO	Fiss. prod. by unit						
NG8=	200	Blocks for d.a. unit									
NL8=	512	Length of d.a. block									

*The words of storage in CSAS are defaulted to 100,000 and can be overridden by using the size= parameter on the analytical sequence specification which then becomes the default value of LNG in KENO V.a.

For example: =CSAS25 PARM=SIZE=200000
or =CSAS25 PARM=(CHECK,SIZE=200000)

Table C4.4.15 (continued)

Summary of array data

ARRAY Format: READ ARRAY array parameters data type orientation data END ARRAY See Sects. F11.5.5, F11.5.6, and F11.5.7.

Repeat the sequence ARRAY PARAMETERS DATA TYPE ORIENTATION DATA for each array used in the problem.

ARRAY PARAMETERS			DATA TYPE
KEYWORD	DEFAULT	DEFINITION	FILL LOOP
ARA=	1	No. defining the array	
NUX=	1	No. of units in X direction	
NUY=	1	No. of units in Y direction	
NUZ=	1	No. of units in Z direction	
GBL=	Maxara	Global, universe, or overall array number**	
COM=	None	Delim comment delim Optional comment is a maximum of 132 characters	

**Can be defaulted by the code. If specified, it need be entered only once per problem.

ORIENTATION DATA FOR FILL

Enter unit numbers to define every position in the array. When entering data utilizing the options in this table, the count field and option field must be adjacent with no imbedded blanks. The operand field may be separated from the option field by one or more blanks. Orientation data for FILL is terminated by entering END FILL.

COUNT FIELD	OPTION FIELD	OPERAND FIELD	COMMENTS
		j	Stores j at the current position in the array
i	R	j	Stores j in the next i positions in the array
i	*	j	Stores j in the next i positions in the array
i	$	j	Stores j in the next i positions in the array
	F	j	Fills remainder of the array with unit no. j starting with the current array position
	A	j	Sets the current position in the array to j
i	S		increments; current position in the array by i allows skipping i positions. The value of i may be positive or negative
i	Q	j	Repeats the previous j entries i times. The default value of i is 1
i	N	j	Repeats the previous j entries i times, inverting the sequence each time. The default value of i is 1
i	B	j	Starting with the entry at -i from the current position, store entries in inverse order until position -(i+j) is reached. Default value of i=1
i	P	j	Alternately stores j and -j in the next i positions of the array
i	I	j k	Provides the end points, j and k, with i entries linearly interpolated between them (i.e., a total of i+2 points). At least one blank must separate j and k. When used for an integer array, the I option should only be used to generate integer steps [i.e., (k-j)/(i+1) should be a whole number].
	T		Terminates the data reading for the array

ORIENTATION DATA FOR LOOP

Enter the unit number and nine numbers that define the position(s) of that unit. Data for each of these ten entries are repeated until every position in the array has been defined. Orientation data for LOOP is terminated by entering END LOOP.

ENTER DATA IN THE FORM:

DATA ENTRY	COMMENTS
LTYPE	The unit or box type. LTYPE must be greater than 1
IX1	Starting position in the X direction. IX1 must be at least 1 and no larger than the value entered for NUX
IX2	Ending position in the X direction. IX2 must be at least 1 and no larger than the value of NUX
INCX	The number of units by which increments are made in the X direction
IY1	The starting position in the Y direction. IY1 must be at least 1 and less than the value entered for NUY
IY2	Ending position int he Y direction. IY2 must be at least 1 and no larger than the value of NUY
INCY	The number of units by which increments are made in the positive Y direction
IZ1	Starting position in the Z direction. IZ1 must be at least 1 and no larger than NUZ
IZ2	Ending position in the Z direction. IZ2 must be at least 1 and no larger than NUZ
INCZ	The number of units by which increments are made in the positive Z direction

Table C4.4.15 (continued)

Summary of biasing data

BIAS (weighting)

Format: READ BIAS keyword correlation data auxiliary END BIAS
See Sects. F11.4.7 and F11.5.8

KEYWORD	DESCRIPTION	
ID=	CORRELATION DATA will be read next.	
	id	Material ID. Enter from table at right to use weighting data from the library
	ibgn	Beginning bias ID
	iend	Ending bias ID
WT=	AUXILIARY DATA will be read next.	
WTS=	AUXILIARY DATA will be read next.	
	wttitl	Material title (12-character maximum)
	id	Material ID
	nsets	Number of sets of group structures
	REPEAT	(thkinc, numinc, ngpwt, wtavg) nsets times
	thkinc	Thickness per increment
	numinc	Number of increments
	ngpwt	Number of energy groups for this set of wts
	wtavg	Enter numinc x ngpwt values of wtavg

MATERIAL	ID	ENERGY GROUPS	THICKNESS/ INCREMENT
Concrete	301	16,27,123	5 cm
Paraffin	400	16,27,123	3 cm
Water	500	16,27,123,218	3 cm
Graphite	6100	16,27,123	20 cm

For CORRELATION DATA, the material ID is chosen from material ID column above (the keyword is ID=).
For AUXILIARY DATA, the material ID is chosen by the user and the keyword is WT= or WTS=.
When AUXILIARY DATA are entered, CORRELATION DATA must also be entered to use the data.
Beginning and ending bias ID's are defined by the user. The geometry specificaiton that has the bias ID equal to the beginning bias ID utilizes the wt avg's from the first interval of material ID.

Table C4.4.15 (continued)

Summary of boundary condition data

BNDS (albedo or boundary conditions)

Format: READ BNDS face code albedo name END BNDS
See Sect. F11.4.7

The sequence FACE CODE ALBEDO NAME is entered as many times as necessary to define the appropriate albedo boundary conditions. The default for all faces is vacuum.

FACE CODES FOR ENTERING BOUNDARY (ALBEDO) CONDITIONS

FACE CODE	DEFINITION	FACE CODE	DEFINITION	FACE CODE	DEFINITION	FACE CODE	DEFINITION
+XB=	Positive X face	XFC=	Both X faces	+YX=	Positive X and Y faces	&ZY=	Positive Y and Z faces
&XB=	Positive X face	YFC=	Both Y faces	&XY=	Positive X and Y faces	-XY=	Negative X and Y faces
-XB=	Negative X face	ZFC=	Both Z faces	&YX=	Positive X and Y faces	=XZ=	Negative X and Z faces
+YB=	Positive Y face	+FC=	All positive faces	+XZ=	Positive X and Z faces	=YZ=	Negative Y and Z faces
&YB=	Positive Y face	&FC=	All positive faces	+ZX=	Positive X and Z faces	YXF=	All X and Y faces
-YB=	Negative Y face	-FC=	All negative faces	&XZ=	Positive X and Z faces	ZXF=	All X and Z faces
+ZB=	Positive Z face	XYF=	All X and Y faces	&ZX=	Positive X and Z faces	ZYF=	All Y and Z faces
&ZB=	Positive Z face	XZF=	All X and Z faces	+YZ=	Positive Y and Z faces	-YX=	Negative X and Y faces
-ZB=	Negative Z face	YZF=	All Y and Z faces	+ZY=	Positive Y and Z faces	-ZX=	Negative X and Z faces
ALL=	All 6 faces	+XY=	Positive X and Y faces	&YZ=	Positive Y and Z faces	-ZY=	Negative Y and Z faces

ALBEDO NAMES AVAILABLE ON THE KENO V ALBEDO LIBRARY, FOR USE WITH THE FACE CODES

ALBEDO NAME	DESCRIPTION	ALBEDO NAME	DESCRIPTION	ALBEDO NAME	DESCRIPTION
DPOH20 DPOH20 DPO DPO	12-in. double PO water differential albedo with 4 incident angles	CONC-4 CON4 CONC4	4-in. concrete differential albedo with 4 incident angles	VACUUM VOID VACU VAC	Vacuum condition
H20 WATER	12-in. water differential albedo with 4 incident angles	CONC-8 CON8 CONC8	8-in. concrete differential albedo with 4 incident angles	SPECULAR MIRROR MIRR	Mirror image reflection
PARAFFIN PARA WAX	12-in. paraffin differential albedo with 4 incident angles	CONC-12 CON12 CONC12	12-in. concrete differential albedo with 4 incident angles	SPEC SPE MIR	
CARBON GRAPHITE C	200-cm carbon differential albedo with 4 incident angles	CONC-16 CON16 CONC16	16-in. concrete differential albedo with 4 incident angles	PERIODIC PERI PER	Periodic boundary condition
ETHYLENE POLY CH2	12-in. polyethylene differential albedo with 4 incident angles	CONC-24 CON24 CONC24	24-in. concrete differential albedo with 4 incident angles		

Table C4.4.15 (continued)

Summary of geometry data

GEOMETRY (region)

Format: READ GEOM enter geometry region data here END GEOM
See Sects. F11.4.4, F11.5.1.2, F11.5.6, and F11.5.7.

GEOMETRY REGION DATA consists of SIMPLE GEOMETRY REGION DATA and EXTENDED GEOMETRY REGION DATA.

ENTER GEOMETRY REGION DATA IN THE FOLLOWING FORM:

OPTIONAL GLOBAL SPECIFICATION
UNIT n
OPTIONAL GEOMETRY COMMENT
SIMPLE GEOMETRY REGION DATA
and/or
EXTENDED GEOMETRY REGION DATA

* * * *

Table C4.4.15 (continued)

Summary of geometry data (continued)

GEOMETRY (region) (cont.)

ENTER EXTENDED GEOMETRY DATA IN THE FOLLOWING FORM:

fgeom ref. ID bias ID thickness per region origin coordinates nreg

EXTENDED GEOMETRY REGION INPUT DATA REQUIREMENTS

TYPE OF DATA	TYPE 1 DATA	TYPE 2 DATA	TYPE 3 DATA
fgeom	ARRAY CORE COREBDY COREBNDS COREBOUN	HOLE	REPLICATE REFLECTOR
Ref. ID	Array no.	Emplaced unit number	Mixture no. in generated regions
Bias ID	Omit for ARRAY	Omit	First bias ID
Thick./reg.	Omit	Omit	Variable*
Origin coord.	Enter the X Y Z coord. of most neg. pt. of array	Enter the X Y Z coord. of origin	Omit
nreg	Omit	Omit	No. of regions to be generated

*The number of dimensions to be entered is the same as the region preceding the replicate or reflector specification because the generated regions have that shape. The value of the dimensions is the thickness of each generated region of material on that surface.

Table C4.4.15 (continued)

Summary of mixing table data

MIXTURES Format: READ MIXT xsec parameters END MIXT

Note: In CSAS, only xsec parameters should be entered.
KENO V.a mixing table data consists of "xsec parameters" and a "mixing table." The "mixing" table" is used to define the materials used in the KENO V.a problem. These data are automatically created by CSAS and provided to KENO V.a. It cannot be overridden.
See Sects. F11.4.10 and F11.5.5.

XSEC PARAMETERS consists of keywords and associated values.
These parameters, if entered, need be entered only once.

KEYWORD	DEFAULT	DEFINITION
SCT=	1	No. of discrete scattering angles 0 is isotropic 1 is P1 2 is P3 3 is P5
EPS=	.00003	Cross-section message cutoff value Use to suppress message No. K5-60

Table C4.4.15 (continued)

Summary of plot data

PLOT — Format: READ PLOT plot parameters END PLOT plot parameters must be entered for each plot that is to be made.
See Sects. F11.4.11 and F11.5.9

KEYWORD	DEFAULT	DEFINITION
TTL=	Prob. title	delim ptitl delim delim is a one-character delimiter that signals the beginning and end of the title. ptitl is the plot title (max. 132 char.)
PIC=	MAT	Type of picture: MIXTURE, UNIT NO. or BIAS ID NO.
		MIXTURE ---------- MAT
		MIX
		MIXT
		MIXTURE
		MEDI
		MEDIA
		UNIT NO. ---------- BOX
		BOXT
		BOXTYPE
		UNT
		UNIT
		UNITTYPE
		BIAS ID NO. ------- IMP
		BIAS
		BIASID
		WTS
		WEIG
		WEIGHTS
		WGT
		WGTS
XUL=	Prev. plot	X coord. of upper left corner of plot
YUL=	Prev. plot	Y coord. of upper left corner of plot
ZUL=	Prev. plot	Z coord. of upper left corner of plot
XLR=	Prev. plot	X coord. of lower right corner of plot
YLR=	Prev. plot	Y coord. of lower right corner of plot
ZLR=	Prev. plot	Z coord. of lower right corner of plot

KEYWORD	DEFAULT	DEFINITION
UAX=	Prev. plot 0 IF VAX OR WAX is read	X component of direction cosine for the AX axis of the plot (across)
VAX=	Prev. plot 0 IF UAX OR WAX is read	Y component of direction cosine for the AX axis of the plot (across)
WAX=	Prev. plot 0 IF UAX OR VAX is read	Z component of direction cosine for the AX axis of the plot (across)
UDN=	Prev. plot 0 IF VDN OR WDN is read	X component of direction cosine for the DN axis of the plot (down)
VDN=	Prev. plot 0 IF UDN OR WDN is read	Y component of direction cosine for the DN axis of the plot (down)
WDN	Prev. plot 0 IF UDN OR VDN is read	Z component of direction cosine for the DN axis of the plot (down)
DLX=		Horizontal spacing between points on plot
DLD=		Vertical spacing between points on plot
NAX=		No. of intervals to be printed across page
NDN=		No. of intervals to be printed down page
LPI=	8	Lines per inch printed down the page
NCH=	CHRS**	Delim CHRS delim, a one character delimiter signals the beginning and end of the character string
RUN=	YES	YES allows the problem to execute NO terminates problem after data checking
PLT=	YES	YES allows the plot(s) to be made NO allows reading the plot data without making a plot

PLOT ORIGIN:

(1) SINGLE UNIT - coincides with origin of geometry description.

(2) BASE ARRAY - at the most negative point of the array (lower left-hand back corner of the global array).

(3) REFLECTED ARRAY - coincides with the origin of the CORE or ARRAY description of the global array.

**default values of CHRS are given below:

MEDIA	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
CHRS		1	2	3	4	5	6	7	8	9	A	B	C	D	E	F	G	H	I	J	K	L	M

MEDIA	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42
CHRS	N	O	P	Q	R	S	T	U	V	W	X	Y	Z	#	,	$	-	+	)	|

MEDIA	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58
CHRS	£	>	:	;	.	-	%	*	"	=	!	(	@	<	/	0

Table C4.4.15 (continued)

Summary of starting data

START Format: READ START enter start data here END START
The default value of start type is zero. See Sect. F11.4.8.

START TYPE	REQUIRED DATA	OPTIONAL DATA	STARTING DISTRIBUTION
0	None	NST	Uniform
		XSM	
		XSP	
		YSM	
		YSP	
		ZSM	
		ZSP	
		RFL	
		PSP	
1	NST	XSM	Cosine
		XSP	
		YSM	
		YSPO	
		ZSM	
		ZSP	
		RFL	
		PSP	
2	NST	XSM	Cosine with
	NXS	XSP	fraction in
	NYS	YSM	specified
	NZS	YSP	unit
	FCT	ZSM	
		ZSP	
		RFL	
		PSP	

START TYPE	REQUIRED DATA	OPTIONAL DATA	STARTING DISTRIBUTION
3	NST	KFS	Spike
	TFX	PSP	
	TFY		
	TFZ		
	NXS		
	NYS		
	NZS		
4	NST	KFS	Multiple
	TFX	PSP	spikes
	TFY		
	TFZ		
	NBX		
5	NST	PSP	In specified
	NBX		units
6	NST	NXS	Arbitrary
	TFX	NYS	points
	TFY	NZS	
	TFZ	KFS	
	LNU*	PS6	
		PSP	

KEYWORD	DEFAULT	DEFINITION
NST=	0	Start type
TFX=	0.0	X coordinate
TFY=	0.0	Y coordinate
TFZ=	0.0	Z coordinate
NXS=	0	X index of unit pos.
NYS=	0	Y index of unit pos.
NZS=	0	Z index of unit pos.
KFS=		Fission spectra
LNU=	0	Number of last neutron
NBX=	0	Source unit number
FCT=	0	Fraction
XSM=	-X	-X of source cuboid
XSP=	+X	+X of source cuboid
YSM=	-Y	-Y of source cuboid
YSP=	+Y	+Y of source cuboid
ZSM=	-Z	-Z of source cuboid
ZSP=	+Z	+Z of source cuboid
RFL=	NO	Start in reflector
PS6=	NO	Print start 6 input
PSP=	NO	Print starting points

*LNU must be the last entry for each set of start 6 data. The LNU of each successive set of data must be larger than the last.

C4.4.10 SEARCH DATA

Search data are required only for CSAS4 and CSAS4X. They are omitted for all other sequences. Search data are entered in the form:

READ SEARCH search data END SEARCH

The words READ SEARCH inform the code that search data are to be read, and the words END SEARCH terminate the search data. The search data options are described in Sects. C4.4.10.1 and C4.4.10.2. Additional information and examples are contained in Sects. C4.5.6 through C4.5.11.

C4.4.10.1 Search Type Specification

The basic search data to define the type of search and various search parameters that set limits for the search are described in this section. These data are listed in Table C4.4.16.

The desired search type must be specified in the search data before the individual search commands can be entered. The desired search type is specified only once in a problem. The data specifications are listed below.

1. Search descriptor

   Enter a word (OPTIMUM, CRITICAL, MINIMUM) to define the basic search mode. A default value is not supplied. The three basic search modes are:

   OPTIMUM initiates a search for the maximum value of k-effective.

   CRITICAL initiates a search for a specified value of k-effective.

   MINIMUM initiates a search for the minimum value of k-effective.

2. Search type

   Enter a word (PITCH, DIMENSION, CONCENTRATION) to specify the variable that is changed during the search. A default value is not supplied. The variables are:

   PITCH causes the pitch (center-to-center spacing in the x and y directions) to vary according to the search parameters.

   DIMENSION causes the dimensions in one or more geometry regions to vary according to the search parameters.

   CONCENTRATION causes the concentration to vary. THIS OPTION IS NOT IMPLEMENTED.

3. Optional search parameters

   Optional search parameters are available for changing default values. They are specified by entering a keyword followed by the desired value. The optional search parameters are listed below.

Table C4.4.16 Outline of search type specification

Entry number	Type of data	Data entry	Comments
1	Search descriptor	OPTIMUM OPT OPTM	Initiates a search for the maximum value of k-effective
		CRITICAL CRTL	Initiates a search for a specified value of k-effective. Initiates a search for the minimum value of k-effective
		MINIMUM MINM MIN	
2	Search type	PITCH PIT PTCH	Vary the pitch
		DIMENSION DIM DMSN	Vary one or more dimensions in one or more regions
		CONCENTRATION CON	NOT IMPLEMENTED
3	Optional search parameters		Optional search parameters allow changing default values. Any or all may be entered in any order
3a	No. of search passes	PAS=	Enter the keyword PAS= followed by the desired number of search passes. default=10
3b	No. of search parameters	NPM=	Enter the keyword NPM= followed by the number of search parameters. Present capability is limited to 1. default=1
3c	Search convergence tolerance	EPS=	Enter the keyword EPS= followed by the desired convergence tolerance. Default=0.005
3d	Desired value of k-effective	KEF=	Enter the keyword KEF= followed by the desired value of k-effective. The default value is 1.000. DO NOT ENTER FOR OPTIMUM OR MINIMUM SEARCHES
3e	Maximum allowed pitch	MAXPITCH=	Enter the keyword MAXPITCH= followed by the maximum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the pitch corresponding to -5.0 times the parameter at the minimum possible pitch
3f	Minimum allowed pitch	MINPITCH=	Enter the keyword MINPITCH= followed by the minimum allowed pitch for a search whose search type, entry 2 above, is PITCH. The default value is the minimum possible pitch (i.e., the pitch at which the shapes in the array touch)
4	Additional search data	MORE	Enter the delimiter MORE. This delimiter ends the optional search commands and initiates the auxiliary search commands found in Table C4.4.17.

3a. PAS= Number of search passes

The number of search passes is the maximum number of times the search will change data and calculate the corresponding k-effective. The default is 10.

3b. NPM= Number of search parameters

The number of search parameters is not fully implemented. The default value is 1 and should not be overridden.

3c. EPS= Search convergence tolerance

The search convergence tolerance is the search convergence criteria. OPTIMUM and MINIMUM searches are terminated when a k-effective is calculated that is within EPS of the optimum or minimum respectively. A CRITICAL search is terminated when a calculated k-effective is within EPS of the target or desired k-effective. The default value is 0.005.

3d. KEF= Desired value of k-effective

This information is entered ONLY for a CRITICAL search. The default value is 1.000.

3e. MAXPITCH= Maximum allowed pitch

The maximum allowed pitch (center-to-center spacing in the x and y directions) is specified using this keyword. It applies to a pitch search type and causes the search to terminate if the specified pitch is exceeded. The default value is the pitch corresponding to -5 times the parameter at the minimum pitch.

3f. MINPITCH= Minimum allowed pitch

The minimum allowed pitch (center-to-center spacing in the x and y directions) is specified using this keyword. It applies to a PITCH search type and causes the search to terminate if the pitch needs to be smaller than MINPITCH. The default value is the pitch at which the pins in the array are touching.

4. More additional search data will follow.

The word MORE terminates the optional search parameters and initiates the individual search commands. Do not enter MORE unless individual search commands are to be entered.

C4.4.10.2 Auxiliary Search Commands and Constraints

Auxiliary search commands are entered ONLY if MORE, item 4, of the search type specification data were entered (see Table C4.4.16). Individual search commands are used to specify search constraints and to communicate to the search program the units that will be altered, the regions that will be altered within those units, and the faces or surfaces of those regions that will be altered. The data comprising the auxiliary search commands are listed in Table C4.4.17. All data except items 1a, 1b, and 1c are keyworded (i.e., the data are entered by specifying a keyword, followed by a value). An explanation of each individual search command follows the table.

Table C4.4.17 Outline of auxiliary search commands and constraints

Entry number	Keyword name	Type of data	Entry requirements	Comments
1a	ALTER ALTR ALT CHANGE CHNG MODIFY MOD MDFY	Begin a new search command	DIMENSION PITCH	These words are used to specify that modifications will be made to the geometry according to subsequent commands (entries 3 through 6 as required to specify the desired changes)
1b	MAINTAIN MNTN	Begin a new search command	DIMENSION PITCH	The spacing (thickness) of the specified geometry regions will be maintained when the interior regions grow or shrink
1c	KEEP HOLD	Begin a new search command	DIMENSION PITCH	This command resets the specified geometry to the original input specifications
2	PAR=	Parameter number	DIMENSION PITCH	Enter the parameter number that the current command (ALTER, MAINTAIN, KEEP) applies to. The present capability is limited. Default=1 and should not be overridden
3	UNIT=	Unit the current command applies to	DIMENSION PITCH	Enter the unit in which regions are to be altered
4	REG=	First region to be altered in the unit	DIMENSION PITCH	Enter the first or only region in the unit that the search constants (entry 6a, b, c and/or d) apply to. Default is the first region
5	TO	Last region to be altered in the unit	DIMENSION PITCH	Enter the last region in the unit that the search constants (entry 6a, b, c and/or d) apply to. Default is the first region NOTE: Entry 4 must be entered in order to alter a single region in a unit. Entries 4 and 5 must both be entered in order to alter more than one region in a unit
6a	ALL=	Search constant for all surfaces (faces) of the region(s)	DIMENSION PITCH	Enter a value for the search constants for the specified regions. This value will be applied to all surfaces of the region(s)
6b	+X=	Search constant for +X face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +X face of a cuboid
	-X=	Search constant for -X face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -X face of a cuboid
	+Y=	Search constant for +Y face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +Y face of a cuboid
	-Y=	Search constant for -Y face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -Y face of a cuboid
	+Z=	Search constant for +Z face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the +Z face of a cuboid
	-Z=	Search constant for -Z face of cuboid	DIMENSION PITCH	Enter a value for the search constant for the -Z face of a cuboid
6c	R=	Search constant for radius	DIMENSION PITCH	Enter a value for the search constant for the radius of a sphere or a cylinder
	+H=	Search constant for + height	DIMENSION PITCH	Enter a value for the search constant for the + height of a cylinder
	-H=	Search constant for - height	DIMENSION PITCH	Enter a value for the search constant for the - height of a cylinder
6d	CH=	Search constant for chord	DIMENSION PITCH	Enter a value for the search constant for the chord face of a hemisphere or hemicylinder
7	+CON=	Maximum constraint	DIMENSION PITCH	Enter the maximum constraint for the current parameter. default=+10E10
8	-CON=	Minimum constraint	DIMENSION PITCH	Enter the minimum constraint for the current parameter. default=-10E10

1. Command definition. A command definition tells the code what action is to be taken. A new search command is initiated whenever an item 1a through 1c is encountered. The code will vary the geometry according to subsequent commands.

1a. ALTER, ALTR, ALT, CHANGE, CHNG, MODIFY, MOD, MDFY — Alter geometry regions. These words specify that modifications will be made to the geometry according to subsequent commands.

1b. MAINTAIN, MNTN — Maintain the thickness. The thickness of the specified geometry region(s) will be maintained when the interior regions grow or shrink (i.e., the specified region will grow or shrink in conjunction with the interior region in such a way as to maintain the original distance between the two regions). This means that the original thickness of the region is preserved. For instance, the inner radius of a pipe can be altered and the wall thickness can be preserved by applying the MAINTAIN command to the region defining the outer radius of the pipe.

1c. KEEP, HOLD — Keep the original specification. This command causes the specified geometry region(s) to be reset to their original input value for every search pass. Therefore they go through the entire search process unchanged.

2. PAR= — Parameter number. The search parameter number is not fully implemented. The default number is 1 and should not be overridden.

3. UNIT= — Geometry unit number. This is the geometry unit to which the previously entered command definition (item 1a, 1b, or 1c) is applied. Items 3, 4, and 5 specify the region(s) within the unit and the surfaces of the region(s) to be altered.

4. REG= — First region to be altered. This is used to specify the first or only region in the unit (specified by item 3) that is to be altered according to the search command (item 1a, 1b, or 1c). The region(s) are altered according to the search constants (items 6a, 6b, 6c, and/or 6d).

5. TO — Last region to be altered. This item is entered to specify the last region to be altered, starting with the region specified by REG=. For example, assume unit 3 contains 8 regions and you wish to make changes to regions 4, 5, 6, 7, and 8. These regions are identified by entering the following data. UNIT=3 REG=4 TO 8

6. Search constants. A search constant is the proportionality factor utilized to alter a geometry region. A search constant must be entered for each surface of a region that is to be altered. A nonzero search constant will cause the region dimension for that surface to be changed. A search constant of 0.0 will cause the region dimension to remain unchanged. The default value of the search constant is 0.0.

6a. ALL= — Search constant for all surfaces. All of the surfaces in a region are altered simultaneously by using this search command.

6b. +X= — Search constant for +X face. This parameter is used to specify the value of the search constant for the +X face of a cuboid.

6b. -X= Search constant for -X face. This parameter is used to specify the value of the search constant for the -X face of a cuboid.

6b. +Y= Search constant for +Y face. This parameter is used to specify the value of the search constant for the +Y face of a cuboid.

6b. -Y= Search constant for -Y face. This parameter is used to specify the value of the search constant for the -Y face of a cuboid.

6b. +Z= Search constant for +Z face. This parameter is used to specify the value of the search constant for the +Z face of a cuboid.

6b. -Z= Search constant for -Z face. This parameter is used to specify the value of the search constant for the -Z face of a cuboid.

NOTE: If it is desirable to change all the faces of a cuboid except the -z face by some amount (search constant of 1.0), items 6a and 6b can be used together as follows: ALL=1.0 -Z=0.0. This is the same as entering +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0. If both z faces are to remain unchanged, items 6a and 6b can be entered as: ALL=1.0 +Z=0.0 -Z=0.0 or as +X=1.0 -X=1.0 +Y=1.0 -Y=1.0.

6c. R= Search constant for radius. This parameter is used to specify the value of the search constant for the radius of a sphere, hemisphere, cylinder, or hemicylinder.

6c. +H= Search constant for +height. This parameter is used to specify the value of the search constant for the +height of a cylinder or hemicylinder.

6c. -H= Search constant for -height. This parameter is used to specify the value of the search constant for the -height of a cylinder or hemicylinder.

6d. CH= Search constant for chord. This parameter is used to specify the value of the search constant for the chord of a hemisphere or hemicylinder.

7. +CON= Maximum constraint. Enter the maximum value you wish to allow the search parameter to obtain. The maximum constraint must be larger than the mimimum constraint but need not be a positive number. The default value of the maximum constraint is 10^{11}. See Sect. C4.5.6.2b for additional information on how to determine constraints.

NOTE: For a PITCH search, the maximum constraint is redefined and is calculated from the data entered for MAXPITCH, item 1. +CON should not be entered if a value was entered for MAXPITCH. If constraints, +CON= and/or -CON= are not entered as data, the code computes the minimum constraint corresponding to the pins touching, and the maximum constraint is then negative five times the magnitude of the minimum constraint.

8. -CON= Minimum constraint. Enter the minimum value you wish to allow the search parameter to obtain. The minimum constraint must be smaller than the maximum constraint but need not be a negative number. The default value of the minimum constraint for a dimension search is -10^{11}. The default value of the minimum constraint for a pitch search is redefined to correspond to the pins in the lattice touching. See Sect. C4.5.6.2b for additional information on how to determine constraints.

C4.5 NOTES FOR CSAS USERS

This section provides tips concerning the use of CSAS and its associated sequences. Section M7.5 provides information about the use of the Material Information Processor, and Sect. F11.7 provides assistance about the use of the KENO V.a data required by CSAS.

C4.5.1 CSAS MODULES

Several CSAS modules are contained in the CSAS family. These modules enable the user to generate and save working format cross sections for use with KENO IV, XSDRNPM, or KENO V.a, or a MORSE/KENO cross-section library for use with MORSE or KENO V.a. Therefore, the user can run different codes using the same cross-section library for comparison purposes. A list of the available modules is given below. Table C4.5.1 lists the I/O devices utilized by CSAS, and Table C4.5.2 lists the type of I/O files utilized by the functional modules invoked by CSAS.

The CSAS input data allow the user to define optional I/O files. The CSAS optional parameter data, Sect. C4.4.8, allow the user to define the following optional files: (1) the unit from which XSDRNPM may read fluxes, (2) the unit on which XSDRNPM may write fluxes, and (3) the unit on which ICE may write an ANISN library. The KENO V.a input data used by CSAS allow the user to define optional logical units used by KENO V.a. See "Logical Unit Numbers" in Sect. F11.4.3. The unit on which a KENO V.a restart data file is written should not be set to 95.

CSASN — Runs BONAMI and NITAWL-II and generates a working format cross-section library on unit 4. The user may save that library for future use or stack a KENO V.a or XSDRNPM problem after it with the input library specified as unit 4. If the user wishes to exercise XSDRNPM options that are not available in CSAS (such as a search or adjoint calculation), an XSDRNPM problem can be stacked immediately after the CSASN problem. When a KENO V.a problem is stacked after a CSASN problem, the parameter LIB=4 should be entered in the KENO V.a parameter data and a mixing table must be entered in order to utilize the working format library from CSASN.

CSAS1X — Runs BONAMI, NITAWL-II, and XSDRNPM. A cell-weighted working format cross-section library is written on unit 3. Note that any mixture utilized in the cell cannot be used in a subsequent KENO V.a calculation because the weighting applied to those mixtures is for the purpose of generating the cell-weighted cross section. This difficulty is circumvented by adding the same mixtures to the CSAS data with different mixture numbers. To utilize the cell-weighted library in a KENO V.a problem following a CSAS1X problem, LIB=3 should be entered in the KENO V.a parameter data, a mixing table must be entered, and the cell-weighted mixture can be used in the geometry.

CSASI — Runs BONAMI, NITAWL-II, and ICE. A working format library is written on unit 2, and a MORSE/KENO mixture cross-section library is written on unit 14. To utilize the MORSE/KENO library in a subsequent KENO V.a problem, the parameter XSC=14 must be entered in the KENO V.a parameter data, and the LIB= parameter should be omitted. The mixing table must be omitted, and the mixtures utilized in the geometry must match the mixtures specified in the CSASI data.

Table C4.5.1 Description of units utilized by the Criticality Safety Analysis Sequence No. 4 control module

Unit number	Type of data	Creating module	User module	Type of file
5	Input	DRIVER	CSAS	Sequential
8	Scratch file	CSAS	CSAS	Direct or random access data
11	Short master cross-section library	CSAS	BONAMI	Sequential
16	Scratch file	CSAS	CSAS	Sequential
17	Scratch file	CSAS	CSAS	Sequential
18	Scratch file	CSAS	CSAS	Sequential
19	Scratch file	CSAS	CSAS	Sequential
70	User-supplied cross sections		CSAS	AMPX master format library
81	16-group cross sections		CSAS	AMPX master format library
82	27-group cross sections		CSAS	AMPX master format library
83	123-group cross sections		CSAS	AMPX master format library
84	218-group cross sections		CSAS	AMPX master format library
85	22 neutron-18 gamma cross sections		CSAS	AMPX master format library
86	18-gamma cross sections		CSAS	AMPX master format library
87	27-group cross sections for burnup		CSAS	AMPX master format library
88	27 neutron-18 gamma cross sections		CSAS	AMPX master format library
89	Standard Composition Library		CSAS	Direct- or random-access data file
90	Search data	CSAS	MODIFY	Direct or random access data
92	ICE input data	CSAS	ICE	Sequential
95	KENO V.a restart data	CSAS MODIFY KENO V.a	KENO V.a MODIFY	Sequential
96	BONAMI input data	CSAS	BONAMI	Sequential
97	NITAWL-II input data	CSAS	NITAWL-II	Sequential
98	XSDRNPM input data	CSAS	XSDRNPM	Sequential
99	Printed output	CSAS MODIFY	CSAS MODIFY	Sequential

Table C4.5.2 Description of units used by the functional modules of CSAS

Unit No.	Module	Action	Type of file
1	BONAMI	WRITE	Microscopic master working format cross sections
	NITAWL-II	READ	Microscopic master working format cross sections
2	ICE	WRITE	Macroscopic working format cross sections
3	XSDRNPM	WRITE	Microscopic cell-weighted working format cross sections
	ICE	READ	Microscopic cell-weighted working format cross sections
	KENO V.a	READ	Microscopic cell-weighted working format cross sections
4	NITAWL-II	WRITE	Microscopic working format cross sections
	ICE	READ	Microscopic working format cross sections
	KENO V.a	READ	Microscopic working format cross sections
	XSDRNPM	READ	Microscopic working format cross sections
6	BONAMI	WRITE	Printed output
	ICE	WRITE	Printed output
	KENO V.a	WRITE	Printed output
	NITAWL-II	WRITE	Printed output
	XSDRNPM	WRITE	Printed output
8	BONAMI	WRITE/READ	Direct- or random-access scratch files
	ICE	WRITE/READ	Direct- or random-access scratch files
	KENO V.a	WRITE/READ	Direct- or random-access scratch files
	XSDRNPM	WRITE/READ	Direct- or random-access scratch files
9	BONAMI	WRITE/READ	Direct- or random-access scratch files
	ICE	WRITE/READ	Direct- or random-access scratch files
	KENO V.a	WRITE/READ	Direct- or random-access scratch files
	NITAWL-II	WRITE/READ	Direct- or random-access scratch files
	XSDRNPM	WRITE/READ	Direct- or random-access scratch files
10	ICE	WRITE/READ	Direct- or random-access scratch files
	KENO V.a	WRITE/READ	Direct- or random-access scratch files
	XSDRNPM	WRITE/READ	Direct- or random-access scratch files
11	BONAMI	READ	Short AMPX master format cross sections
14	ICE	WRITE	Monte Carlo-formatted macroscopic cross sections
	KENO V.a*	READ/WRITE	Monte Carlo-formatted macroscopic cross sections
16	KENO V.a	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Angular flux file
17	XSDRNPM	WRITE/READ	Sequential scratch file
18	BONAMI	WRITE/READ	Sequential scratch file
	NITAWL-II	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Sequential scratch file
19	BONAMI	WRITE/READ	Sequential scratch file
	NITAWL-II	WRITE/READ	Sequential scratch file
	XSDRNPM	WRITE/READ	Sequential scratch file
79	KENO V.a	READ	KENO V.a albedo file
80	KENO V.a	READ	KENO V.a weighting file
92	ICE	READ	Binary input file
95	KENO V.a	READ	Binary input file
96	BONAMI	READ	Binary input file
97	NITAWL-II	READ	Binary input file
98	XSDRNPM	READ	Binary input file

*KENO V.a always reads from unit 14. If microscopic input cross sections are used, KENO V.a prepares macroscopic cross sections and writes them on unit 14 to be read later.

CSASIX — Runs BONAMI, NITAWL-II, XSDRNPM, and ICE. A working format library is written on unit 2, and a MORSE/KENO mixture cross-section library, including the cell-weighted mixture 500, is written on unit 14. To utilize the MORSE/KENO library in KENO V.a, the parameter XSC=14 must be entered in the KENO V.a parameter data, and the LIB= parameter should be omitted. The mixing table must be omitted, and the mixtures utilized in the geometry must match the mixtures specified in the CSASIX data.

CSAS25 — Runs BONAMI, NITAWL-II, and KENO V.a. A working format library is written on unit 4, and a MORSE/KENO mixture cross-section library is written on unit 14. Either or both of these libraries can be saved for future use. Because KENO V.a data are entered as part of the CSAS25 data, LIB= and XSC= should not be specified in the KENO V.a parameter data, and the mixing table should be omitted from the KENO V.a data. All KENO V.a options are available through CSAS25.

CSAS2X — Runs BONAMI, NITAWL-II, XSDRNPM, and KENO V.a. A working format library is written on unit 3, and a MORSE/KENO mixture cross-section library is written on unit 14. The cell-weighted mixture 500 is included on unit 14. Either or both of these libraries can be saved for future use. Because KENO V.a data are entered as part of the CSAS25 data, LIB= and XSC= should not be specified in the KENO V.a parameter data, and the mixing table should be omitted from the KENO V.a data. All KENO V.a options are available through CSAS2X. To process cross sections and run KENO V.a, CSAS25 should be used unless use of a cell-weighted mixture in KENO V.a is planned.

CSAS4 — Runs BONAMI, NITAWL-II, KENO V.a, and MODIFY. Use CSAS to perform an automatic search on dimensions or pitch. CSAS is an iterative procedure in which the KENO V.a geometry data is modified and KENO V.a is run until the convergence criteria is met or the problem runs out of time. A working format library is written on unit 4, and a MORSE/KENO mixture cross-section library is written on unit 14. Either or both of these libraries can be saved for future use. Because KENO V.a data are entered as part of the CSAS data, LIB= and XSC= should not be specified in the KENO V.a parameter data, and the mixing table should be omitted from the KENO V.a data. All KENO V.a options are available through CSAS. The search data follow the KENO V.a data.

CSAS4X — Runs BONAMI, NITAWL-II, XSDRNPM, KENO V.a, and MODIFY. Use CSAS4X for search problems where the geometry utilizes a cell-weighted cross section and an automatic search on the KENO V.a geometry dimensions or pitch is desired. CSAS4X is an iterative procedure in which KENO V.a geometry data are modified and KENO V.a is run until the convergence criteria is met or the problem runs out of time. A working format library is written on unit 3, and a MORSE/KENO mixture cross-section library is written on unit 14. The cell-weighted mixture 500 is included on unit 14. Either or both of these libraries can be saved for future use. Because the KENO V.a data is entered as part of the CSAS data, LIB= and XSC= should not be specified in the KENO V.a parameter data, and the mixing table should be omitted from the KENO V.a data. All KENO V.a options are available through CSAS4X. The search data follows the KENO V.a data.

C4.5.2 AUTOMATIC CROSS-SECTION PROCESSING FOR CRITICALITY CALCULATIONS

The CSAS family of control modules can prepare an AMPX working format problem-dependent cross-section library for use by KENO V.a. CSAS25, CSAS2X, CSAS4, and CSAS4X can be used to prepare an AMPX working format cross-section library and run KENO V.a without the necessity of having to enter the mixing table data in KENO V.a. Examples are given in Sects. C4.5.2.1 through C4.5.2.4.

C4.5.2.1 Run KENO V.a using CSAS25 or CSAS4

CSAS25 and CSAS4 create a microscopic working format library and a mixing table that is passed to KENO V.a. CSAS25 executes KENO V.a and calculates k-effective for the problem. CSAS4 executes KENO V.a repeatedly to perform a search as specified in the search data.

EXAMPLE 1. CSAS25 - Determine the k-effective of a system.

Consider a problem consisting of four uranium metal cylinders that are 93.2% wt enriched, having a density of 18.76 g/cc. The cylinders are arranged in a 2 × 2 × 2 array. Each has a radius of 5.748 cm and a height of 10.765 cm. The center-to-center spacing in the horizontal plane (X-Y) is 13.74 cm and the vertical center-to-center spacing is 13.01 cm. The input data for this problem follow. The calculated k-effective for this critical experiment was 0.9934 ± 0.0045.

```
=CSAS25
SET UP 2C8 IN CSAS25
HANSEN-ROACH  INFHOMMEDIUM
URANIUM  1 DEN=18.76 1 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
END COMP
KENO V.a SAMPLE PROBLEM 1  CASE 2C8 BARE
READ PARAMETERS  TME=1.0 FLX=YES FDN=YES FAR=YES
END PARAMETERS
READ GEOMETRY
CYLINDER 1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.87 -6.87 6.87 -6.87 6.505 -6.505
END GEOMETRY
READ ARRAY  NUX=2 NUY=2 NUZ=2  END ARRAY
END DATA
END
```

EXAMPLE 2. CSAS - Determine the unit size for k-eff= 0.95.

Consider the problem of example 1 above. Determine the size of the uranium metal pieces that will yield a k-effective of 0.95 ± 0.005. Maintain the H/D ratio of the cylinders and the original center-to-center spacings. The input data are

```
=CSAS4
SET UP 2C8 IN CSAS25
HANSEN-ROACH  INFHOMMEDIUM
URANIUM  1 DEN=18.76 1 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
END COMP
CRITICAL DIMENSION SEARCH FOR CASE 2C8 BARE
READ PARAMETERS  TME=1.0 FLX=YES FDN=YES FAR=YES
END PARAMETERS
READ GEOMETRY
CYLINDER 1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.87 -6.87 6.87 -6.87 6.505 -6.505
END GEOMETRY
READ ARRAY  NUX=2 NUY=2 NUZ=2  END ARRAY
END DATA
```

```
READ SEARCH  CRITICAL DIMENSION KEF=0.95 EPS=0.005
MORE
ALTER  UNIT=1 REG=1  ALL=1.0
+CON=0.0  -CON=-0.25
END SEARCH
END
```

The calculated results for this search are the following:

```
SEARCH PASS1  KEFF=9.95561E-01  +OR - 4.36660E-03  PARAMETER=0.00000E+00
SEARCH PASS2  KEFF=6.69976E-01  +OR - 3.95561E-03  PARAMETER=-2.50000E-01
SEARCH PASS3  KEFF=9.46110E-01  +OR - 4.09973E-03  PARAMETER=-3.49840E-02
```

The final configuration for region 1 is:

```
CYLINDER  1 1  5.5469  5.1942  -5.1942
```

EXAMPLE 3. CSAS25 - Determine the k-effective of an array of fuel assemblies.

Consider a 4 × 4 × 1 array of fuel assemblies in a square aluminum cask. Each assembly consists of a 17 × 17 × 1 array of zirconium-clad, 2.35%-enriched UO_2 fuel pins in a square pitched array. The UO_2 has a density of 9.21 g/cc. The pin diameter is 0.8 cm and is 366 cm long. The clad is 0.07 cm thick, and the pitch is 1.3 cm. Each fuel bundle is contained in a 0.65-cm-thick boral sheath. The bundles are separated by an edge-to-edge spacing of 1 cm. The array of bundles is centered in a 10-cm-thick aluminum cask whose inside dimensions are 0.5 cm beyond the outer edges of the fuel bundles. Determine the k-effective of a dry cask. Input data for this cask follow. The calculated k-effective for this system is 0.7940 ± 0.0035.

```
=CSAS25
SQUARE FUEL CASK EXAMPLE
HANSEN-ROACH LATTICECELL
UO2  1 DEN=9.21 1.0 293. 92235 2.35 92238 97.65 END
ZR  2 1 END
H2O  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
H2O  6 1 END
AL  5 1 END
END COMP
SQUAREPITCH  1.3 .8 1 3 .94 2 END
SQUARE FUEL CASK EXAMPLE USING DETAILED MOCKUP
READ PARAM  TME=12.0  NUB=YES FAR=YES GEN=153
END PARAM
READ GEOM
UNIT  1
COM='FUEL PIN'
CYLINDER 1 1 0.4  2P183.0
CYLINDER 2 1 0.47 2P183.07
CUBOID   3 1 4P0.65 2P183.07
```

```
UNIT 2
COM='FUEL ASSEMBLY'
ARRAY 1 2R-11.05 -183.07
REPLICATE 4 1 6*0.65 1
REPLICATE 3 1 6*0.5 1
GLOBAL
UNIT 3
COM='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'
ARRAY 2 2R-48.8 -184.22
REPLICATE 5 1 6R10.0 1
END GEOM
READ ARRAY ARA=1 NUX=17 NUY=17 NUZ=1 FILL F1 END FILL
ARA=2 NUX=4 NUY=4 NUZ=1 FILL F2 END FILL
END ARRAY
END DATA
END
```

EXAMPLE 4. CSAS - Determine the optimum pitch for an array of fuel assemblies

Consider the 4 × 4 × 1 array of fuel assemblies in a square aluminum cask described in example 3 above. Search for the assembly spacing that yields the maximum value of k-effective. Because the spacing between the assemblies is to be altered, the last region of unit 2 will be altered. In order to do this, the fuel assembly shroud cannot be defined as a replicate, because the code does not know the size of the array until later. In order to perform a pitch or dimension search, the code calculates the distance between the outermost region of the unit and the region interior to it. Therefore, the fuel assembly gap must be defined as a cuboid, and the water gap between assemblies can be entered as either a cuboid or a replicate. This search has been defined as an optimum dimension search. The calculated k-effectives for this system are listed after the following input data:

```
=CSAS4
SAMPLE FUEL CASK EXAMPLE
HANSEN-ROACH LATTICECELL
UO2 1 DEN=9.21 1.0 293. 92235 2.35 92238 97.65 END
ZR 2 1 END
H2O 3 1 END
B4C 4 0.367 END
AL 4 0.636 END
AL 5 1 END
END COMP
SQUAREPITCH 1.3 .8 1 3 .94 2 END
SQUARE FUEL CASK EXAMPLE WITH DETAILED MOCKUP
READ PARAM TME=6.0 NUB=YES FAR=YES GEN=103
END PARAM
READ GEOM
UNIT 1
COM='FUEL PIN'
CYLINDER 1 1 0.4 2P183.0
CYLINDER 2 1 0.47 2P183.07
CUBOID 3 1 4P0.65 2P183.07
```

```
UNIT 2
COM='FUEL ASSEMBLY'
ARRAY 1 2R-11.05 -183.07
CUBOID 4 1 4P11.7 2P183.72
REPLICATE 3 1 6*0.5 1
GLOBAL
UNIT 3
COM='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'
ARRAY 2 2R-48.8 -184.22
REPLICATE 5 1 6R10.0 1
END GEOM
READ ARRAY ARA=1 NUX=17 NUY=17 NUZ=1 FILL F1 END FILL
ARA=2 NUX=4 NUY=4 NUZ=1 FILL F2 END FILL
END ARRAY
END DATA
READ SEARCH OPTIMUM DIMENSION MORE
ALTER UNIT=2 REG=3 +X=1 -X=1 +Y=1 -Y=1
+CON=0.204918     -CON=-0.0409836
END SEARCH
END
```

The calculated results for this search are:

```
SEARCH PASS 1 KEFF=7.9334-01 + OR - 4.0541-03  PARAMETER= 0.00000E+00
SEARCH PASS 2 KEFF=8.4564-01 + OR - 4.0814-03  PARAMETER=-4.09836E-02
SEARCH PASS 3 KEFF=6.6002-01 + OR - 4.0889-03  PARAMETER= 2.04918E-01
SEARCH PASS 4 KEFF=6.9373-01 + OR - 3.9071-03  PARAMETER= 1.02459E-01
SEARCH PASS 5 KEFF=8.1896-01 + OR - 3.8378-03  PARAMETER=-2.04918E-02
CONVERGENCE WAS ACHIEVED ON PASS 2
```

The corresponding geometry for unit 2 was:

```
ARRAY NUMBER 1 1 11.05 -11.05 11.05 -11.05 183.07 -183.07
CUBOID           4 1 11.70 -11.70 11.70 -11.70 183.72 -183.72
CUBOID           3 1 11.70 -11.70 11.70 -11.70 183.72 -183.72
```

The highest k-effective is achieved on PASS number two, when the fuel assemblies are touching.

An alternative method of entering the search data for this problem is to define the search as an optimum pitch search and require that the spacing of the fuel pin cells remain unchanged. Because a pitch search is always conducted at the lowest array level, in this case the spacing between the pins in the fuel assembly (the outer region of unit 1), it is necessary to countermand the automatic alteration of the outer region of unit 1 by entering the KEEP command. Search constants must be entered for the X and Y faces to instruct the code to KEEP those dimensions unchanged. It is easier to use the keyword ALL, which applies the KEEP command to all of the faces since the optimum pitch search would have changed only the X and Y faces leaving the Z faces unchanged. The ALTER command must then be entered to instruct the search to alter the spacing between the fuel assemblies (region 3 of unit 2). Only the X and Y dimensions are to be altered; so the search constants are entered individually for those dimensions. It is acceptable to enter ALL=1 +Z=0 -Z=0 rather than +X=1 -X=1 +Y=1 -Y=1. It is not necessary to enter the constraints for an optimum pitch search (+CON= and -CON=). They were entered in this case to ensure that the alternative

data more nearly duplicate the optimum dimension search data of example 4. These alternative search data are:

```
READ SEARCH  OPTIMUM PITCH MORE
KEEP UNIT=1 REG=3 ALL=1
ALTER UNIT=2 REG=3 +X=1 -X=1 +Y=1 -Y=1
END SEARCH
```

C4.5.2.2 Run KENO V.a using CSAS2X or CSAS4X

CSAS2X and CSAS4X create a microscopic working format library and a mixing table that is passed to KENO V.a. The microscopic cross sections of the nuclides used in the unit cell geometry description are cell- weighted for use in mixture 500. Mixture 500 utilizes the cell-weighted cross sections that represent the heterogeneous system. CSAS2X executes KENO V.a and calculates k-effective for the problem. CSAS4X executes KENO V.a repeatedly to perform a search as specified in the search data.

EXAMPLE 1. CSAS2X - Calculate the k-effective of an array of fuel assemblies using cell-weighted cross sections.

Consider the 4 × 4 × 1 array of fuel assemblies in a square aluminum cask described in Sect. C4.5.2.1, example 3. Calculate the k-effective of the system by using the cell-weighted mixture 500 to represent the fuel pins in the fuel assembly. Note that mixtures 1, 2, and 3, representing UO_2, zirconium, and water, respectively, are used in the unit cell description. Cell-weighting is applied to the microscopic cross sections that are used in the cell, making them incorrect for use elsewhere. Because water is used both inside the cell and between the fuel assemblies, an additional mixture, mixture 6, has been added to represent the water between the fuel assemblies. The input data for this problem follow. The calculated k-effective is 0.79400 ± 0.0030.

```
=CSAS2X
SQUARE FUEL CASK EXAMPLE
HANSEN-ROACH LATTICECELL
UO2  1 DEN=9.21 1.0 293. 92235 2.35 92238 97.65 END
ZR  2 1 END
H2O  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
AL  5 1 END
H2O  6 1 END
END COMP
SQUAREPITCH  1.3 .8 1 3 .94 2 END
SAMPLE SQUARE FUEL CASK USING HOMOGENEOUS MOCKUP
READ PARAM  TME=12.0  NUB=YES FAR=YES GEN=153
END PARAM
READ GEOM
UNIT  2
COM='FUEL ASSEMBLY'
CUBOID  500 1 4P11.05 2P183.07
REPLICATE  4 1 6*0.65 1
REPLICATE  6 1 6*0.5 1
GLOBAL
UNIT 3
```

```
COM='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'
ARRAY  1 2R-48.8 -184.22
REPLICATE 5 1 6R10.0 1
END GEOM
READ ARRAY ARA=1 NUX=4 NUY=4 NUZ=1 FILL F2 END FILL
END ARRAY
END DATA
END
```

EXAMPLE 2. CSAS4X - Determine the optimum pitch for an array of fuel assemblies using cell-weighted cross sections.

Consider the 4 × 4 × 1 array of fuel assemblies in a square aluminum cask described using cell-weighted cross sections in example 3 above. Search for the assembly spacing that yields the maximum value of k-effective. The calculated k-effectives for this system are listed after the following input data.

```
=CSAS4X
SQUARE FUEL CASK EXAMPLE
HANSEN-ROACH LATTICECELL
UO2  1 DEN=9.21 1.0 293. 92235 2.35 92238 97.65 END
ZR  2 1 END
H2O  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
AL  5 1 END
H2O  6 1 END
END COMP
SQUAREPITCH  1.3 .8 1 3 .94 2 END
SAMPLE SQUARE FUEL CASK USING HOMOGENIZED MOCKUP
READ PARAM  TME=5.0  NUB=YES FAR=YES GEN=103
END PARAM
READ GEOM
UNIT  2
COM='FUEL ASSEMBLY'
CUBOID  500 1 4P11.05 2P183.07
REPLICATE  4 1 6*0.65 1
REPLICATE  6 1 6*0.5 1
GLOBAL
UNIT 3
COM='FUEL CASK CONTAINING 4X4 ARRAY OF ASSEMBLIES'
ARRAY  1 2R-48.8 -184.22
REPLICATE 5 1 6R10.0 1
END GEOM
READ ARRAY ARA=1 NUX=4 NUY=4 NUZ=1 FILL F2 END FILL
END ARRAY
END DATA
READ SEARCH  OPTIMUM PITCH  END SEARCH
END
```

The calculated results for this search are:

```
SEARCH PASS 1 KEFF=7.9303-01 + OR - 3.6699-03  PARAMETER= 0.00000E+00
SEARCH PASS 2 KEFF=8.4365-01 + OR - 3.9363-03  PARAMETER=-4.09836E-02
SEARCH PASS 3 KEFF=6.5431-01 + OR - 3.9188-03  PARAMETER= 2.04918E-01
SEARCH PASS 4 KEFF=7.0925-01 + OR - 3.6657-03  PARAMETER= 1.02459E-01
CONVERGENCE WAS ACHIEVED ON PASS 2
```

The corresponding geometry for unit 2 was:

```
CUBOID 500 1 11.05 -11.05 11.05 -11.05 183.07 -183.07
CUBOID   4 1 11.70 -11.70 11.70 -11.70 183.72 -183.72
CUBOID   6 1 11.70 -11.70 11.70 -11.70 184.22 -184.22
```

Thus, the highest k-effective is achieved when the fuel assemblies are touching.

C4.5.2.3 Run XSDRNPM using CSAS1X

XSDRNPM can be utilized to calculate the eigenvalue of a system without the necessity of manually preparing the cross sections and mixing table data by executing CSAS1X as shown in example 1 below.

EXAMPLE 1. CSAS1X - Calculate the eigenvalue of a system.

This example is a critical experiment of plutonium nitrate solution in a spherical stainless steel tank reflected by water. The plutonium is 95.4% wt ^{239}Pu, the remainder being ^{240}Pu. The fuel is a 0.52-M nitric acid solution of plutonium-nitrate, containing 24.4 g of heavy metal per liter of solution. Optional parameters were entered to decrease the number of mesh intervals and to use an S_4 calculation rather than S_8. The input data for this problem follow. The eigenvalue calculated by XSDRNPM is 1.00946.

```
=CSAS1X
CRITICAL PU(NO3)4 SOLUTION IN A SS SPHERICAL TANK REFLECTED BY WATER
HANSEN-ROACH  MULTIREGION
SOLNPU(NO3)4   1 24.4 .52 1 295 94239 95.4 94240 4.6 END
SS304  2 1.0  END
H2O  3 1  END
END COMP
SPHERICAL  VACUUM  REFLECTED  0  END
1 19.304 ONEEXTERMOD  2 19.426 ONEEXTERMOD  3 39.746 NOEXTERMOD
END ZONE
MORE DATA  ISN=4 SZF=1.5 END
END
```

C4.5.3 AUTOMATED CROSS-SECTION PREPARATION FOR USE BY SUBSEQUENT CODES

Many of the control modules available through the CSAS family of codes are used primarily to process cross sections for use by other codes. Some of these applications are described in the following subsections.

C4.5.3.1 Create a Microscopic AMPX Working Format Cross-Section Library for Use by KENO V.a

This example demonstrates the use of CSASN to create a microscopic, AMPX working format library on unit 4. KENO V.a can be executed as part of the same job and use the created cross sections, or the cross-section data set on unit 4 can be saved for later use. It should be noted that the cross-section library created by CSASN is a problem-dependent cross-section library containing only those nuclides specified in the problem. The resonance corrections applied to these cross sections are appropriate only for the specified problem. A simple demonstration of the use of CSASN to create the library and its use by KENO V.a is given in example 1.

EXAMPLE 1

Consider a problem consisting of four uranium metal cylinders that are 93.2% wt enriched, having a density of 18.76 g/cc. The cylinders are arranged in a 2 × 2 × 2 array. Each has a radius of 5.748 cm and a height of 10.765 cm. The center-to-center spacing in the horizontal plane (X-Y) is 13.74 cm, and the vertical center-to-center spacing is 13.01 cm. Use CSASN to create the microscopic, AMPX working format library for use by KENO V.a. The input data for this problem are:

```
=CSASN
CREATE A MICROSCOPIC AMPX WORKING FMT LIBRARY FOR 2C8
HANSEN-ROACH  INFHOMMEDIUM
URANIUM  1 DEN=18.76 1 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
END COMP
END
=KENOV
KENO V.A SAMPLE PROBLEM 1   CASE 2C8 BARE
READ PARAMETERS  TME=1.0 FLX=YES FDN=YES FAR=YES LIB=4
END PARAMETERS
READ MIXT MIX=1 92235 4.48006-2 92238 2.6578-3 92234 4.827-4
92236 9.57-5 END MIXT
READ GEOMETRY
CYLINDER 1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.87 -6.87 6.87 -6.87 6.505 -6.505
END GEOMETRY
READ ARRAY  NUX=2 NUY=2 NUZ=2  END ARRAY
END DATA
END
```

Note that the KENO V.a data given above are the same as those given in Sect. C4.5.2.1 except (1) the parameter data specify LIB=4 to instruct KENO V.a where to obtain the cross-section library and (2) the mixing table data must be supplied to KENO V.a. The number densities in the above data were hand-calculated. An easy method of obtaining the mixing table is to run the CSASN problem with PARM=CHECK, capture the output, and delete everything except the mixing table, which is shown in Fig. C4.5.1. This mixing table can then be edited into the correct format for the KENO V.a mixing table as shown in Figs. C4.5.2 and C4.5.3. Either of these mixing tables can be used in the place of the mixing table shown in example 1.

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY	N.I.T. POINTER
1	92235	4.48072E-02	274
1	92238	2.65827E-03	276
1	92234	4.82825E-04	273
1	92236	9.57448E-05	275

Figure C4.5.1 Mixing table from CSASN with PARM=CHECK

```
READ MIXT
MIX=1       92235  4.48072E-02
            92238  2.65827E-03
            92234  4.82825E-04
            92236  9.57448E-05
END MIXT
```

Figure C4.5.2 Mixing table from CSASN edited to KENO V.a format

```
READ MIXT
  MIX=1     92235  4.48072E-02
  MIX=1     92238  2.65827E-03
  MIX=1     92234  4.82825E-04
  MIX=1     92236  9.57448E-05
END MIXT
```

Figure C4.5.3 Mixing table from CSASN edited to KENO V.a format

C4.5.3.2 Create a Microscopic Cell-Weighted AMPX Working Format Cross-Section Library

EXAMPLE 1. Use CSAS1X to create a microscopic cell-weighted library.

This example demonstrates the use of CSAS1X to create a microscopic, cell-weighted, AMPX working format, cross-section library for use with KENO V.a. CSAS1X produces the microscopic, cell-weighted AMPX working format library on unit 3. All nuclides that are used in the mixtures specified in the unit cell are flux-weighted according to the characteristics of the unit cell and therefore should not be used in any mixtures utilized in KENO V.a other than the cell-weighted mixture. To utilize this cross-section library in KENO V.a, LIB=3 must be specified in the parameter data and an appropriate mixing table must be supplied. The input data for a CSAS1X problem follow:

```
=CSAS1X
PWR 15x15 LATTICECELL CALCULATION AT OPER. T&P
HANSEN-ROACH  LATTICECELL
UO2  1 0.95 1000.0 92235 3.3 92238 96.7 END
ZIRCALLOY  2 1.0 605.0 END
H2O  3 0.719 581.0 END
END COMP
SQUAREPITCH  1.430 0.92964 1 3 1.07188 2 0.94844 0 END
END
```

Because the printed mixing tables from CSASN and CSAS1X with PARM=CHECK do not contain mixing table data for the cell-weighted mixture, the number densities can be calculated by hand or another sequence (CSASIX or CSAS2X with PARM=CHECK) can be used to obtain the mixing table.

EXAMPLE 2. Use CSASIX to create a microscopic cell-weighted library.

A microscopic, cell-weighted, AMPX format library is created on unit 3 when CSASIX is run. The number densities of the cell-weighted mixture are volume averaged. To obtain the mixing table, CSASIX can be run with PARM=CHECK. The second mixing table (labeled COMPLETE MIXING TABLE) will contain the data for the cell-weighted mixture, but the mixture number will not be designated as mixture 500. Instead, it will be one larger than the largest mixture specified in the standard compositions data for the problem. In example 2, the cell-weighted mixture will be designated as mixture 4 in the complete mixing table. The CSASIX data are the following:

```
=CSASIX
PWR 15x15 LATTICECELL CALCULATION AT OPER. T&P
HANSEN-ROACH  LATTICECELL
UO2  1 0.95 1000.0 92235 3.3 92238 96.7 END
ZIRCALLOY  2 1.0 605.0 END
H2O  3 0.719 581.0 END
END COMP
SQUAREPITCH  1.430 0.92964 1 3 1.07188 2 0.94844 0 END
END
```

The second mixing table from CSASIX is shown in Fig. C4.5.4. In this problem, mixtures 1, 2, and 3 are the only mixtures defined in the input data, and all of them are used in the unit cell description. The cell-weighted mixture is always one larger than the largest defined mixture number; in this case the cell-weighted mixture is mixture 4. All of the mixtures defined in the standard compositions data are used in the unit cell description. Therefore, all of the nuclides used in this problem are cell-weighted, and it is not valid to use them in any mixture other than the cell-weighted mixture. In Fig. C4.5.5, the cell-weighted mixture is mixture 4. In KENO V.a, LIB=3 must be specified in the parameter data in order to access the cell-weighted cross sections. The cell-weighted mixture is usually defined as mixture 500 in KENO V.a.

The mixing table shown in Fig. C4.5.4 can be edited for use in KENO V.a as shown in Fig. C4.5.5. Because mixtures 1, 2, and 3 were used in the unit cell description, they should not be used in KENO V.a. The mixing table shown in Fig. C4.5.4 can be edited by eliminating the ENTRY column and inserting MIX= in front of each mixture number, and inserting a READ MIXT at the beginning of the data and an END MIXT at the end of the data. Since mixtures 1, 2, and 3 should not be used in KENO V.a, they can be edited out as shown in Fig. C4.5.5, or they can be left in the mixing table and not used in the KENO V.a geometry. It should be noted that the easiest way to use a cell-weighted mixture in KENO V.a is to run CSAS2X and utilize mixture number 500 to designate the cell-weighted mixture in the KENO V.a geometry data so the user does not need to create a mixing table.

COMPLETE MIXING TABLE

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY
1	92235	7.76007E-04
4	92235	2.57581E-04
1	92238	2.24522E-02
4	92238	7.45257E-03
1	8016	4.64564E-02
4	8016	1.54203E-02
3	308016	2.39971E-02
4	308016	1.34078E-02
2	40302	4.25156E-02
4	40302	4.07230E-03
3	1001	4.79943E-02
4	1001	2.68156E-02

Figure C4.5.4 Second mixing table from CSASIX

```
READ MIXT   MIX=500
  92235          2.57581E-04
  92238          7.45257E-03
   8016          1.54203E-02
 308016          1.34078E-02
  40302          4.07230E-03
   1001          2.68156E-02
END MIXT
```

Figure C4.5.5 Mixing table from CSASIX edited to KENO V.a format

EXAMPLE 3. Use CSASIX to create a microscopic cell-weighted library with extra mixtures.

This example is identical to example 2 except water and Zircaloy are to be used in the KENO V.a geometry description in addition to the cell-weighted mixture. The temperature of this water and Zircaloy is 450 K. Note that even if the temperatures of the water and Zircaloy were identical to the temperatures specified for the mixtures that are used in the LATTICECELL description, they would have to be specified again with a different mixture number in order to use them in the KENO V.a geometry data. The input data for this example are the following:

```
=CSASIX
PWR 15X15 LATTICECELL CALCULATION AT OPER. T&P
HANSEN-ROACH  LATTICECELL
UO2  1 0.95 1000.0 92235 3.3 92238 96.7 END
ZIRCALLOY  2 1.0 605.0 END
H2O  3 0.719 581.0 END
ZIRCALLOY  4 1.0 450.0 END
H2O  5 0.847 450.0 END
```

```
END COMP
SQUAREPITCH  1.430 0.92964 1 3 1.07188 2 0.94844 0 END
END
```

In this example, the cell-weighted mixture will be identified as mixture 7. The mixing tables from CSASIX are shown in Fig. C4.5.6.

MIXING TABLE FROM STANDARD COMPOSITIONS DATA

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY	N.I.T. POINTER
1	92235	7.76007E-04	274
1	92238	2.24522E-02	276
1	8016	4.64564E-02	21
3	308016	2.39971E-02	21
5	508016	2.39971E-02	21
2	40302	4.25156E-02	95
4	440302	4.25156E-02	95
3	1001	4.79943E-02	4
5	501001	4.79943E-02	4

COMPLETE MIXING TABLE

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY
1	92235	7.76007E-04
6	92235	2.57581E-04
1	92238	2.24522E-02
6	92238	7.45257E-03
1	8016	4.64564E-02
6	8016	1.54203E-02
3	308016	2.39971E-02
6	308016	1.34078E-02
5	508016	2.82692E-02
2	40302	4.25156E-02
6	40302	4.07230E-03
4	440302	4.25156E-02
3	1001	4.79943E-02
6	1001	2.68156E-02
5	501001	5.65385E-02

Figure C4.5.6 Mixing tables from CSASIX

In order to use the microscopic, cell-weighted, cross-section library in KENO V.a, LIB=3 must be specified in the KENO V.a parameter data because the CSAS sequences whose names contain an X write the microscopic, cell-weighted, cross-section library on unit 3. The appropriate mixing table for KENO V.a can be created by capturing and editing the COMPLETE MIXING TABLE. The order of scatter should be specified in the KENO V.a mixing table. KENO V.a always defaults to P1 scattering, but CSAS sets the order of scattering based on the cross-section library (presently P1 for the Hansen-Roach 16-group library and P3

for all other libraries). In KENO V.a the order of scattering is set using the parameter SCT= in the mixing table data. The resultant mixing table is shown in Figs. C4.5.7 through C4.5.9 below.

```
READ MIXT        SCT=1
  MIX=1          92235      7.76007E-04
  MIX=500        92235      2.57581E-04
  MIX=1          92238      2.24522E-02
  MIX=500        92238      7.45257E-03
  MIX=1          8016       4.64564E-02
  MIX=500        8016       1.54203E-02
  MIX=3          308016     2.39971E-02
  MIX=500        308016     1.34078E-02
  MIX=5          508016     2.82692E-02
  MIX=2          40302      4.25156E-02
  MIX=500        40302      4.07230E-03
  MIX=4          440302     4.25156E-02
  MIX=3          1001       4.79943E-02
  MIX=500        1001       2.68156E-02
  MIX=5          501001     5.65385E-02
END MIXT
```

Figure C4.5.7 KENO V.a mixing table using all CSASIX entries

In Fig. C4.5.7 all of the entries from the CSASIX COMPLETE MIXING TABLE have been edited to conform to the KENO V.a format. In the CSASIX output, mixture 6 is the cell-weighted mixture. Its mixture number has been changed to 500, but it is not necessary to do so. CSASIX, CSAS2X, and CSAS4X automatically label the cell-weighted mixture cross section as mixture 500 on the macroscopic, cross-section library. This example arbitrarily redefined mixture 6 to be mixture 500 so a user would recognize that cell-weighted cross sections were used in the geometry. MIXTURES 1, 2, AND 3 SHOULD NOT BE USED IN THE KENO V.a GEOMETRY DATA BECAUSE THEY HAVE BEEN FLUX-WEIGHTED OVER THE CELL TO CREATE A CELL-WEIGHTED CROSS SECTION THAT ALLOWS THE HETEROGENEOUS SYSTEM TO BE REPRESENTED AS A HOMOGENEOUS MATERIAL.

```
READ MIXT        SCT=1
  MIX=500        92235      2.57581E-04
  MIX=500        92238      7.45257E-03
  MIX=500        8016       1.54203E-02
  MIX=500        308016     1.34078E-02
  MIX=5          508016     2.82692E-02
  MIX=500        40302      4.07230E-03
  MIX=4          440302     4.25156E-02
  MIX=500        1001       2.68156E-02
  MIX=5          501001     5.65385E-02
END MIXT
```

Figure C4.5.8 KENO V.a mixing table using only mixtures 4, 5 and 6 from CSASIX

In Fig C4.5.8, mixtures 1, 2, and 3 have been removed because they should not be used in the KENO V.a geometry description.

```
READ MIXT          SCT=1
  MIX=4            440302      4.25156E-02
  MIX=5            508016      2.82692E-02
                   501001      5.65385E-02
  MIX=500          92235       2.57581E-04
                   92238       7.45257E-03
                   8016        1.54203E-02
                   308016      1.34078E-02
                   40302       4.07230E-03
                   1001        2.68156E-02
END MIXT
```

Figure C4.5.9 Condensed KENO V.a mixing table using only mixtures 4, 5, and 6 from CSASIX

The mixing table shown in Fig. C4.5.9 has been abbreviated by reordering the data to group all of the components of a mixture together and specifying the mixture number only once for each mixture.

C4.5.3.3 Create a Macroscopic, AMPX Working Format, Cross-Section Library and a Macroscopic, MORSE/KENO, Cross-Section Library

Example 1 illustrates the use of CSASI to produce a macroscopic, AMPX working format, cross-section library on unit 2 for use by KENO V.a. The ID numbers in this library are the mixtures specified in the standard composition data. To utilize this library in KENO V.a, LIB=2 must be entered in the parameter data, and a mixing table must be provided. The mixing table nuclide ID numbers are the mixture numbers used in the CSASI problem. The number density is a multiplication factor applied to the macroscopic cross sections. Entering a number density of 1.0 causes the cross sections to remain unchanged. Consider a CSASI problem that defines three mixtures and mixture 2 is full-density water. If KENO V.a is to use these cross sections and needs to use half-density water in addition to all of the other defined mixtures, mixture 4 can be defined as half-density water, and the mixing table for KENO V.a would be:

```
READ MIXT MIX=1 1 1.0 MIX=2 2 1.0 MIX=3 3 1.0 MIX=4 2 0.5 END MIXT
```

LIB=2 would be entered in the parameter data.

EXAMPLE 1

Consider a problem that consists of four 20.96-kg, 93.2% enriched uranium metal cylinders, density 18.76 g/cc, and four 5-l Plexiglas bottles filled with highly enriched uranyl nitrate solution at 415 g/l, a specific gravity of 1.555, and 0.39 mg of excess nitrate per gram of solution. The isotopic content of the uranium metal is 93.2% wt ^{235}U, 5.6% wt ^{238}U, 1.0% wt ^{234}U, and 0.2% wt ^{236}U. The uranium isotopic content of the nitrate solution is 92.6% wt ^{235}U, 5.9% wt ^{238}U, 1.0% wt ^{234}U, and 0.5% wt ^{236}U. Each metal unit has a diameter of 11.496 cm, a height of 10.765 cm, and an edge-to-edge spacing of 1.684 cm horizontally and 1.685 cm vertically. The uranyl nitrate solution is contained in a Plexiglas cylinder having an ID of 19.05 cm and an inside height of 17.78 cm. The Plexiglas walls are 0.635 cm thick. The solution units have an edge-to-edge spacing of 1.43 cm horizontally and vertically. The center-to-center spacing between the metal and solution units is 17.465 cm.

CSASI creates a macroscopic, AMPX working format library on unit 2 and a macroscopic, MORSE/KENO library on unit 14. To use the macroscopic, AMPX working format library in KENO V.a, enter LIB=2 in the parameter data, and enter the following mixing table:

READ MIXT MIX=1 1 1.0 MIX=2 2 1.0 MIX=3 3 1.0 END MIXT

The total input data to run CSASI, followed by KENO V.a are given below:

```
=CSASI
SET UP 4AQUEOUS 4 METAL IN CSAS25
HANSEN-ROACH   INFHOMMEDIUM
URANIUM        1 0.985 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
SOLNUO2(NO3)2  2 415 9.783-3 SPG=1.555 1.0 293 92235 92.6 92238 5.9
                                    92234 1.0  92236 0.5 END
PLEXIGLAS     3 END
END COMP
END
=KENOV
KENO VA  4 AQUEOUS 4 METAL MIXED UNITS USING CSASI MACRO WORKING LIBR
READ PARAM  FLX=YES FDN=YES  TME=2.0 LIB=2
END PARAM
READ MIXT MIX=1 1 1.0 MIX=2 2 1.0 MIX=3 3 1.0 END MIXT
READ GEOM
BOX TYPE 1
CYLINDER  2 1 9.525 8.89 -8.89
CYLINDER  3 1 10.16 9.525 -9.525
CUBOID  0 1 10.875 -10.875 10.875 -10.875 10.24 -10.24
BOX TYPE  2
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 6.59 -15.16 6.225 -14.255
BOX TYPE  3
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 15.16 -6.59 6.225 -14.255
BOX TYPE  4
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 6.59 -15.16 14.255 -6.225
BOX TYPE  5
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 15.16 -6.59 14.255 -6.225
END GEOM  READ ARRAY  NUX=2 NUY=2 NUZ=2  LOOP
1 3R2 1 2 1 1 2 1  2 9R1  3 3R1 2 2 1 3R1  4 6R1 2 2 1  5 3R1 2 2 1 2 2 1
END ARRAY
END DATA
END
```

Example 2 illustrates the use of CSASI to produce a macroscopic, MORSE/KENO format, cross-section library on unit 14 for use by KENO V.a. The ID numbers in this library are the mixtures specified in the standard composition data. To utilize this library in KENO V.a, XSC=14 must be entered in the parameter data, and a mixing table is not provided. The mixtures used in the KENO V.a geometry must correspond to the mixtures defined in the CSASI data.

EXAMPLE 2

Consider the problem described in example 1. Produce a macroscopic, MORSE/KENO format, cross-section library on unit 14 for use by KENO V.a. To utilize this library in KENO V.a, XSC=14 must be entered in the parameter data, and a mixing table is not provided. The mixture numbers used in the KENO V.a geometry must correspond to the mixtures defined in the standard composition data of CSASI. The input data required to run this problem are the following:

```
=CSASI
SET UP 4AQUEOUS 4 METAL IN CSAS25
HANSEN-ROACH   INFHOMMEDIUM
URANIUM        1 0.985 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
SOLNUO2(NO3)2  2 415 9.783-3 SPG=1.555 1.0 293 92235 92.6 92238 5.9
                                       92234 1.0  92236 0.5 END
PLEXIGLAS      3 END
END COMP
END
=KENOV
KENO VA   4 AQUEOUS 4 METAL MIXED UNITS USING CSASI MACRO WORKING LIBR
READ PARAM  FLX=YES FDN=YES  TME=2.0 XSC=14
END PARAM
READ GEOM
BOX TYPE 1
CYLINDER  2 1 9.525 8.89 -8.89
CYLINDER  3 1 10.16 9.525 -9.525
CUBOID  0 1 10.875 -10.875 10.875 -10.875 10.24 -10.24
BOX TYPE  2
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 6.59 -15.16 6.225 -14.255
BOX TYPE  3
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 15.16 -6.59 6.225 -14.255
BOX TYPE  4
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 6.59 -15.16 14.255 -6.225
BOX TYPE  5
CYLINDER  1 1 5.748 5.3825 -5.3825
CUBOID  0 1 6.59 -15.16 15.16 -6.59 14.255 -6.225
END GEOM  READ ARRAY  NUX=2 NUY=2 NUZ=2  LOOP
1 3R2 1 2 1 1 2 1  2 9R1  3 3R1 2 2 1 3R1  4 6R1 2 2 1  5 3R1 2 2 1 2 2 1
END ARRAY
END DATA
END
```

The cross-section libraries created by CSASI are

1. a macroscopic AMPX working format library on unit 2,
2. a macroscopic MORSE/KENO format library on unit 14, and
3. a microscopic AMPX working format library on unit 4.

C4.5.3.4. Create a Macroscopic, Cell-Weighted, AMPX Working Format Library and a Macroscopic, Cell-Weighted, MORSE/KENO Library

This section illustrates the use of CSASIX to produce cell-weighted, macroscopic libraries for use with a subsequent code. The problem-dependent cross-section libraries created by CSASIX are:

1. A macroscopic, cell-weighted, AMPX working format library on unit 2.
   To use this library in KENO V.a, set LIB=2 in the parameter data and enter a mixing table using the mixture numbers as the nuclide ID's and number densities of 1.0.

2. A microscopic, cell-weighted, AMPX working format library on unit 3.
   To use this library in KENO V.a, set LIB=3 in the parameter data and enter a mixing table using the appropriate nuclide IDs and number densities. If the cell-weighted mixture is to be used, its component nuclides and correct number densities must be included in the mixing table.

3. A microscopic, AMPX working format library on unit 4.
   To use this library in KENO V.a, set LIB=4 in the parameter data and enter the mixing table data. None of the cross sections in this library are cell weighted.

4. A macroscopic cell-weighted MORSE/KENO format library on unit 14.
   To use this library in KENO V.a, set XSC=14 in the parameter data and omit LIB. Do not provide a mixing table. The cell-weighted cross section is mixture 500.

Example 1 shows the use of the macroscopic, cell-weighted, AMPX working format library. Example 2 shows the use of the macroscopic, cell-weighted, MORSE/KENO library.

EXAMPLE 1

This example illustrates the use of CSASIX to create a cell-weighted macroscopic library for use in KENO V.a. The CSASIX data define the materials used to describe a flooded 3 × 3 array of PWR fuel assemblies. The center-to-center spacing between the assemblies is 12 cm. Each fuel assembly is a 17 × 17 array of fuel pins contained in a 0.29-cm-thick boral sheath. The fuel is 3.2% enriched UO_2, density = 10.41 g/cc. The fuel OD is 0.819 cm, the gap OD is 0.836 cm, and the clad OD is 9.50 cm. The fuel pin pitch is 1.26 cm. The fuel pin length is 375 cm.

Note that the cell-weighted macroscopic library is specified in KENO V.a by entering LIB=2 in the parameter data and entering mixing table data. The KENO V.a geometry uses mixture 500 to represent the homogenized pin cells inside each fuel assembly. Unit 1 in the geometry describes the fuel assembly and the spacing cuboid that define the center-to-center spacing between assemblies. Unit 2 defines the water-reflected array of fuel assemblies. Because mixture 3 was used in the unit cell definition in CSASIX, another water, mixture 5, was defined to be used in the KENO V.a geometry because mixtures 1, 2, and 3 have been cell-weighted and cannot be used in the geometry. The input data are the following:

```
=CSASIX
FLOODED PWR FUEL ASSEMBLY (17x17) AT ROOM TEMP
27GROUPNDF4  LATTICECELL
UO2  1  DEN=10.41 1.0 293. 92235 3.2 92238 96.8 END
ZIRCALLOY  2  1.0  END
H2O  3  1.0  END
ARBMTL-B4C  2.64  2  1  1  0  5000  4  6012  1  4  0.015  END
```

```
ARBMTL-AL 2.64 1 0 0 0 13027 100.0 4 0.985 END
H2O 5 1.0 END
END COMP
SQUAREPITCH 1.26 0.819 1 3 0.950 2 0.836 0 END
END
=KENOV
3 X 3 ARRAY OF FLOODED FUEL ASSEMBLIES
READ PARAM LIB=2 TME=5.0 END PARAM
READ MIXT MIX=1 1 1.0 MIX=2 2 1.0 MIX=3 3 1.0 MIX=4 4 1.0 MIX=5 5 1.0
END MIXT
READ GEOM
UNIT 1
COM='HOMOGENIZED FUEL ASSEMBLY'
CUBOID 500 1 4P10.71 375.0 0.0
CUBOID 4 1 4P11.0 375.29 -0.29
CUBOID 5 1 4P12.0 375.29 -0.29
GLOBAL UNIT 2
COM='WATER REFLECTED 3X3 ARRAY OF FUEL ASSEMBLIES'
ARRAY 1 3*0.0
REPLICATE 5 2 6P3.0 10
END GEOM
READ ARRAY ARA=1 NUX=3 NUY=3 NUZ=1 FILL F1 END FILL END ARRAY
READ BIAS ID=500 2 11 END BIAS
END
```

EXAMPLE 2

This example is the same as example 1 except the KENO V.a problem will use the macroscopic, MORSE/KENO library. The input data for CSASIX and KENO V.a are given below. Note that XSC=14 is specified in the KENO V.a data, and a mixing table is not entered. However, the mixture numbers used in the geometry correspond to the mixture numbers defined in the standard composition library. Because water, mixture 3, was used in the unit cell definition in CSASIX, another water, mixture 5, has to be defined to be used in the KENO V.a geometry because mixture 3 has been cell-weighted along with mixtures 1 and 2. The input data follow:

```
=CSASIX
FLOODED PWR FUEL ASSEMBLY (17x17) AT ROOM TEMP
27GROUPNDF4 LATTICECELL
UO2 1 DEN=10.41 1.0 293. 92235 3.2 92238 96.8 END
ZIRCALLOY 2 1.0 END
H2O 3 1.0 END
ARBMTL-B4C 2.64 2 1 1 0 5000 4 6012 1 4 0.015 END
ARBMTL-AL 2.64 1 0 0 0 13027 100.0 4 0.985 END
H2O 5 1.0 END
END COMP
SQUAREPITCH 1.26 0.819 1 3 0.950 2 0.836 0 END
END
=KENOV
3 X 3 ARRAY OF FLOODED FUEL ASSEMBLIES USING MORSE/KENO LIBRARY
READ PARAM XSC=14 TME=5.0 END PARAM
```

```
READ GEOM
UNIT 1
COM='HOMOGENIZED FUEL ASSEMBLY'
CUBOID  500 1 4P10.71 375.0 0.0
CUBOID    4 1 4P11.0  375.29 -0.29
CUBOID    5 1 4P12.0  375.29 -0.29
GLOBAL UNIT 2
COM='WATER REFLECTED 3X3 ARRAY OF FUEL ASSEMBLIES'
ARRAY 1 3*0.0
REPLICATE 5 2 6R3.0 10
END GEOM
READ ARRAY  ARA=1 NUX=3 NUY=3 NUZ=1 FILL F1 END FILL END ARRAY
READ BIAS ID=500 2 11 END BIAS
END
```

C4.5.4 CREATE AND USE TWO CELL-WEIGHTED MIXTURES IN A PROBLEM

Consider a problem in which a stainless steel cylinder with an ID of 56 cm and an inside height of 91 cm is filled with pellets of UO_2 in borated water. The steel is 0.125 cm thick. The spherical 2.57%-enriched UO_2 pellets have a diameter of 1.07 cm and are arranged in a triangular pitch array with a pitch of 1.13 cm. The spherical 2.96%-enriched UO_2 pellets have a diameter of 1.07 cm and are arranged in a triangular pitch array with a pitch of 1.12 cm. The cylindrical tank is filled half full of the 2.96% pellets in borated water, and the remainder is filled with the 2.57%-enriched pellets in borated water.

Example 1 demonstrates how this problem can be calculated by running a CSASIX case for each of the pellet arrays, combining the macroscopic, AMPX working format, cell-weighted libraries using the AMPX module WAX to combine the two libraries. The combined AMPX working format library can then be used to run the KENO V.a problem. It should be noted that this procedure cannot be stacked together to run in a single SCALE execution because the second CSASIX would destroy the library created by the first CSASIX. Example 2 demonstrates how to add an additional WAX step to move the library created by the first CSASIX so that the steps can be stacked together to run in a single SCALE execution.

EXAMPLE 1

STEP 1. Run CSASIX to obtain a macroscopic, cell-weighted, AMPX working format library on unit 2. The mixture 500 on this library represents the 2.57%- enriched pellets in borated water. The input data for this step are given below. The user must save the library that is created on unit 2. The input data are

```
=CSASIX
2.57% ENR UO2 PELLETS IN 3500 PPM BORATED WATER
27GROUPNDF4  LATTICECELL
UO2    1  .925  283 92235 2.57 92238 97.43 END
H2O  2 1.0 283 END
ARBMBACID  2.0017-2 3 1 1 0 5000 1 1001 3 8016 3  2  1.0
          283 5010 18.32 5011 81.68 END
END COMP
SPHTRIANGP 1.13 1.07  1  2 END
END
```

STEP 2. Run CSASIX to obtain a macroscopic, cell-weighted, AMPX working format library on unit 2. The mixture 500 on this library represents the 2.96%-enriched pellets in borated water. The input data for this step are given below. The user must save the library that is created on unit 2. Note that the problem that is to be run by KENO V.a must have stainless steel available to define the cylindrical container. Therefore, stainless steel must be defined in one of the CSASIX problems. The input data are the following:

```
=CSASIX
2.96% ENR UO2 PELLETS IN 3500 PPM BORATED WATER
27GROUPNDF4  LATTICECELL
UO2    1  .925  283 92235 2.96 92238 97.04 END
H2O  2 1.0 283 END
ARBMBACID  2.0017-2 3 1 1 0 5000 1 1001 3 8016 3  2  1.0
          283 5010 18.32 5011 81.68 END
SS304 3 1.0 283 END
END COMP
SPHTRIANGP 1.12   1.07  1  2 END
END
```

STEP 3. Run WAX to combine the macroscopic, cell-weighted, AMPX working format libraries and rename the mixture 500s to distinguish between them. In this case, mixture 500 for the 2.57%-enriched pellets has been renamed to 501 and mixture 500 for the 2.96%-enriched pellets has been renamed to 502. The 2.57% library is mounted on unit 33, the 2.96% library is mounted on unit 34, and the combined library is written out on unit 4. It is not necessary to rename both of the mixture 500s. One of them can be carried through as 500; the other one, as some other number. WAX can be used to rename all of the mixtures on the library. The cell-weighted mixture created by the CSAS modules is always mixture 500, but WAX can be used to rename it to any desired number. The mixture numbers on the WAX library are the nuclide ID numbers that must be used in the KENO V.a mixing table when multiple cell-weighted mixtures are used. The user must save the library that is created on unit 4 so that it will be available for use in KENO V.a. The input data follow:

```
=WAX
0$$ 4 34
1$$ 2   1T
2$$ 33 1  2T
3$$ 500
4$$ 501    3T
2$$ 34 2  2T
3$$ 3 500
4$$ 3 502   3T
END
```

STEP 4. Use the combined macroscopic, AMPX working format library to run KENO V.a. Use mixture 501 for the homogenized, cell-weighted, 2.57%-enriched pellets, and use mixture 502 for the homogenized, cell-weighted, 2.96%-enriched pellets. The KENO V.a data are:

```
=KENOV
PROBLEM USING TWO CELL_WEIGHTED MIXTURES (502 IS 2.96% & 501 IS 2.57%)
READ PARAM  FLX=YES LIB=4    END PARAM
READ MIXT  MIX=3 3 1.0 MIX=501 501 1.0  MIX=502 502 1.0 END MIXT
```

```
READ GEOM
CYLINDER 502 1 38.0 45.5 0.0
CYLINDER 501 1 38.0 91.0 0.0
CYLINDER   3 1 38.125 91.0 -0.125
END GEOM
END DATA
END
```

Alternatively, KENO V.a could have been set up to define mixtures 1 and 2 as the cell-weighted mixtures as follows:

```
=KENOV
PROBLEM USING TWO CELL_WEIGHTED MIXTURES (502 IS 2.96% & 501 IS 2.57%)
READ PARAM  FLX=YES LIB=4    END PARAM
READ MIXT  MIX=3 3 1.0 MIX=1 501 1.0  MIX=2 502 1.0 END MIXT
READ GEOM
CYLINDER   2 1 38.0 45.5 0.0
CYLINDER   1 1 38.0 91.0 0.0
CYLINDER   3 1 38.125 91.0 -0.125
END GEOM
END DATA
END
```

EXAMPLE 2

This example is the same as example 1 except a WAX step has been added to move the library created by the first CSASIX from unit 2 to unit 12 so that the steps can be stacked together and run in a single SCALE execution. Because all of the steps are stacked together, unit 12 is used instead of unit 33 because unit 12 is defined in the SCALE procedure and will be automatically passed to the next step. The SCALE input data are:

```
=CSASIX
2.57% ENR UO2 PELLETS IN 3500 PPM BORATED WATER
27GROUPNDF4  LATTICECELL
UO2    1  .925  283 92235 2.57 92238 97.43 END
H2O  2 1.0 283 END
ARBMBACID  2.0017-2 3 1 1 0 5000 1 1001 3 8016 3  2  1.0
          283 5010 18.32 5011 81.68 END
END COMP
SPHTRIANGP 1.13 1.07  1  2 END
END
=WAX
0$$ 12 2
1$$ 1   1T
2$$ 2  1  2T
3$$ 500
4$$ 500     3T
END
=CSASIX
2.96% ENR UO2 PELLETS IN 3500 PPM BORATED WATER
27GROUPNDF4  LATTICECELL
```

```
UO2   1  .925  283 92235 2.96 92238 97.04 END
H2O  2 1.0 283 END
ARBMBACID  2.0017-2 3 1 1 0 5000 1 1001 3 8016 3  2  1.0
          283 5010 18.32 5011 81.68 END
SS304 3 1.0 283 END
END COMP
SPHTRIANGP 1.12   1.07  1  2 END
END
=WAX
0$$ 4  2
1$$ 2   1T
'RENAME MIXTURE 500 TO MIXTURE 501
2$$ 12 1  2T
3$$ 500
4$$ 501     3T
'RENAME MIXTURE 500 TO MIXTURE 502.  MIXTURE 3 REMAINS MIXTURE 3
2$$ 2  2  2T
3$$ 3 500
4$$ 3 502   3T
END
=KENOV
PROBLEM USING TWO CELL-WEIGHTED MIXTURES (502 IS 2.96% & 501 IS 2.57%)
READ PARAM  FLX=YES LIB=4    END PARAM
READ MIXT  MIX=3 3 1.0 MIX=501 501 1.0  MIX=502 502 1.0 END MIXT
READ GEOM
CYLINDER 502 1 38.0 45.5 0.0
CYLINDER 501 1 38.0 91.0 0.0
CYLINDER   3 1 38.125 91.0 -0.125
END GEOM
END DATA
END
```

C4.5.5. CREATE A CELL-WEIGHTED MIXTURE REPRESENTING A NONHOMOGENEOUS FUEL ASSEMBLY

Calculate the k-effective of a 3 × 3 × 3 array of the fuel assembly shown in Fig. C4.5.10. The spacing between the assemblies is 2 cm and is filled with water. The array is reflected by 31 cm of water on all faces. Each assembly is a 15 × 15 array of fuel pins with 16 water holes and a central instrumentation hole. The fuel pins are 1.98%-enriched UO_2 at 10.138 g/cc and are 0.94 cm in diameter. The active fuel length is 365.76 cm. The zircaloy-4 clad is 0.545 cm OR × 0.4875 cm IR. The fuel rod pitch is 1.44 cm.

The fuel assembly shrouds are 0.16-cm-thick 304 stainless steel. The IDs are 21.6 cm in cross section. The interstices between the rods are filled with water.

To obtain the correct cell-weighted cross sections for this assembly, run CSASIX to define the cell-weighted fuel pin cell. Then run XSDRNPM to account for the water holes.

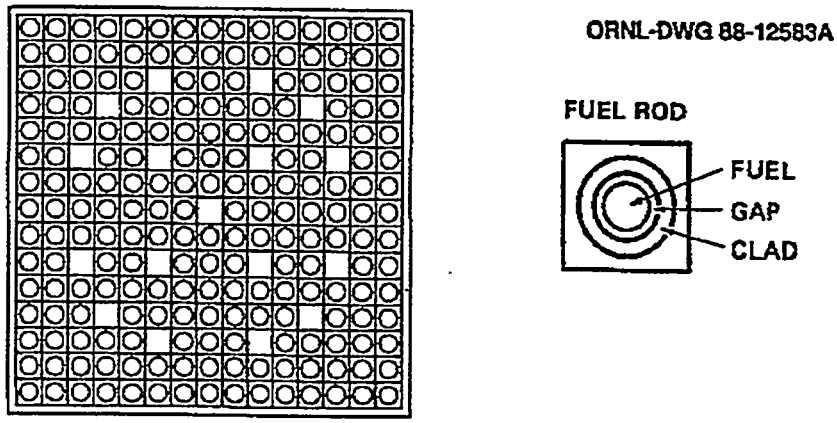


Figure C4.5.10 1.98% enriched UO_2 fuel assembly

The input data for CSASIX are given below. Mixtures 1, 2, and 3 are used in the unit cell description, causing them to be cell-weighted and therefore unacceptable for use by a subsequent code. The cross sections for the stainless steel shroud and water holes must be defined so they will be available for use by a subsequent code, XSDRNPM in this case. Mixture 4 is the stainless steel for the fuel assembly shroud, and mixture 5 is the water for the instrumentation hole and water holes. XSDRNPM will create a cell-weighted cross section representing the interior of the fuel assembly. This procedure will use the cell-weighted cross section from CSASIX and the mixture 5 water. Therefore mixture 5 will be cell-weighted and cannot be used in a subsequent code. Since water is to be used in the KENO V.a calculation that uses the cell-weighted cross sections from XSDRNPM, a mixture 6 that is identical to mixtures 3 and 5 must be added to the CSASIX data. The input data follow:

```
=CSASIX
CREATE CELL WEIGHTED CROSS SECTION FOR FUEL PIN CELL
27GROUPNDF4  LATTICECELL
UO2       1 .925   293 92235 1.98 92238 98.02 END
ZIRCALLOY  2 1.0    293 END
H2O       3 1.0    293 END
SS304     4 1.0    293 END
H2O       5 1.0    293 END
H2O       6 1.0    293 END
END COMP
SQUAREPITCH  1.44 .94 1 3 1.09 2 .975 0 END
END
```

The input data for XSDRNPM are given below. Each assembly contains 225 units, 17 of which are water holes (the instrumentation hole is treated as a water hole). The geometry for XSDRNPM is an infinite cylinder of water having an area equal to the area of the central instrumentation hole. The ratio of fuel to water in the assembly is (225-17)/17; so the area of the fuel region surrounding the water is (225-17)/17 times the area of the water region. The OR of the water hole is 0.81243 cm, and the OR of the fuel region is 2.95566 cm. XSDRNPM will use the macroscopic, cell-weighted, cross-section library that was created by CSASIX on unit 2 and will create a new macroscopic cell-weighted cross-section library on unit 3 as specified

in the 0$$ array. Note that XSDRNPM will process only those mixtures that are used in the problem. All mixtures that are to be passed through XSDRNPM for use by a subsequent code must be included in every mixture used in XSDRNPM and should have a very small number density (1.0–20). Therefore, mixtures 4 and 6 must be added to both the water (mixture 5 from CSASIX) and the cell-weighted pin cell mixture (mixture 500 from CSASIX) with a negligible number density. The macroscopic, cell-weighted, cross-section library from CSASIX is read from unit 2, and the resultant cell-weighted cross-section library is written on unit 3. The 3$$ array must specify that a weighting calculation is to be done.

```
=XSDRNPM
USE CELL WTD PIN CELL XSECS AND CREATE CELL WTD FUEL ASSMBLY XSECS
0$$ A3 2 E
1$$  2 2 20 1 3 4 6 8 3 1 E
2$$  A7 -1 E
3$$  1 E
4$$  -1 27 E  1T
13$$   1   2  1 2 1 2
14$$   5 500  4 4 6 6
15** 1.0 1.0  4R1.-20   2T
33## F1.0 4T
35** 9I0 9I0.812433 2.95566
36$$ 10R1 10R2
51$$ 25I1 27 5T
END
```

The input data for KENO V.a are given below. The cell-weighted cross-section library is read from unit 3. This library contains mixtures 5, 500, 4, and 6. Mixtures 5 and 500 have been cell-weighted to represent the heterogeneous fuel assembly. To create a cell-weighted mixture that represents the fuel assembly, the number densities associated with mixtures 5 and 500 are their respective volume fractions in the fuel assembly. In this problem, mixture 1 is the homogenized fuel assembly mixture. Mixture 4 is the stainless steel shroud, and mixture 6 is water. The number density is 1.0 for mixtures 4 and 6.

```
=KENOVA
WATER REFLECTED 3X3X3 ARRAY OF HOMOGENIZED FUEL ASSEMBLIES
READ PARAM LIB=3 TME=10 END PARAM
READ MIXT MIX=1 5 0.075556 500 0.924444  MIX=4 4 1.0 MIX=6 6 1.0 END MIXT
READ GEOM
UNIT 1
COM='CELL-WEIGHTED HOMOGENIZED FUEL ASSEMBLY WITH ZIRCALLOY SHROUD
AND H2O'
CUBOID 1 1 4P10.8 365.76 0.0
REPLICATE 4 1 6R0.16 1
REPLICATE 6 1 6R1.0 1
GLOBAL UNIT 2
ARRAY 1 3*0.0
REPLICATE 6 2 6R3.0 10
END GEOM
READ ARRAY NUX=3 NUY=3 NUZ=3 FILL F1 END FILL END ARRAY
READ BIAS ID=500 2 11 END BIAS
END DATA
END
```

C4.5.6 SEARCH DATA

Search data must be entered for CSAS4 and CSAS4X. The search data enable the code to perform a search according to the instructions specified by the user. The code begins reading search data when it encounters the words READ SEARCH and continues reading search data until it encounters the words END SEARCH. Search data consist of the search type specification and auxiliary search commands.

C4.5.6.1. Search Type Specification

These data are used to define the type of search and to set the parameters that provide limits for the search. The search type specification data consist of (a) a search descriptor, (b) the search type, and (c) optional search parameters as described below.

C4.5.6.1a SEARCH DESCRIPTOR is used to define the search mode.
Use OPTIMUM, OPTI, OPT, or OPTM if the maximum value of k-effective is to be determined.
Use CRITICAL, CRIT, or CRTL if a specified value of k-effective is to be obtained.
Use MINIMUM, MINI, MINM, or MIN if the minimum value of k-effective is to be determined.

C4.5.6.1b SEARCH TYPE is used to specify the variable that is to be changed during the search procedure.
Use PITCH, PIT, PITC, or PTCH to alter the center-to-center spacing between the units at the lowest array level. By default only the spacing in the X and Y directions will be altered.
Use DIMENSION, DIME, DIM, or DMSN to alter the dimensions of one or more geometry regions.

The combination of the search descriptor and the search type defines the search method. An OPTIMUM PITCH search will search for the pitch that gives the maximum value of k-effective. By default only the X and Y spacing will be altered. Auxiliary search commands can be used to instruct the code to also vary the z spacing. An OPTIMUM DIMENSION search will alter the dimensions of one or more geometry regions in accordance with the specified auxiliary search commands and determine the maximum value of k-effective. A CRITICAL PITCH search alters the spacing between units in the same manner as an optimum pitch search to achieve the specified value of k-effective. A CRITICAL DIMENSION search alters the dimensions of one or more geometry regions in accordance with the specified auxiliary search commands to achieve the specified value of k-effective. A MINIMUM PITCH search will search for the pitch that gives the minimum value of k-effective. A MINIMUM DIMENSION search alters the dimensions of one or more geometry regions in accordance with the specified auxiliary search commands to achieve the minimum value of k-effective. Only one combination of SEARCH DESCRIPTOR and SEARCH TYPE is allowed in a problem.

C4.5.6.1c OPTIONAL SEARCH PARAMETERS are entered after the SEARCH DESCRIPTOR AND SEARCH TYPE and are used to alter the default values of the optional search parameters. Only one set of optional search parameters can be entered for a problem. The optional search parameters are listed below.

PAS=nn is used to set the maximum number of times the search will calculate k-effective. The first pass calculates the k-effective corresponding to the initial geometry dimensions. The second pass calculates the k-effective corresponding to one of the constraints, and the third pass often corresponds to the other constraint. The default value of nn is 10.

NPM=nn is used to set the number of search parameters. The default value is 1 and should not be overridden.

EPS=ff is used to set the search convergence tolerance (the amount by which k-effective is allowed to vary from the desired k-effective). An optimum or minimum search is terminated when the calculated k-effective is within EPS of the optimum or minimum value as indicated by the mathematical fit to the calculated points. A critical search is terminated when the calculated k-effective is within EPS of the specified k-effective. The default value of ff is 0.005.

KEF=ff is used only for a critical search and is used to specify the desired value of k-effective. The default value of ff is 1.000.

MAXPITCH=ff is allowed ONLY for a PITCH search. It is used to specify the maximum allowed pitch (center-to-center spacing in the x and y directions) between units in an array. The search will terminate if the specified pitch is exceeded. The default value of ff is the pitch corresponding to -5 times the parameter that corresponds to the minimum pitch. It is much easier to specify a maximum allowed pitch than to calculate the appropriate value of the maximum constraint.

MINPITCH=ff is allowed ONLY for a PITCH search. It is used to specify the minimum allowed pitch (center-to-center spacing in the x and y directions) between the units in an array. The search will terminate if the pitch becomes smaller than the specified minimum pitch. The default value of ff is the pitch at which the region immediately inside the spacing region touches the spacing region. It is much easier to specify the minimum allowed pitch than to calculate the appropriate value of the minimum constraint.

MORE is used to terminate the optional search parameters and initiate the auxiliary search commands. Do not enter MORE unless auxiliary search commands are to be entered.

C4.5.6.2 Auxiliary Search Commands

Auxiliary search commands are entered ONLY if the word MORE was entered in the search type specification data. These data are used to define the method the search will use to alter the geometry data and to set the constraints for the parameter search. The auxiliary search commands consist of (1) INDIVIDUAL SEARCH COMMANDS and (2) SEARCH PARAMETER CONSTRAINTS.

C4.5.6.2a An INDIVIDUAL SEARCH COMMAND consists of (1) a command definition, (2) the geometry unit number, (3) the region(s) to be altered, and (4) search constants for each dimension that is to be altered in the specified region(s). A series of individual search commands can be entered for a problem to govern the search process. A new search command is initiated whenever a command definition, item (1) above, is encountered.

The COMMAND DEFINITION tells the code what action is to be taken for a specified geometry region or range of regions. ALTER, CHANGE, or MODIFY are used to cause the specified geometry region(s) to be modified. MAINTAIN is used to maintain the thickness of the specified geometry region(s). KEEP or HOLD are used to cause the specified geometry region(s) to be reset to its original value. The available command definitions are listed below.

ALTER
ALTR
ALT
CHANGE
CHNG
MODIFY
MOD
MDFY

The list of commands to the left are command definitions, item (1) above. These commands are used to instruct the code to make changes to the specified geometry region(s). The regions that are to be changed are specified using items (2) and (3) above. The amount of change is governed by the search constants, item (4) above.

MAINTAIN
MNTN

The list of commands to the left are command definitions, item (1) above. These commands commands are used to instruct the code to maintain the thickness of the specified region(s) noted in items (2) and (3) above. The search constants, item (4) above, must be nonzero to cause the thickness of the region(s) to be preserved. It should be noted that the thickness of a region can be maintained using this command ONLY when the interior boundary of the region is being altered. If the exterior boundary is being altered, the code is unable to maintain the thickness between it and the boundary interior to it. For example, consider a spherical stainless steel tank with a wall thickness of 1/4 in., filled with a fissile solution. Region 1 is a sphere of solution, and region 2 is the stainless steel. If the search data specifies that region 1 is to be altered and region 2 is to be maintained, the search will maintain a tight-fitting, 1/4-in.-thick, stainless steel region around the fissile solution sphere as it changes sizes. However, if the search data specify only that region 2 is to be altered, the size of the solution sphere will be unchanged and the thickness of the stainless steel spherical shell will vary. If the search data specify that region 1 is to be maintained and region 2 is to be altered, the size of the solution sphere will remain unchanged and the thickness of the stainless-steel container will vary. If the search data specify only that region 2 is to be maintained, no changes will be made and neither region will be changed.

KEEP
HOLD

The list of commands to the left are command definitions, item (1) above. These commands are used to instruct the code to preserve the original dimensions of the specified region(s) noted in items (2) and (3) above. The search constants, item (4) above, must be nonzero in order to preserve the original dimensions of the region(s).

THE GEOMETRY UNIT NUMBER, item (2) above, is used to define the unit or box type that contains the geometry region(s) to which the command definition pertains. The geometry unit number is specified by entering the keyword UNIT= followed by the desired unit number.

UNIT=nn is used to define the geometry unit to which the previously entered command definition is to be applied. The keyword UNIT= is entered, followed by the unit number, nn. There is no default value of nn.

THE REGION(S) TO BE ALTERED, item (3) above, defines the region(s) in unit nn to which the command definition pertains. A single geometry region is specified by entering the keyword REG=, followed by the desired region number, nn. A range of regions is specified by entering the keyword REG=, followed by the first region to which the search commands pertain. The last region in the range is specified by entering the keyword TO and the last region of the range.

REG=nn is used to define the first geometry region to which the previously entered command definition is to be applied. The keyword REG= is entered, followed by the region number, nn. There is no default value of nn.

TO mm is used to define the final geometry region of the range to which the previously entered command definition applies. The keyword TO is entered, followed by the last region number of the range, mm. There is no default value of mm.

For example, if region 3 of unit 2 is to be altered, items 1, 2, and 3 would be entered as:

ALTER UNIT=2 REG=3

If regions 3, 4, 5, and 6 of unit 2 are to be altered, items 1, 2, and 3 would be entered as:

ALTER UNIT=2 REG=3 TO 6

THE SEARCH CONSTANTS, item (4) above, are proportionality factors that are applied to the specified dimensions of the specified region(s) to which the command definition applies. The search constants define both the dimension to which the search command pertains and the value of the corresponding search constant. Search constants are entered by using a keyword to define the appropriate dimension, followed by a proportionality constant, pc. The default value of pc is 0.0. A nonzero value of pc causes the dimension(s) specified by the keyword to have the search command applied to it. A list of search constant keywords follows.

ALL= is used to define the search constant for all of the dimensions of the region or range of regions defined by items (2) and (3) above. ALL= changes the +X, -X, +Y, -Y, +Z, and -Z dimensions of a cuboid; the radius and +Height and -Height of a cylinder; and the radius of a sphere.

+X= is used to define the search constant for the positive X dimension of a cuboid.

-X= is used to define the search constant for the negative X dimension of a cuboid.

+Y= is used to define the search constant for the positive Y dimension of a cuboid.

-Y= is used to define the search constant for the negative Y dimension of a cuboid.

+Z= is used to define the search constant for the positive Z dimension of a cuboid.

-Z= is used to define the search constant for the negative Z dimension of a cuboid.

R= is used to define the search constant for the radius of a sphere or a cylinder.

+H= is used to define the search constant for the positive height of a cylinder.

-H= is used to define the search constant for the negative height of a cylinder.

CH= is used to define the search constant for the chord of a hemisphere or hemicylinder.

ENTERING AUXILIARY SEARCH COMMANDS IN THE SEARCH DATA

EXAMPLE 1

Consider an example in which region 2 of unit 1 is a cuboid and all of the dimensions of the cuboid are to be altered. The search data could be entered as:

```
ALTER UNIT=1 REG=2 ALL=1.0
```
or
```
ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
```

Because all of the search constants are nonzero, all of the dimensions will be changed. Because the search constants are identical, the original relationship between the dimensions will be preserved as they are altered.

For example, if region 2 of unit 1 is a cylinder and if all the dimensions of the cylinder are to be altered, the search data could be entered as:

```
ALTER UNIT=1 REG=2 ALL=1.0
```
or
```
ALTER UNIT=1 REG=2 R=1.0 +H=1.0 -H=1.0
```

Because all of the search constants are nonzero, all of the dimensions will be changed. Because the search constants are identical, the original relationship between the dimensions will be preserved as they are altered. If the original height-to-diameter ratio is 1.5, that ratio will be preserved throughout the search only if the search constants for the radius and + and - height are identical.

Search constants can be entered sequentially with each new entry overriding only identical previous entries. For example, if region 2 of unit 1 is a cuboid and if all of the dimensions except the -Z dimension are to be altered, the search data could be entered as:

```
ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0
```
or
```
ALTER UNIT=1 REG=2 ALL=1.0 -Z=0.0
```

In the second example, all of the search constants corresponding to the cuboid's dimensions are set to 1.0 by using the ALL= command. This includes the -Z dimension. To reset the search constant for the -Z dimension to zero, -Z=0.0 is added following the ALL=1.0 command. If the search commands are reversed, -Z=0.0 ALL=1.0, the -Z dimension will also be altered because the -Z portion of the ALL= command will override the previously entered -Z=0.0 command.

EXAMPLE 2

A search command must be entered for each unit and region specification. Consider a problem having units 1, 2, and 3. Unit 1 consists of 3 concentric spheres in a cuboid. Unit 2 consists of a single sphere in a cuboid, and unit 3 contains 3 concentric cuboids. A search is to be made that changes the exterior dimensions of the 3 units, the inner sphere of unit 1, and the sphere of unit 2. The thicknesses of the outer spheres of unit 1 are to be maintained, and the two inner cuboids of unit 3 are to remain unchanged. The search data for this problem can be entered as follows:

```
ALTER UNIT=1 REG=1 ALL=1.0
ALTER UNIT=1 REG=4 ALL=1.0
ALTER UNIT=2 REG=1 TO 2 ALL=1.0
ALTER UNIT=3 REG=3 ALL=1.0
MAINTAIN UNIT=1 REG=2 TO 3 ALL=1.0
```

C4.5.6.2b SEARCH PARAMETER CONSTRAINTS set the parameter limits for the search. The minimum constraint is the minimum value of the parameter allowed in the search. The maximum constraint is the maximum value of the parameter allowed in the search. The initial geometry configuration corresponds to a parameter value of 0.0. A physical limit occurs when the value of the parameter causes geometry intersections. Constraints should be entered for a DIMENSION search.

For a DIMENSION search, the constraints are given by Eqs. (C4.5.1) and (C4.5.2):

$$C_{min} = ((D_{min}/D_i) - 1.0)/SC \qquad (C4.5.1)$$

$$C_{max} = ((D_{max}/D_i) - 1.0)/SC\,, \qquad (C4.5.2)$$

where

C_{min} is the minimum constraint for the search
C_{max} is the maximum constraint for the search
D_{min} is the minimum allowed dimension for the search [For a chord, $D_{min} = (Radius_{min} + Chord_{min})/2\ Radius_{min}$]
D_{max} is the maximum allowed dimension for the search [For a chord, $D_{max} = (Radius_{max} + Chord_{max})/2\ Radius_{max}$]
D_i is the initial dimension [For a chord, $D_i = (Radius_{initial} + Chord_{initial})/2\ Radius_{initial}$]
SC is the search constant for that dimension

For example, the initial radius of a sphere is 6 cm, and a search is to be conducted to determine the radius at which the sphere is critical. The minimum radius the user wishes to allow is 3 cm, and the maximum radius to be allowed is 9 cm. A nonzero search constant must be entered to cause the radius to be changed. A search constant of 1.0 will be used for the radius. The constraints calculated from Eqs. (C4.5.1) and (C4.5.2) are:

$C_{min} = ((3.0/6.0)-1.0)/1.0 = -0.5$

$C_{max} = ((9.0/6.0)-1.0)/1.0 = 0.5$

The constraints would be entered in the problem by entering the following data:

-CON=-0.5 +CON=0.5

For a PITCH search, the minimum constraint defines the limit for shrinking the system, and the maximum constraint defines the limit for expanding the system:

$$C_{min} = \underset{i=1}{\overset{i=\text{number of faces}}{MAX}}\left[D_+, D_-\right] \text{ for shrinking}$$

$$C_{max} = \underset{i=1}{\overset{i=\text{number of faces}}{MIN}}\left[D_+, D_-\right] \text{ for expanding}$$

where

C_{min} is the minimum constraint,
C_{max} is the maximum constraint,
D_+ are face constraints for the positive dimensions,
D_- are face constraints for the negative dimensions.

Face constraints must be calculated for each face using Eqs. (C4.5.3) and (C4.5.4):

$$D_+ = \frac{(X_{d+} - X_{i+})(SC_+ \times del_+ + SC_- \times del_-)}{(X_{i+} - X_{i-})(SC_+ **2 \times del_+)}, \qquad \text{(C4.5.3)}$$

$$D_- = \frac{-(X_{d-} - X_{i-})(SC_+ \times del_+ + SC_- \times del_-)}{(X_{i+} - X_{i-})(SC_- **2 \times del_-)}, \qquad \text{(C4.5.4)}$$

where

X_{d+} is the desired limit of the positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

X_{i+} is the initial positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

X_{d-} is the desired limit of the negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

X_{i-} is the initial negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

SC_+ is the search constant for the positive dimension of the spacing cuboid in that direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

SC_- is the search constant for the negative dimension of the spacing cuboid in that direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)
NOTE: Using a search constant of 1.0 simplifies the determination of C_{max} and C_{min} when the dimensions are to change proportionately.

del_+ is the initial distance from the spacing cuboid to the closest interior region in the positive direction (positive dimension of X, Y, or Z, whichever dimension is under consideration)

del_- is the initial distance from the spacing cuboid to the closest interior region in the negative direction (negative dimension of X, Y, or Z, whichever dimension is under consideration)

The search parameter constraints are entered using the following keywords:

-CON=pp is used to set the minimum constraint for the current parameter. The value of pp is defaulted to -10E10 for a dimension search. The value of pp is defaulted to a value that allows geometry regions to touch for a pitch search unless a value was entered for MINPITCH, in which case the parameter corresponding to that pitch is calculated and used.

+CON=rr is used to set the maximum constraint for the current parameter. The value of rr is defaulted to +10E10 for a dimension search and to -5 x pp for a pitch search.

NOTE: A search will reset a constraint (entered using the keyword +CON= or -CON=) that falls outside the default range to the default value. If a PITCH search is specified and if a value has been entered for MAXPITCH and/or MINPITCH, values should not be entered for the constraints. If values are entered for +CON= and/or -CON= for a PITCH search and if MAXPITCH and/or MINPITCH were specified in the optional search parameters, the maximum and minimum constraints will be set to the values corresponding to MAXPITCH and MINPITCH, even though the value of MINPITCH may result in an intersection.

C4.5.7 SEARCH CONSIDERATIONS

Both DIMENSION searches and PITCH searches can be performed using CSAS4 and CSAS4X. A DIMENSION search alters only those regions specified in the search data. A PITCH search alters the center-to-center spacing of units in an array.

By default, a pitch search is performed at the lowest array level, and only the spacing in the x and y directions will be changed. For example, if an array of fuel assemblies is described in the geometry, the lowest array level is the array of fuel pins comprising an assembly. Therefore, an optimum pitch search would alter the spacing between the fuel pins within the assembly. The spacing can be expanded until the array intersects the first region external to it. The exterior size of the fuel pin array would grow or shrink within the confines of the exterior region (fuel assembly shroud). If the external regions are described using replicate regions, the array can grow or shrink within the confines of the maximum and minimum constraints.

If replicate regions are used outside an altered region or an array whose spacing units are altered, the dimensions of the replicate regions are recalculated (maintaining the thickness) at each search pass without having to enter search data for those regions. However, geometry regions specified by a geometry shape (sphere, cuboid, cylinder, etc.) that exist outside an altered region or an array whose spacing units are being altered will remain unchanged unless search data are provided for them. In other words, REPLICATE regions will grow and shrink in response to changes in the dimensions of the interior region, but other geometry shapes will not.

Some of the limitations applicable to a search are:

1. A pitch search is performed only at the lowest array level unless search commands are entered to keep the lowest array level unit unchanged and other commands are entered to cause other units to be altered.

2. A pitch search alters the +X, -X, +Y, and -Y dimensions by default. Appropriate search commands can be entered to alter the +Z and -Z dimensions if it is desirable to do so. Entering a search constant of zero for +X, -X, +Y, and/or -Y will keep the corresponding dimension from being altered.

3. A pitch search alters only the outer region of the unit(s) used in the array at the lowest array level unless the search data specifying otherwise is input.

4. A search cannot alter a region whose boundaries are set by the code (i.e., an ARRAY, CORE BOUNDARY, or REPLICATE following an ARRAY). If the dimensions of a replicate region are to be altered, the dimensions of the region interior to it must be explicitly defined. For example, the interior region can be a standard geometry shape (sphere, cylinder, cuboid, etc.), but cannot be a replicate following an array or core boundary.

5. All searches allow auxiliary search data as described in Sect. C4.4.10.2.

C4.5.8 OPTIMUM PITCH SEARCH

An optimum pitch search searches for the pitch that yields the highest value of k-effective. An optimum pitch search is activated by entering "OPTIMUM PITCH" in the search data. By default, the search is performed at the lowest array level, and only the spacing in the x and y directions (the x and y dimensions of the outermost region of the unit(s) used in the array at the lowest array level) will be changed. The search constants are defaulted to 1.0 for the +X, -X, +Y, and -Y dimensions of the region. The dimensions of other geometry regions will not be changed (their search constants are defaulted to 0.0) unless additional search data containing appropriate instructions are supplied.

The limits for an optimum pitch search can be set using either the MAXPITCH=/MINPITCH= option in the optional search parameters (Sect. C4.5.6.1c) or the +CON=/-CON= in the search parameter constraints of the auxiliary search commands (Sect. C4.5.6.2b). MAXPITCH=/MINPITCH= are used to enter a value of the maximum allowed pitch and minimum allowed pitch respectively. +CON=/-CON= are used to enter values for the parameter constraints (i.e., the maximum and minimum allowed value of the search parameter). Typically, it is easier to set the maximum allowed pitch and minimum allowed pitch using MAXPITCH=/MINPITCH= than it is to calculate the value of the parameter corresponding to those pitches.

The default minimum constraint corresponds to MINPITCH, the pitch at which the largest interior region of a unit used in the array is in contact with the spacing cuboid of that unit. The maximum constraint is defaulted to -5 times the minimum constraint. The code calculates k-effective for the initial geometry first. Then the dimensions corresponding to the minimum constraint and maximum constraint are calculated.

A simple optimum pitch search is demonstrated in example 1:

EXAMPLE 1

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. Search data and results for some optimum pitch searches using this example are given in methods 1 through 6 below.

DEFAULT OPTIMUM PITCH SEARCH

The search data for a default optimum pitch search are as follows:

READ SEARCH OPTIMUM PITCH END SEARCH

These data will cause the code to alter the +X, -X, +Y, and -Y dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The +Z and -Z dimensions will remain unchanged, thereby preserving the original spacing between the z layers. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 1

Define unit 1 so the sphere is centered in the unit. The geometry region data and search data for this example are:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  OPTIMUM PITCH  END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.4990 ± 0.0033   Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
SECOND PASS..k-effective=1.9127 ± 0.0045   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2861 ± 0.0025  Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P14.0 2P4.0
```

METHOD 2

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case follow:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH  OPTIMUM PITCH  END SEARCH
```

A summary of the code results follows:

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=0.9127 ± 0.0045 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2837 ± 0.0028 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 2P14.0 2P4.0

METHOD 3

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH OPTIMUM PITCH END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.5054 ± 0.0036 Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=0.9094 ± 0.0044 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2825 ± 0.0031 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 6.0 -2.0

OPTIMUM PITCH SEARCH IN ALL THREE DIMENSIONS

Search data for an optimum pitch search that alters the Z dimensions as well as the X and Y dimensions are given below.

READ SEARCH
OPTIMUM PITCH MORE ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH

These data will cause the code to alter the +X, -X, +Y, -Y, +Z, and -Z dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The original relationship between the dimensions is preserved (i.e., original ratio of the X to Y to Z dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 4

Define unit 1 so the sphere is centered in the unit. The geometry region data and search data for this example are:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH
OPTIMUM PITCH MORE ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.4990 ± 0.0033   Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0

SECOND PASS..k-effective=1.2771 ± 0.0048   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2609 ± 0.0020   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P14.0
```

METHOD 5

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH
OPTIMUM PITCH MORE ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH
```

A summary of the code results follows:

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=1.2771 ± 0.0048 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2570 ± 0.0024 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 4P14.0

METHOD 6

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are the following:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH
OPTIMUM PITCH MORE ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.5054 ± 0.0036 Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=1.2771 ± 0.0048 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2596 ± 0.0021 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 26.0 -2.0

C4.5.9 OPTIMUM DIMENSION SEARCH

An optimum dimension search searches for the geometry dimensions that yield the highest value of k-effective. An optimum dimension search is activated by entering "OPTIMUM DIMENSION" in the search data. There are no defaulted search data in a dimension search. The user must specify the dimensions to be changed and the manner in which they will be changed as described in the auxiliary search commands (Sect. C4.5.6.2).

A dimension search is performed by altering the regions having nonzero search constants specified in the auxiliary search commands portion of the search data. By default, the search constants for every dimension in the problem is zero. Only those dimensions having a nonzero search constant are altered by the code.

By default, a dimension search sets the minimum constraint to -10E10 and the maximum constraint to +10E10. The relationship between the constraints and the search constants are given in Eqs. (C4.5.1) and (C4.5.2). If the default values of the constraints are used, appropriate search constants must be calculated using these equations. It may be simpler to set the search constants to 1.0 and calculate the corresponding maximum and minimum constraints.

A simple optimum dimension search is demonstrated in example 1.

EXAMPLE 1

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. Search data and results for some optimum dimension searches using this example are given in methods 1 through 6 below.

OPTIMUM DIMENSION SEARCH IN X AND Y

The search data for an optimum dimension search that alters only the x and y dimensions of region 2 of unit 1 are given as follows. The constraints are set to be consistent with those of the optimum pitch search above.

```
READ SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

These data will cause the code to alter the +X, -X, +Y, and -Y dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The +Z and -Z dimensions will remain unchanged, thereby preserving the original spacing between the z layers. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 1

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example are:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

FIRST PASS...k-effective=0.4990 ± 0.0033 Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE 0 1 2P4.0

SECOND PASS..k-effective=0.9027 ± 0.0043 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2861 ± 0.0025 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P14.0 2P4.0

METHOD 2

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are the following:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=0.9032 ± 0.0042 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2837 ± 0.0028 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 2P14.0 2P4.0

METHOD 3

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are the following:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5054 ± 0.0036  Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS...k-effective=0.9009 ± 0.0044  Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0

THIRD PASS...k-effective=0.2596 ± 0.0021  Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 2P14.0 2P4.0
```

OPTIMUM DIMENSION SEARCH IN ALL THREE DIMENSIONS

Search data for an optimum dimension search that alters the X, Y, and Z dimensions follow. The constraints are set to be consistent with the optimum pitch search above.

```
REACH SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

These data will cause the code to alter the +X, -X, +Y, -Y, +Z, and -Z dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y to Z dimensions of the cuboid is preserved throughout the search). Because this is an optimum dimension search, the sphere dimensions will not be altered unless search data are entered for region 1 of unit 1. For this particular example, results for only three passes are given.

METHOD 4

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example are:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
```

-CON=-0.5 +CON=2.5
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.4990 ± 0.0033 Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE 0 1 2P4.0

SECOND PASS...k-effective=1.2743 ± 0.0053 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2609 ± 0.0020 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P14.0

METHOD 5

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS...k-effective=1.2854 ± 0.0047 Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2570 ± 0.0024 Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 4P14.0

METHOD 6

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are given below:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH  OPTIMUM DIMENSION
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5054 ± 0.0036   Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=1.2778 ± 0.0045   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

THIRD PASS...k-effective=0.2596 ± 0.0021   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 26.0 -2.0
```

C4.5.10 CRITICAL PITCH SEARCH

A critical pitch search alters the outer region of the unit or units at the lowest array level in search of a specified value of k-effective. A critical pitch search is activated by entering "CRITICAL PITCH" in the search data. By default, the search is performed at the lowest array level, and only the spacing in the x and y directions (the x and y dimensions of the outermost region of the unit(s) used in the array at the lowest array level) will be changed. The search constants are defaulted to 1.0 for the +X, -X, +Y, and -Y dimensions of the region. The dimensions of other geometry regions will not be changed (their search constants are defaulted to 0.0) unless additional search data containing appropriate instructions are supplied.

The limits for a critical pitch search can be set using either the MAXPITCH=/MINPITCH= option in the optional search parameters (Sect. C4.5.6.1c) or the +CON=/-CON= in the search parameter constraints of the auxiliary search commands (Sect. C4.5.6.2b). MAXPITCH+/MINPITCH= are used to enter a value of the maximum allowed pitch and minimum allowed pitch respectively. +CON=/-CON= are used to enter values for the parameter constraints (i.e., the maximum and minimum allowed value of the search parameter). Typically, it is easier to set the maximum allowed pitch and minimum allowed pitch using MAXPITCH=/MINPITCH= than it is to calculate the value of the parameter corresponding to those pitches.

The default minimum constraint corresponds to MINPITCH, the pitch at which the largest interior region of a unit used in the array is in contact with the spacing cuboid of that unit. The maximum constraint is defaulted to -5 times the minimum constraint. The code calculates k-effective for the initial geometry first. Then the dimensions corresponding to the minimum constraint and maximum constraint are calculated.

A simple critical pitch search is demonstrated in example 1.

EXAMPLE 1

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. Search data and results for some critical pitch searches using this example are given in methods 1 through 6.

DEFAULT CRITICAL PITCH SEARCH

The search data for a critical pitch search that alters the +X, –X, +Y, and –Y dimensions in search of a k-effective of 0.93 are:

```
READ SEARCH  CRITICAL PITCH KEF=0.93  END SEARCH
```

These data will cause the code to alter the +X, –X, +Y, and –Y dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The +Z and –Z dimensions will remain unchanged, thereby preserving the original spacing between the z layers. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y dimensions of the cuboid is preserved throughout the search). Because this is a critical pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 1

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example follow:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  CRITICAL PITCH KEF=0.93  END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.4990 ± 0.0033   Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0

SECOND PASS..k-effective=0.2861 ± 0.0025   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P14.0 2P4.0

THIRD PASS...k-effective=0.9127 ± 0.0045   Parameter=–0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0
```

After the third pass, the code recognizes that the desired k-effective of 0.93 lies outside the range of the parameter constraints. Messages CS-85 and CS-83 are printed and execution is terminated.

METHOD 2

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH  CRITICAL PITCH KEF=0.93  END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5017 ± 0.0036   Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=0.2837 ± 0.0028   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 2P14.0 2P4.0

THIRD PASS..k-effective=0.9127 ± 0.0045   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0
```

After the third pass, the code recognizes that the desired k-effective of 0.93 lies outside the range of the parameter constraints. Messages CS-85 and CS-83 are printed and execution is terminated.

METHOD 3

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0 READ SEARCH
CRITICAL PITCH KEF=0.93  END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5054 ± 0.0036   Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=0.2825 ± 0.0031   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 6.0 -2.0
```

THIRD PASS...k-effective=0.9094 ± 0.0044 . Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 6.0 -2.0

After the third pass, the code recognizes that the desired k-effective of 0.93 lies outside the range of the parameter constraints. Messages CS-85 and CS-83 are printed and execution is terminated.

CRITICAL PITCH SEARCH IN ALL THREE DIMENSIONS

Search data for a critical pitch search that alters the Z dimensions as well as the X and Y dimensions follow:

READ SEARCH
CRITICAL PITCH MORE KEF=0.93 ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH

These data will cause the code to alter the +X, -X, +Y, -Y, +Z, and -Z dimensions of the outer region of unit 1 and search for the dimensions that give a k-effective of 0.93. The original relationship between the dimensions is preserved (i.e., original ratio of the X to Y to Z dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 4

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example are given below:

UNIT 1
SPHERE 1 1 2.0
CUBE 0 1 2P4.0
READ SEARCH
CRITICAL PITCH MORE KEF=0.93 ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.4990 ± 0.0033 Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE 0 1 2P4.0

SECOND PASS..k-effective=0.2609 ± 0.0020 Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P14.0

THIRD PASS...k-effective=1.2771 ± 0.0048 Parameter=-0.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

FOURTH PASS..k-effective=0.7643 ± 0.0047 Parameter=–0.2769
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.8922

FIFTH PASS...k-effective=0.9226 ± 0.0041 Parameter=–0.3643
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.5426

METHOD 5

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are given below:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 –2.0 4P4.0
READ SEARCH
CRITICAL PITCH MORE KEF=0.93 ALTER UNIT=1 REG=2 +Z=1.0 –Z=1.0
END SEARCH

The code results are summarized below.

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.0000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 –2.0 4P4.0

SECOND PASS..k-effective=0.2570 ± 0.0024 Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 –2.0 4P14.0

THIRD PASS...k-effective=1.2771 ± 0.0048 Parameter=–0.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

FOURTH PASS..k-effective=0.7616 ± 0.0040 Parameter=–0.2762
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.7906 –2.0 4P2.8953

FIFTH PASS...k-effective=0.9221 ± 0.0042 Parameter=–0.3650
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.0801 –2.0 4P2.54

METHOD 6

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case follow:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
CRITICAL PITCH MORE KEF=0.93 ALTER UNIT=1 REG=2 +Z=1.0 -Z=1.0
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5054 ± 0.0036  Parameter=0.0000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS...k-effective=0.2596 ± 0.0021  Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 26.0 -2.0

THIRD PASS...k-effective=1.2771 ± 0.0048  Parameter=-0.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

FOURTH PASS...k-effective=0.7598 ± 0.0042  Parameter=-0.2751
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.7992 -2.0 3.7992 -2.0 3.7992 -2.0

FIFTH PASS...k-effective=0.9183 ± 0.0047  Parameter=-0.3652
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.0783 -2.0 3.0783 -2.0 3.0783 -2.0
```

C4.5.11 CRITICAL DIMENSION SEARCH

A critical dimension search searches for the geometry dimensions that yield a specified value of k-effective. A critical dimension search is activated by entering "CRITICAL DIMENSION" in the search data. No defaulted search data are in a dimension search. The user must specify the dimensions to be changed and the manner in which they will be changed.

A dimension search is performed by altering the regions having nonzero search constants specified in the individual search commands portion of the search data. By default, the search constants for every dimension in the problem is zero. Only those dimensions having a nonzero search constant are altered by the code.

By default, a dimension search sets the minimum constraint to -10E10 and the maximum constraint to +10E10. The relationship between the constraints and the search constants is given in Eqs. (C4.5.1) and (C4.5.2). If the default values of the constraints are used, appropriate search constants must be calculated using these equations. It may be simpler to set the search constants to 1.0 and calculate the corresponding maximum and minimum constraints.

A simple critical dimension search is demonstrated using example 1 with methods 1 through 6. A more complicated critical dimension search is given in example 2.

EXAMPLE 1

Consider a 10 × 10 × 10 array of uranium spheres arranged in an array having a "square" pitch. The uranium spheres are 2 cm in radius, and the center-to-center spacing is 8 cm. The uranium spheres and their associated spacing are defined to be unit 1, and the 10 × 10 × 10 array is defined to be array 1. Search data and results for some optimum dimension searches using this example are given in methods 1 through 6.

CRITICAL DIMENSION SEARCH IN X AND Y

The search data for a critical dimension search that alter only the x and y dimensions of region 2 of unit 1 follow. The constraints are set to be consistent with those of the optimum pitch search above.

```
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

These data will cause the code to alter the +X, -X, +Y, and -Y dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The +Z and -Z dimensions will remain unchanged, thereby preserving the original spacing between the z layers. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y dimensions of the cuboid is preserved throughout the search). Because this is an optimum pitch search, the sphere dimensions will not be changed. For this particular example, results for only three passes are given.

METHOD 1

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example are:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.4990 ± 0.0033   Parameter=0.000
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0

SECOND PASS..k-effective=0.2861 ± 0.0025   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P14.0 2P4.0
```

```
THIRD PASS...k-effective=0.9028 ± 0.0043   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0
```

After the third pass, the code recognizes that the desired k-effective of 0.93 lies outside the range of the parameter constraints. Messages CS-85 and CS-83 are printed and execution is terminated.

METHOD 2

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are the following:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5017 ± 0.0036   Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=0.2837 ± 0.0028   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 2P14.0 2P4.0

THIRD PASS...k-effective=0.9032 ± 0.0042   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 2P4.0
```

After the third pass, the code recognizes that the desired k-effective of 0.93 lies outside the range of the parameter constraints. Messages CS-85 and CS-83 are printed and execution is terminated.

METHOD 3

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case are given below.

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.5054 ± 0.0036   Parameter=0.000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=0.2825 ± 0.0031   Parameter=2.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 6.0 -2.0

THIRD PASS...k-effective=0.9009 ± 0.0044   Parameter=-0.500
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 4P2.0 6.0 -2.0
```

CRITICAL DIMENSION SEARCH IN ALL THREE DIMENSIONS

Search data for a critical dimension search that alters the X, Y, and Z dimensions follow. The constraints are set to be consistent with the critical pitch search above.

```
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

These data will cause the code to alter the +X, -X, +Y, -Y, +Z, and -Z dimensions of the outer region of unit 1 and search for the dimensions that give the maximum k-effective. The original relationship between the dimensions is preserved (i.e., the original ratio of the X to Y to Z dimensions of the cuboid is preserved throughout the search). Because this is a critical dimension search, the sphere dimensions will not be altered unless search data are entered for region 1 of unit 1. For this particular example results for only three passes are given.

METHOD 4

Define unit 1 so that the sphere is centered in the unit. The geometry region data and search data for this example follow:

```
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
READ SEARCH  CRITICAL DIMENSION  KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

```
FIRST PASS...k-effective=0.4990 ± 0.0033   Parameter=0.0000
UNIT 1
SPHERE 1 1 2.0
CUBE   0 1 2P4.0
```

SECOND PASS..k-effective=0.2609 ± 0.0020 Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P14.0

THIRD PASS...k-effective=1.2742 ± 0.0054 Parameter=-0.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

FOURTH PASS..k-effective=0.7687 ± 0.0043 Parameter=-0.2780
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.8881

FIFTH PASS...k-effective=0.9211 ± 0.0039 Parameter=-0.3637
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.5454

METHOD 5

Define unit 1 so that the sphere is offset in the unit in the X direction but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case follow:

UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0
READ SEARCH CRITICAL DIMENSION KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH

A summary of the code results follows:

FIRST PASS...k-effective=0.5017 ± 0.0036 Parameter=0.0000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 4P4.0

SECOND PASS..k-effective=0.2569 ± 0.0024 Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 4P14.0

THIRD PASS...k-effective=0.7557 ± 0.0042 Parameter=-0.2733
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.8139 -2.0 4P2.9069

FOURTH PASS..k-effective=0.9142 ± 0.0042 Parameter=-0.3644
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.0851 -2.0 4P2.54

FIFTH PASS...k-effective=0.9228 ± 0.0041 Parameter=-0.3665
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

METHOD 6

Define unit 1 so that the sphere is offset in the unit in X, Y, and Z but the center-to-center spacing is retained at 8.0 cm. The geometry region data for this case follow:

```
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0
READ SEARCH CRITICAL DIMENSION KEF=0.93
MORE ALTER UNIT=1 REG=2 +X=1.0 -X=1.0 +Y=1.0 -Y=1.0 +Z=1.0 -Z=1.0
-CON=-0.5 +CON=2.5
END SEARCH
```

A summary of the code results follows:

FIRST PASS...k-effective=0.5054 ± 0.0036 Parameter=0.0000
SPHERE 1 1 2.0
CUBOID 0 1 6.0 -2.0 6.0 -2.0 6.0 -2.0

SECOND PASS..k-effective=0.2596 ± 0.0021 Parameter=2.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 26.0 -2.0 26.0 -2.0 26.0 -2.0

THIRD PASS...k-effective=1.2778 ± 0.0045 Parameter=-0.5000
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 6P2.0

FOURTH PASS..k-effective=0.7556 ± 0.0042 Parameter=-0.2748
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.8012 -2.0 3.8012 -2.0 3.8012 -2.0

FIFTH PASS...k-effective=0.9228 ± 0.0041 Parameter=-0.3665
UNIT 1
SPHERE 1 1 2.0
CUBOID 0 1 3.0678 -2.0 3.0678 -2.0 3.0678 -2.0

EXAMPLE 2

Consider a problem having units 1, 2, and 3. Unit 1 consists of three concentric spheres in a cuboid. Unit 2 consists of a single sphere in a cuboid, and Unit 3 contains three concentric cuboids. A search is to be made that changes the exterior dimensions of the three units, the inner sphere of unit 1, and the sphere of unit 2. The thicknesses of the outer spheres of unit 1 are to be maintained, and the two inner cuboids of unit 3 are to remain unchanged. The search data for this problem are the following:

```
READ SEARCH CRITICAL DIMENSION
KEF=1.000 EPS=0.005
MORE
ALTER UNIT=1 REG=1 ALL=1.0
ALTER UNIT=1 REG=4 ALL=1.0
ALTER UNIT=2 REG=1 TO 2 ALL=1.0
ALTER UNIT=3 REG=3 ALL=1.0
MAINTAIN UNIT=1 REG=2 TO 3 ALL=1.0
+CON=2.0  -CON=-0.5
END SEARCH
```

The complete input data for this problem are:

```
=CSAS4
SEARCH DEMONSTRATION OF CRITICAL DIMENSION SEARCH
HANSEN-ROACH  INFHOMMEDIUM
URANIUM  1 0.985 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
PLEXIGLASS  2 END
SS304  3 END
END COMP
SEARCH DEMONSTRATION OF CRITICAL DIMENSION SEARCH
READ PARAMETERS  TME=1.0 GEN=53
END PARAMETERS
READ GEOMETRY

UNIT 1
SPHERE 1 1 3.0
SPHERE 0 1 3.25
SPHERE 2 1 3.5
CUBE  0 1 2P5.0
UNIT 2
SPHERE 1 1 3.0
CUBE  0 1 2P5.0
UNIT 3
CUBE  0 1 2P4.9
CUBE  3 1 2P5.0
CUBE  0 1 2P5.0
END GEOMETRY
READ ARRAY ARA=1 NUX=3 NUY=3 NUZ=3 FILL
1 3 2 3 2 3 2 3 1
3 2 3 1 3 2 3 1 3
2 3 1 3 1 3 1 3 2
END FILL END ARRAY
END DATA
```

```
READ SEARCH   CRITICAL DIMENSION
KEF=1.000  EPS=0.005
MORE
ALTER UNIT=1 REG=1 ALL=1.0
ALTER UNIT=1 REG=4 ALL=1.0
ALTER UNIT=2 REG=1 TO 2 ALL=1.0
ALTER UNIT=3 REG=3 ALL=1.0
MAINTAIN UNIT=1 REG=2 TO 3 ALL=1.0
+CON=2.0  -CON=-0.5
END SEARCH
END
```

The results of this search are

```
FIRST PASS...k-effective=0.4075    Parameter=0.000
UNIT 1
SPHERE 1 1 3.0
SPHERE 0 1 3.25
SPHERE 2 1 3.5
CUBE   0 1 2P5.0
UNIT 2
SPHERE 1 1 3.0
CUBE   0 1 2P5.0
UNIT 3
CUBE   0 1 2P4.9
CUBE   3 1 2P5.0
CUBE   0 1 2P5.0

SECOND PASS..k-effective=1.0744    Parameter=2.000
UNIT 1
SPHERE 1 1 9.0
SPHERE 0 1 9.25
SPHERE 2 1 9.5
CUBE   0 1 2P15.0
UNIT 2
SPHERE 1 1 9.0
CUBE   0 1 2P15.0
UNIT 3
CUBE   0 1 2P4.9
CUBE   3 1 2P5.0
CUBE   0 1 2P15.0

THIRD PASS...k-effective=1.0159    Parameter=1.777
UNIT 1
SPHERE 1 1 8.3307
SPHERE 0 1 8.5807
SPHERE 2 1 3.8307
CUBE   0 1 2P13.885
UNIT 2
SPHERE 1 1 8.33017
CUBE   0 1 2P13.8856
UNIT 3
```

```
CUBE   0 1 2P4.9
CUBE   3 1 2P5.0
CUBE   0 1 2P13.885

FOURTH PASS..k-effective=0.9952    Parameter=1.716
UNIT 1
SPHERE 1 1 8.1490
SPHERE 0 1 8.3990
SPHERE 2 1 8.6490
CUBE   0 1 2P13.583
UNIT 2
SPHERE 1 1 8.1490
CUBE   0 1 2P13.582
UNIT 3
CUBE   0 1 2P4.9
CUBE   3 1 2P5.0
CUBE   0 1 2P13.582
```

Convergence was achieved on the fourth pass. Based on the preceding data, the best estimate of the parameter is 1.730 with the following corresponding geometry:

```
UNIT 1
SPHERE 1 1 8.1901
SPHERE 0 1 8.4401
SPHERE 2 1 8.6901
CUBE   0 1 2P13.650

UNIT 2
SPHERE 1 1 8.1901
CUBE   0 1 2P13.650
UNIT 3
CUBE   0 1 2P4.9
CUBE   3 1 2P5.0
CUBE   0 1 2P13.650
```

In the search data of the above example, note that the search command, ALTER, must be entered each time. If it were entered only once regions 1 and 2 of unit 3 would be altered; no changes would be made to unit 1 or unit 2:

```
ALTER UNIT=1 REG=1 ALL=1.0
    UNIT=1 REG=4 ALL=1.0
    UNIT=2 REG=1 TO 2 ALL=1.0
    UNIT=3 REG=1 TO 2 ALL=1.0
MAINTAIN UNIT=1 REG=2 TO 3 ALL=1.0
```

The following data are equivalent to the above data:

```
ALTER UNIT=3 REG=1 TO 2 ALL=1.0
```

C4.6 DESCRIPTION OF OUTPUT

This section describes the output from the CSAS control sequences. The output files that are created when the CSAS control sequences are executed consist of (1) output from the control module, (2) output from the functional modules invoked by the control module, and (3) a listing of the input data. The order in which these output files appear is system dependent. If PARM=CHECK is specified on the analytical sequence indicator, there will be no output from the functional mudules are described in the section pertaining to the module (see Table C4.6.1).

Table C4.6.1 Location of functional module output

Functional module	Section
BONAMI	F1.6
NITAWL-II	F2.8.2
XSDRN	F3.7
ICE	F8.5
KENO V.a	F11.6

C4.6.1 CONTROL MODULE HEADER PAGE

The control module header page, shown in Fig. C4.6.1, prints the name of the control module in block letters. The job name from the job control language, the date (month/day.year), and the time at execution (hour:minute:second) are also printed. This time is given in terms of a 24-h clock, with midnight being 2400 h.

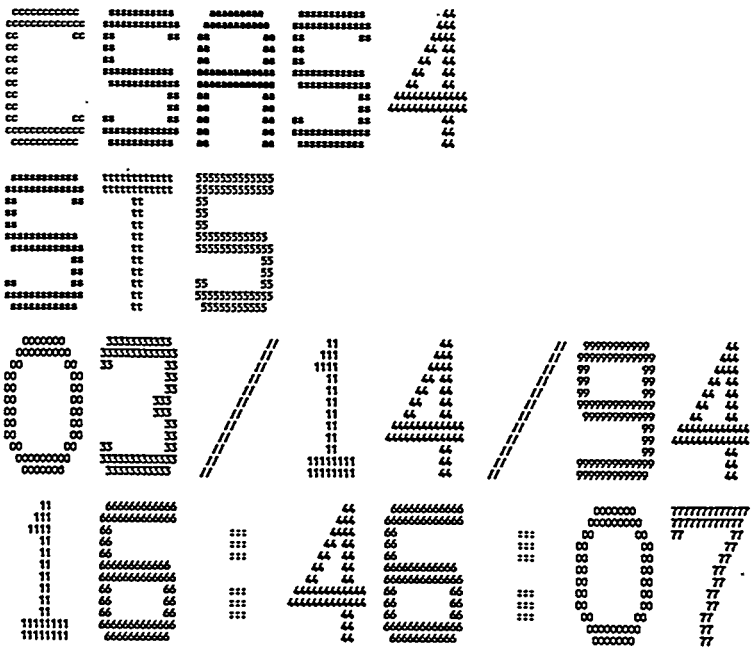


Figure C4.6.1 Sample control module header page

C4.6.2 CONTROL MODULE PROGRAM VERIFICATION TABLE

The control module program verification information table, shown in Fig. C4.6.2, is printed after the header page. It lists the name of the control module that is being executed, the date the load module was created, the library that contains the load module, the computer code name from the configuration control table, and the revision number. Some computers do not store load modules in a library, in which case the library entry is left blank. The job name, date, and time of execution are also printed. This information may be useful for quality assurance purposes.

```
 sssssssssss     ccccccccccc       aaaaaaaaa      ll              eeeeeeeeeeee
ssssssssssssss  ccccccccccccc     aaaaaaaaaaa     ll              eeeeeeeeeeee
ss          ss  cc          cc   aa          aa   ll              ee
ss              cc               aa          aa   ll              ee
ss              cc               aa          aa   ll              ee
ssssssssssss    cc               aaaaaaaaaaaaa    ll              eeeeeeeee
 ssssssssssss   cc               aaaaaaaaaaaaa    ll              eeeeeeeee
          ss    cc               aa          aa   ll              ee
          ss    cc               aa          aa   ll              ee
ss        ss    cc          cc   aa          aa   ll              ee
ssssssssssssss  ccccccccccccc    aa          aa   lllllllllllll   eeeeeeeeeeee
 sssssssssss     ccccccccccc     aa          aa   lllllllllllll   eeeeeeeeeeee
```

```
*****                                                                        *****
*****                  program verification information                     *****
*****                                                                        *****
*****                 code system:    scale  version:    4.2               *****
*****                                                                        *****
*****                                                                        *****
*****                                                                        *****
*****                                                                        *****
*****              program:  csas                                            *****
*****                                                                        *****
*****        creation date:  12/01/93                                        *****
*****                                                                        *****
*****              library:  /scale4.2p/exe                                  *****
*****                                                                        *****
*****                                                                        *****
*****      production code:  csas                                            *****
*****                                                                        *****
*****              version:  2.2                                             *****
*****                                                                        *****
*****              jobname:  st5                                             *****
*****                                                                        *****
*****    date of execution:  03/14/94                                        *****
*****                                                                        *****
*****    time of execution:  16:46:07                                        *****
*****                                                                        *****
```

Figure C4.6.2 Sample control module program verification table

C4.6.3 MATERIAL INFORMATION PROCESSOR OUTPUT

The Material Information Processor output is printed immediately after the program verification table. This output is discussed in detail in Sects. M7.6.1 through M7.6.6. An example of this output is given in Figs. C4.6.3 and C4.6.4.

```
sample problem 4  set up 2c8 in csas25

**** problem parameters ****

lib hansen-roach library
mxx            1 mixtures
msc            1 composition specifications
izm            1 material zones
ge  infhommedium geometry
more           0 0/1 do not read/read optional parameter data
msln           0 fuel solutions

**** problem composition description ****

sc  uranium      standard composition
mx             1 mixture no.
vf         .9850 volume fraction
roth     19.0500 theoretical density
temp       293.0 deg kelvin
           92235  93.20%
           92238   5.60%
           92234   1.00%
           92236    .20%
end

**** problem geometry ****

**** infinite homogeneous medium ****
mfuel          1 mixture no. of the infinite homogeneous medium
```

Figure C4.6.3 Part 1 of Material Information Processor printout

```
*** sample problem 4  set up 2c8 in csas25 ***

*** ********** data library information ********** ***

***   unit                                  volume                                ***
***  number          data set name          name      unit function              ***
***  ------          -------------          ----      -------------              ***
***    89   /scale4.2p/datalib/scale.rev05.sclib      standard composition library ***
***    81   /scale4.2p/datalib/scale.rev02.xn16       cross section library        ***
***    11   ft11f001                                  short cross section library  ***

*** standard composition library data ***
***  ---------------------------------  ***

***  unit number  :  89                                                          ***
***  dataset name :  /scale4.2p/datalib/scale.rev05.sclib                        ***
***  library title:  scale-4 standard composition library                        ***
***                  386 standard compositions, 332 nuclides                     ***
***                  10 elements with variable isotopic distrbutions.            ***
***  creation date:   1/25/94                                                    ***

*** cross section library data ***
***  --------------------------  ***

***  unit number  :  81                                                          ***
***  dataset name :  /scale4.2p/datalib/scale.rev02.xn16                         ***
***  library title:  scale 4 - 16 neutron group criticality safety library       ***
***                   hansen-roach data with knight modifications and some endf/b 4 data ***
***                     compiled for nrc       1/27/89                          ***
***                       last updated        10/12/89                          ***
***                          l.m.petrie       ornl                              ***
```

Figure C4.6.4 Part 2 of Material Information Processor printout

C4.6.4 KENO V.a OUTPUT

Output from KENO V.a is printed if the control sequence expects to execute KENO V.a and PARM=CHECK is specified on the analytical sequence indicator. See Sects. F11.6.3 through F11.6.20 for an explanation of the KENO V.a output.

If the control sequence expects to execute KENO V.a and if PARM=CHECK is not specified on the analytical sequence indicator, the KENO V.a output consists of a set of cryptic statements indicating the number of I/Os used to process the KENO V.a data as shown in Fig. C4.6.5.

```
........    0 io's were used before reading keno v data     ........

........    0 io's were used reading the keno v parameter data     ........

*************** data reading completed ***************

........    0 io's were used preparing the keno v input data     ........

........    0 io's were used loading the keno v data     ........

........    0 io's were used loading the data     ........

........    0 io's were used checking the keno v geometry data     ........
*****  restart data has been written on unit 95  *****

........    0 io's were used writing the keno v - csas data     ........

........    0 io's were used before reading search data     ........

........    0 io's were used processing csas input data     ........
```

Figure C4.6.5 Summary of KENO V.a I/O usage by CSAS control module

The first line of Fig. C4.6.5, the number of I/Os used before reading KENO V.a data, is always printed for the analytical sequences contained in the CSAS family of control modules. It is the only line of Fig. C4.6.5 that is printed for CSASN, CSAS1X, CSASI, and CSASIX. The next to the last line of Fig. C4.6.5 is printed only for control modules that expect to perform a search by executing the control module MODIFY (i.e., CSAS4 and CSAS4X). All other lines of Fig. C4.6.5 are printed by control modules that expect to execute KENO V.a (i.e., CSAS25, CSAS2X, CSAS4, and CSAS4X).

C4.6.5 PROGRAM VERIFICATION TABLE FOR THE CONTROL MODULE MODIFY

If a search is to be performed, the control module MODIFY is invoked to alter the KENO V.a geometry data and execute KENO V.a using the new data. This procedure is repeated until the problem achieves convergence, runs out of time or I/Os, or completes the specified number of search passes.

The program verification information table for MODIFY is shown in Fig. C4.6.6. It lists the name of the control module, the date the load module was created, the library that contains the load module, the computer code name from the configuration control table, and the revision number. Some computers do not store load modules in a library, in which case the library entry is left blank. The job name, date, and time of execution are also printed. This information may be useful for quality assurance purposes.

```
 ssssssssss     ccccccccccc      aaaaaaaaa     ll             eeeeeeeeeeee
ssssssssssss   ccccccccccccc    aaaaaaaaaaa    ll             eeeeeeeeeeee
ss         ss  cc          cc  aa         aa   ll             ee
ss             cc              aa         aa   ll             ee
ss             cc              aa         aa   ll             ee
ssssssssssss   cc              aaaaaaaaaaaaa   ll             eeeeeeeee
 ssssssssssss  cc              aaaaaaaaaaaaa   ll             eeeeeeeee
          ss   cc              aa         aa   ll             ee
          ss   cc              aa         aa   ll             ee
ss        ss   cc          cc  aa         aa   ll             ee
ssssssssssss   ccccccccccccc   aa         aa   lllllllllllll  eeeeeeeeeeee
 ssssssssss     ccccccccccc    aa         aa   lllllllllllll  eeeeeeeeeeee

*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                  program verification information                *****
*****                                                                     *****
*****                 code system:    scale  version:    4.2           *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  modify                                       *****
*****                                                                     *****
*****         creation date:  10/25/93                                    *****
*****                                                                     *****
*****              library:  /scale4.2p/exe                               *****
*****                                                                     *****
*****                                                                     *****
*****       production code:  modify                                      *****
*****                                                                     *****
*****              version:  2.1                                          *****
*****                                                                     *****
*****              jobname:  st5                                          *****
*****                                                                     *****
*****     date of execution:  03/14/94                                    *****
*****                                                                     *****
*****     time of execution:  16:46:26                                    *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

Figure C4.6.6 Program verification table for MODIFY

C4.6.6 TABLE OF SEARCH DATA

The table of search data, shown in Fig. C4.6.7, lists the search data for the problem. The KENO V.a title is printed at the top of the table. The search parameters are printed in the top portion of the table after the KENO V.a title and below the heading "SEARCH DATA." The search type is the first entry in the search parameters and defines the type of search to be performed. In this example, a critical pitch search is to be performed. PAS is the number of search passes to be performed. The default value is 10. NPM, the number of search parameters, is defaulted to 1 and should not be changed. EPS is the search convergence tolerance and is defaulted to 0.005. If a critical pitch or critical dimension search is to be performed, KEF, the desired value of k-effective, is printed. It is omitted for "optimum" and "minimum" searches. -CON is the value of the minimum constraint and +CON is the value of the maximum constraint. If a "pitch" search is performed and if values are entered for the minimum allowed pitch, MINPITCH, and the maximum allowed pitch, MAXPITCH, they are printed following +CON.

```
*** critical pitch search for case 2c8 bare ***

****** search data ******

search type                                  critical pitch
pas    number of search passes                      10
npm    number of search parameters                   1
eps    search convergence tolerance                .0050
kef    desired k-effective                         1.0000
-con   minimum constraint                          -.2070
+con   maximum constraint                           .0693

                unit   first  last
command         number region region  ---------- search constants ----------
                                      +x or r  -x or +h  +y or -h  -y  +z  -z
                unit   reg=__ to __
alter/change/modify   1      2      2    1.00     1.00     1.00    1.00  .00  .00
alter/change/modify   1      2      2     .00      .00      .00     .00 1.00 1.00
```

Figure C4.6.7 Table of search data

The bottom portion of the table of search data lists the search command, the unit number, the range of regions in the unit the search command is applicable to, and the search constants for each dimension of those regions. A search constant of 0.0 means the search command should be ignored for that particular dimension. In Fig. C4.6.7, all six dimensions (+X, –X, +Y, –Y, +Z, –Z) of region 2 of unit 1 will be altered.

C4.6.7 SEARCH PASS ITERATION DATA

This portion of the search output is created as the search progresses. At the end of each KENO V.a calculation, the pass number, k-effective, and deviation are printed, followed by the value of the search parameter. The third line is a statement that modified KENO V.a data have been written on unit 95 to provide data for the next pass to KENO V.a. These three lines are printed for every completed search pass. However, the third line is not printed when convergence is achieved. This output is illustrated in Fig. C4.6.8.

```
********** search pass  1    keff=  9.62581E-01 + or -  4.66186E-03  **********
                   the parameter was  0.00000E+00
          *****  modified keno v data has been rewritten on unit 95  *****

********** search pass  2    keff=  9.26968E-01 + or -  4.76267E-03  **********
                   the parameter was  6.92605E-02
          *****  modified keno v data has been rewritten on unit 95  *****

********** search pass  3    keff=  1.01030E+00 + or -  4.65530E-03  **********
                   the parameter was -7.27719E-02
          *****  modified keno v data has been rewritten on unit 95  *****

********** search pass  4    keff=  1.00968E+00 + or -  4.18861E-03  **********
                   the parameter was -5.70604E-02
          *****  modified keno v data has been rewritten on unit 95  *****

********** search pass  5    keff=  9.80129E-01 + or -  5.04216E-03  **********
                   the parameter was -3.87869E-02
          *****  modified keno v data has been rewritten on unit 95  *****

********** search pass  6    keff=  9.98210E-01 + or -  4.21917E-03  **********
                   the parameter was -5.09593E-02
```

Figure C4.6.8 Search pass iteration data

C4.6.8 SEARCH CONVERGENCE INFORMATION

If a search achieves convergence, the search convergence information table is printed as shown in Fig. C4.6.9. The KENO V.a title is the first line printed. The pass at which convergence was achieved is printed followed by the equation used in the search to determine k-effective in terms of the parameter, P. The k-effective and deviation from the converged pass are printed, followed by the geometry description from the converged pass.

```
                                critical pitch search for case 2c8 bare
**********************************************************************************************************************************
**********************************************************************************************************************************

                          convergence was achieved on pass  6  the parameter was  -5.09593E-02

                          the equation used in the search was:

                          k-eff = +9.39989E-01 -9.76969E-01*p +7.86001E+00*p**2 +8.33712E+01*p**3

                          k-effective=  9.98210E-01 + or -  4.21917E-03   the corresponding geometry follows;

             media bias       geometry description for those units utilized in this problem
region        num   id

                                                    -----  unit     1  -----

1 cylinder      1  1  radius =  5.7480   +z =  5.3825   -z = -5.3825   centerline is at  x = 0.00000E+00  y = 0.00000E+00

2 cuboid        0  1       +x =  6.8786   -x = -6.8786   +y =  6.8786   -y = -6.8786     +z =  6.5318     -z = -6.5318
**********************************************************************************************************************************
**********************************************************************************************************************************
```

Figure C4.6.9 Search pass iteration data

C4.6.9 EXTRAPOLATION OF CONVERGED DATA

If a search achieves convergence and has run four or more passes, the data from the search are used to provide an estimate of the parameter that is used to determine the geometry corresponding to the best estimate of the parameter. This last information printed for a search is shown in Fig. C4.6.10.

```
                                critical pitch search for case 2c8 bare

                          based on the preceding data, the best estimate of the parameter is   -5.17118E-02

                          the geometry corresponding to this parameter follows:

             media bias       geometry description for those units utilized in this problem
region        num   id

                                                    -----  unit     1  -----

1 cylinder  1  1  radius = 5.7480  +z = 5.3825  -z = -5.3825  centerline is at  x = 0.00000E+00  y = 0.00000E+00

2 cuboid    0  1       +x = 6.8732  -x = -6.8732 +y =  6.8732  -y = -6.8732     +z =  6.5266     -z = -6.5266
**********************************************************************************************************************************
**********************************************************************************************************************************
                           *****  modified keno v data has been rewritten on unit 95  *****

*****  convergence has been achieved in the search package.  *****

 control module modify   is complete.
```

Figure C4.6.10 Best estimate of the parameter and geometry

C4.7 WARNING AND ERROR MESSAGES

CSAS4 contains two types of warning and error messages. The first type of message is from the Material Information Processor which is common to many of the SCALE analytical sequences. These messages are prefixed by MP- followed by a number. The Material Information Processor messages are listed in numerical order in Sect. C4.7.1. The second type of message pertaining to CSAS4 is identified by CS- followed by a number. These messages are listed in numerical order in Sect. C4.7.2. For additional information concerning a message, simply look up the number in this section.

Warning messages appear when a possible error is encountered. It is the responsibility of the user to verify whether or not the data are correct when a warning message is encountered. The functional modules activated by CSAS4 and related sequences will be executed even though a warning message has been generated.

When an error is recognized, an error message is written and an error flag is set so the functional modules will not be activated. The code stops immediately if the error is too severe to allow continuation of input. However, it will continue to read and check the data if it is able. When the data reading is completed, execution is terminated if an error flag was set when the data were being processed. If the error flag has not been set, execution continues. The STOP codes associated with the severe error messages are listed in Sect. C4.7.3.

C4.7.1 MATERIAL INFORMATION PROCESSOR MESSAGES

The following messages originate in the Material Information Processor, that portion of the analytical sequence that reads the parameter data, standard compositions specification data, and geometry data necessary for preparing the required information for the cross-section processing codes:

MP-1 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 300 is executed when this message is printed.

MP-2 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 310 is executed when this message is printed.

MP-3 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine KNIGHT indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 320 is executed when this message is printed.

MP-4 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine SETUPA indicates that the allocated computer storage will not hold the directories and isotope information tables. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 330 is executed when this message is printed.

MP-5 ***ERROR***SYSTEM GEOMETRY NAME INCORRECT. INSTEAD OF (____), THE USER SHOULD HAVE ENTERED LATTICECELL, MULTIREGION, OR INFHOMMEDIUM AS THE SECOND ITEM ON THE PARAMETER CARD. CHECK SPELLING.

This self-explanatory message is from subroutine SETUPB. The user has misspelled the word defining the type of calculation to be performed, or the parameter data preceding it were entered incorrectly. See Sect. C4.4.3 for assistance in correctly specifying the parameter data.

MP-6 ***ERROR*** _____ NOT FOUND IN STANDARD COMPOSITION LIBRARY. MAKE SURE THE COMPOSITION NAME USED IS IN THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message from subroutine STDCMP indicates that a standard composition name is misspelled, the standard composition specification data were out of order, or the "END" has been omitted from the preceding standard composition specification. Check the standard composition specification data carefully. See Sect. C4.4.4 for assistance with standard composition specification cards. See Sect. M8 for the materials available in the Standard Composition Library.

MP-7 ***ERROR*** THE USER ENTERED A VOLUME FRACTION (VF) OF 0.0 FOR ONE OF THE STANDARD COMPOSITIONS (_____). THIS INDICATES THAT HE INTENDS TO ENTER A NUMBER DENSITY FOR THE STANDARD COMPOSITION. THAT, HOWEVER, CAN ONLY BE DONE WHEN THE STANDARD COMPOSITION NAME REPRESENTS A SINGLE NUCLIDE (LIKE H, O, PB, B-10, U-238, ETC.). CHECK THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message is from subroutine STDCMP. Check the Standard Composition Library, Sect. M8, for the available standard composition names. See Sect. C4.4.4 for the correct method of specifying standard composition specification data.

MP-8 ***ERROR*** CELL TYPE NAME (_____) IS INCORRECT. CHECK THE SPELLING. THE ALLOWED NAMES ARE: SQUAREPITCH, TRIANGPITCH, SPHSQUAREP, SPHTRIANGP, SYMMSLABCELL, ASYMSLABCELL, ASQUAREPITCH, ATRIANGPITCH, ASPHSQUAREP, ASPHTRIANGP, ASQP, ATRP, ASSP, ASTP.

This self-explanatory message is from subroutine LATCEL. The data are misspelled or out of order. Some data items may be missing, or extra ones may have been entered. Errors in the standard composition specification data can cause this message to be printed. See Sect. C4.4.6 for additional assistance.

MP-9 ***ERROR*** THE NUMBER OF ZONES (IZM=_____) IS INCORRECT FOR ASYMSLABCELL GEOMETRY. FOR AN ASYMMETRIC LATTICECELL CALCULATION, ONE SHOULD HAVE IZM=3, 5, OR 7, DEPENDING ON THE MATERIALS PRESENT.

This self-explanatory message is from subroutine LATCEL. See Sect. C4.4.6 for an explanation of the ASYMSLABCELL geometry data. A code error is responsible for this message.

MP-10 ***ERROR*** INSUFFICIENT DATA SUPPLIED ON THE GEOMETRY DESCRIPTION CARD.

This message from subroutine LATCEL can be caused by having an error in the standard composition specification data, thereby causing the reading routines to get out of phase. If no error messages precede this message, it may indicate that a code error exists. The number of material zones (IZM) has been destroyed or altered in some manner.

MP-11 ***ERROR*** MIXTURE _____ IN THE CSAS GEOMETRY DESCRIPTION WAS NOT SPECIFIED IN THE STANDARD COMPOSITION DATA.

This message from subroutine LATCEL indicates that a mixture number used in the geometry description was not defined in the standard composition specification data. Check the input data for consistency. If the specified mixture number is zero and if the problem is a LATTICELL problem using mixture zero for the clad or moderator, it will be necessary to specify a low-density mixture in the standard composition data and use it in the cell specification.

MP-12 ***ERROR*** THE GAP WAS SPECIFIED AS MIXTURE _____ ON THE LATTICECELL. IT SHOULD BE ZERO OR A VALID MIXTURE NUMBER.

This message from subroutine LATCEL indicates that the mixture number used for the GAP was not defined in the standard composition specification data. Check the input data for consistency.

MP-13 **WARNING** NUMBER OF ENTRIES ON THE GEOMETRY DESCRIPTION CARD EXCEEDS THE NUMBER EXPECTED. THIS MESSAGE MAY BE GENERATED IF THE USER FORGOT TO ENTER THE END ON THE GEOMETRY DESCRIPTION CARD.

This message from subroutine LATCEL may result from a code error or from omitting the word "END" from the geometry description card.

MP-14 ***ERROR*** THE COORDINATE SYSTEM NAME (_____) IS INCORRECT. FOR THIS MULTIREGION CALCULATION, THE USER SHOULD HAVE ENTERED SLAB, CYLINDRICAL, SPHERICAL, BUCKLEDSLAB OR BUCKLEDCYL ON THE GEOMETRY DESCRIPTION CARD. CHECK SPELLING.

This self-explanatory message is from subroutine MULTRG.

MP-15 ***ERROR*** ALPHANUMERIC DESCRIPTION OF THE RIGHT-HAND BOUNDARY CONDITION (_____) IS INCORRECT. ONLY VACUUM, REFLECTED, PERIODIC, AND WHITE BOUNDARY CONDITIONS ARE ALLOWED. CHECK SPELLING. CHECK GEOMETRY DESCRIPTION CARD INPUT INSTRUCTIONS FOR ADDITIONAL ASSISTANCE.

This self-explanatory message is from subroutine MULTRG. See Sect. C4.4.6 for additional assistance.

MP-16 ***ERROR*** ALPHANUMERIC DESCRIPTION OF THE LEFT-HAND BOUNDARY CONDITION (_____) IS INCORRECT. ONLY VACUUM, REFLECTED, PERIODIC, AND WHITE BOUNDARY CONDITIONS ARE ALLOWED IN SLAB GEOMETRY. IN THE CASE OF CYLINDRICAL OR SPHERICAL GEOMETRY, ONLY THE REFLECTED BOUNDARY CONDITION IS ALLOWED ON THE LEFT. CHECK SPELLING. CHECK GEOMETRY DESCRIPTION CARD INPUT INSTRUCTIONS FOR ADDITIONAL INSTRUCTIONS.

This self-explanatory message is from subroutine MULTRG. See Sect. C4.4.6 for additional assistance.

MP-17 ***ERROR*** MIXTURE _____ FROM THE MULTIREGION DATA WAS NOT SPECIFIED IN THE STANDARD COMPOSITION DATA.

This message is from subroutine MULTRG. It indicates that a mixture number specified in the multiregion data was not defined in the standard composition specification data. Check the input data for consistency.

MP-18 ***ERROR*** USER MADE AT LEAST _____ DATA ERRORS. PROBLEM WILL NOT BE RUN. HOPEFULLY, EACH OF THESE ERRORS WILL HAVE GENERATED ITS OWN SELF-EXPLANATORY ERROR MESSAGE. IF NOT, CHECK DATA CAREFULLY BEFORE RESUBMITTING.

This self-explanatory message is from subroutine SETUPB. Check through the problem printout and correct all errors that have occurred.

MP-19 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message is from subroutine SETUPB. It indicates that the allocated computer storage will not hold the data that must be loaded to calculate the information that must be passed to BONAMI. The first number is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that is required to hold these data. The third number is the minimum additional words of storage required to hold these data. Subsequent portions of the program may require even more storage. Increase the region size in the "go step" of the job control language and resubmit the problem. A STOP 390 is executed when this message is printed.

MP-20 ***ERROR*** MIXTURE NUMBER _____ ON A STANDARD COMPOSITION CARD IS LESS THAN 1.

This message is from subroutine SETUPB. A mixture number specified on a standard composition specification card must always be greater than zero. This message is triggered if a MP-6 message is printed. Fixing the MP-6 error should eliminate this message. If the printed mixture number is a positive number, a code error is responsible for the message.

MP-21 ***WARNING*** STANDARD COMPOSITION CARD NUMBER _____ IMPLIES THAT MIXTURE NUMBER _____ HAS A TEMPERATURE OF _____ DEGREES KELVIN, WHEREAS STANDARD COMPOSITION SPECIFICATION CARD _____ IMPLIES THAT MIXTURE NUMBER _____ HAS A TEMPERATURE OF _____ DEGREES KELVIN. (ONE OF THESE MAY HAVE BEEN THE VALUE SPECIFIED BY DEFAULT.) THE CODE WILL ASSUME THE HIGHER OF THE TWO AND PROCEED. IF THIS IS NOT SATISFACTORY, THE USER SHOULD ENTER THE CORRECT TEMPERATURE ON EACH OF THE STANDARD COMPOSITION SPECIFICATION CARDS INDICATED.

This self-explanatory message is from subroutine SETUPB.

MP-22 **WARNING** STANDARD COMPOSITION SPECIFICATION CARD(S) MISSING FOR MIXTURE NUMBER _____.

This message from SETUPB is printed to remind the user that the mixture numbers specified in the standard composition specification data are not contiguous. This may result in wasted storage space, but is not necessarily indicative of an error.

MP-23 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MTABLE indicates that the allocated computer storage will not hold the nuclide ID numbers that will be processed by subroutine IDENTS. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 340 is executed when this message is printed.

MP-24 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 350 is executed when this message is printed.

MP-25 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 360 is executed when this message is printed.

MP-26 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine MIXTAB indicates that the allocated computer storage will not hold the three mixing table arrays that will be processed by subroutine ARRAY3. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage needed to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 370 is executed when this message is printed.

MP-27 ***ERROR*** THE NUMBER OF MIXTURES FOUND IN THE MIXING TABLE IS INCONSISTENT WITH THE INPUT DATA. THE NUMBER FOUND IS _____, BUT THE INPUT DATA INDICATED _____.

This message from subroutine REORDR indicates that an error was found in the mixing table during operations to reorder and load it in permanent storage. The number of mixtures found in the mixing table should be the same as the number indicated by the input data. A code error is the likely cause of this message. A STOP 380 is executed when this message is printed.

MP-28 ***ERROR*** NUCLIDE ID _____ SPECIFIED IN THE INPUT DATA WAS NOT FOUND IN THE STANDARD COMPOSITION LIBRARY.

This message is from subroutine IDENTS or subroutine SLNS. A STOP 395 is printed with this message. Check the standard compositions specification data, Sect. C4.4.4, and ensure that the "ZA" ID numbers were entered correctly. This message is also printed if an arbitrary material specifies a value other than 0 or 1 for the MULTIPLE ISOTOPE INDICATOR (IVIS in Sect. C4.4.4).

MP-29 ***ERROR*** AN ARGUMENT OF _____ IS INVALID FOR AN ARCSIN OR ARCCOS.

This message from subroutine ARCHK is indicative of a code error. ARCHK is called from subroutine DAN to ensure that proper arguments are supplied to the ARCSIN and ARCCOS functions in determining cylinder Dancoff factors. This error can be caused by specifying a center-to-center spacing that is smaller than is physically possible.

MP-30 ***ERROR*** THE MATRIX WAS SINGULAR WHEN THE NUMBER FRACTION OF AN ISOTOPE IN AN ELEMENT WAS BEING DETERMINED. MAKE SURE THE SPECIFIED ISOTOPE DISTRIBUTION (WEIGHT PERCENT) SUMS TO 100.0.

This message from subroutine NOFRAC is caused by an isotope distribution that does not sum to 100% for an element. Entry A7 of Sects. C4.4.4 or M7.4.4 illustrates the correct procedure for specifying the weight percent of the various isotopes in an element.

MP-31 ***ERROR*** THE CALCULATED NUMBER FRACTIONS DO NOT REPRODUCE THE WEIGHT PERCENTS ENTERED AS INPUT DATA OR OBTAINED FROM THE STANDARD COMPOSITION LIBRARY.

WTFRAC=nnnnnnnnnn NOFRAC=mmmmmmmmmm MASS=ℓℓℓℓℓℓℓℓℓℓ

This message is printed from subroutine NOFRAC. WTFRAC, NOFRAC, and MASS are printed for each isotope in the standard composition. WTFRAC is the specified input weight percent for the isotope converted to weight fraction instead of weight percent. NOFRAC is the adjusted atom percent converted to atom fraction for the isotope corresponding to a total weight percent of 100% for the isotopes in the standard composition. MASS is the atomic weight of the isotope. The adjusted isotopic weight percents are not printed in MP-31 but can be calculated according to:

$$ADJ_i = \frac{NOFRAC_i \times MASS_i}{\sum_i NOFRAC_i \times MASS_i} \times 100, \qquad \text{(C4.7.1)}$$

where

ADJ_i is the adjusted weight percent of isotope i,

$NOFRAC_i$ is the number fraction of isotope i printed in MP-31,

$MASS_i$ is the atomic weight of isotope i printed in MP-31.

Message MP-31 is printed if the adjusted weight percent of an isotope differs by 0.4% or more from the isotopic weight percent specified for that particular isotope in the standard composition data. An error flag is set, and the problem will not execute. If the isotopic weight percents specified in the input data do not sum to 100%, the weight percent of the first isotope whose specified weight percent is greater than 0.1% is adjusted to force the total weight percent to sum to 100%. If this adjustment results in a calculated weight percent for that isotope that is less than 0.4% different from that specified in the input data, the problem is run using the adjusted data. If message MP-31 is printed, correct the isotopic weight percents specified in the standard composition input data to sum to 100 or specify the isotope with the largest weight percent first, and resubmit the problem.

MP-32 ***ERROR*** END COMP WAS EXPECTED, BUT _____ WAS READ INSTEAD.

This message from subroutine SETUPA is printed if the data is out of order or the keywords END COMP or END COMPOSITIONS are omitted after the last standard composition specification. An END followed by blanks is also allowed. Check the data and the spelling of the END COMP. See Sect. C4.4.4.

MP-33 ***ERROR*** END OF FILE WAS ENCOUNTERED WHILE READING MULTIREGION ZONE DESCRIPTION. VERIFY THAT THE END ZONE CARD WAS ENTERED.

This self-explanatory message from subroutine SETUPA is printed if the END ZONE is omitted following the MULTIREGION zone description data. See Sect. C4.4.7.

MP-34 ***ERROR*** END ZONE WAS EXPECTED, BUT _____ WAS READ INSTEAD.

This message from subroutine SETUPA is printed if data is out of order or the keywords END ZONE are omitted at the end of the MULTIREGION zone description data. Check the data and the spelling of the END ZONE. See Sect. C4.4.7.

MP-35 ***ERROR*** END OF FILE WAS ENCOUNTERED WHEN THE GEOMETRY DESCRIPTION CARD WAS EXPECTED.

This self-explanatory message from subroutine SETUPA is printed if data are omitted or out of order. See Sect. C4.4.

MP-36 ***ERROR*** ILLEGAL SOLUTION NAME _____. ALLOWED NAMES INCLUDE SOLNUO2F2, SOLNUO2(NO3)2 AND SOLNPU(NO3)4.

This self-explanatory message from subroutines SLNS and SLNAME is printed if a solution name is misspelled or data are out of order. See Sect. C4.4.4 for assistance in specifying solution names correctly.

MP-37 ***ERROR*** _____ IS AN INVALID NAME WHEN READING MORE DATA.

This message is printed from subroutine MOREDT when extra parameter data is to be entered as explained in Sect. C4.4.8. The data are out of order, or a parameter name is misspelled.

MP-38 ***ERROR*** INVALID GEOMETRY WORD _____. ONLY INFHOMMEDIUM, MULTIREGION, OR LATTICECELL ARE ALLOWED.

This self-explanatory message is from subroutine SETUPA. Correct the input data and resubmit the problem. Check the spelling of the geometry word, ensure that the data are in order, and resubmit the problem.

MP-39 ***WARNING*** AN END DATA WAS READ BEFORE IT WAS EXPECTED. AN END WAS PROBABLY OMITTED FROM A STANDARD COMPOSITION.

This message from subroutine SETUPA indicates that an "END" was omitted from a standard composition specification or that the END for a standard composition specification was followed by COMP. The first four characters following the END on a standard composition specification card cannot be COMP. The words END COMP terminate the standard composition specification data. Check the standard composition specification data carefully.

MP-40 ***ERROR*** NUCLIDE ID _____ IN MIXTURE _____ DOES NOT OCCUR IN THE STANDARD COMPOSITION LIBRARY.

This self-explanatory message is from subroutine REORDR. A STOP 385 is executed in conjunction with this message.

MP-41 ***ERROR*** A NUCLIDE ID OF _____ IS INVALID FOR _____ IN THE FOLLOWING STANDARD COMPOSITION SPECIFICATION.

This message from subroutine STDCMP indicates that a nuclide ID is not compatible with a standard composition name. For example: UO2 3 1 300 94240 50 94238 50 END would cause this error because plutonium is invalid for a uranium standard composition specification. If this message is printed for a solution, the specific gravity of the solution may have been entered without the required keyword SPG=.

MP-42 ***ERROR*** AN END WAS ENCOUNTERED BEFORE MORE DATA WAS COMPLETED.

This message from MOREDT indicates incomplete input for MORE DATA. See Sect. C4.4.8 or M7.4.8 for assistance.

MP-43 ***WARNING*** BAL=_____ IS AN INVALID BALANCE TABLE SPECIFICATION. ALL BALANCE TABLES WILL BE PRINTED.

This message from subroutine MOREDT indicates that the value entered following BAL= is incorrect. Available options are NONE, FINE, and ALL. If any other value is entered, this message will be printed.

MP-44 *** ERROR *** NUCLIDE _____ IS NOT A MULTIPLE ISOTOPE NUCLIDE ***ERROR***.

This message from subroutine STDCMP indicates that a value greater than zero was entered for the multiple isotope indicator (IVIS) in an arbitrary material and that the first ID NUMBER (NCZA) is not a multiple isotope nuclide (see Sect. C4.4.4). When this message is printed, an error flag is set to prevent execution and IVIS is set to zero to allow the code to continue checking the remaining input data. If an arbitrary material was not specified, this message indicates that the Standard Composition Library is in error for the standard composition printed immediately following this message.

MP-45 ***** ERROR ***** _____ IS NOT A VALID CALCULATION TYPE. USE INFHOMMEDIUM, LATTICECELL, OR MULTIREGION. EXECUTION IS TERMINATED.

This message from subroutine CSPARM indicates that the TYPE OF CALCULATION (see item 3 of Sect. C4.4.3) was spelled incorrectly, entered out of order, or was improperly specified.

MP-46 *** ERROR *** THE FUELOD CANNOT BE GREATER THAN THE PITCH.

This self-explanatory message from subroutine LATCEL results from an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem (see Sect. C4.4.6). The value of PITCH must be at least as large as the value of FUELOD.

MP-47 *** ERROR *** THE CLADOD CANNOT BE LESS THAN THE FUELOD, NOR GREATER THAN THE PITCH.

This message from subroutine LATCEL indicates an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem. See Sect. C4.4.5 and verify the values of PITCH, FUELOD, and CLADOD.

MP-48 *** ERROR *** THE GAPOD CANNOT BE LESS THAN THE FUELOD, NOR GREATER THAN THE CLADOD.

This message from subroutine LATCEL indicates an error in the UNIT CELL SPECIFICATION for a LATTICECELL problem. See Sect. C4.4.6 and verify the values of FUELOD, CLADOD, and CLADID (note that CLADID is the GAPOD and is equal to FUELOD + twice the gap thickness).

MP-49 *** ERROR *** THE ABOVE RADIUS MUST BE GREATER THAN THE PREVIOUS RADIUS.

This message from subroutine MULTRG indicates an error in the GEOMETRY SPECIFICATION for a MULTIREGION problem. See Sect. C4.4.7 and check to ensure that each value of RZ is greater than the previous value of RZ.

MP-50 *** WARNING *** IN MORE DATA, RESONANCE INFORMATION (RES=) WAS SUPPLIED FOR MIXTURE _____. IT WILL NOT BE USED BECAUSE THAT MIXTURE OCCURS IN THE CELL DESCRIPTION.

This message from subroutine MOREDT is printed if resonance data (RES=) are entered for a mixture in MORE DATA (Sect. C4.4.8) and are also used in the cell description (Sects. C4.4.6 and C4.4.7).

MP-51 *** ERROR *** IN MORE DATA _____ IS AN INVALID GEOMETRY TYPE FOR USE IN SPECIFYING RESONANCE DATA.
CYLINDER, SPHERE, OR SLAB MUST BE ENTERED.

This message from subroutine MOREDT is printed if resonance data (RES=) are entered in MORE DATA (Sect. C4.4.8) and an incorrect shape is specified. The correct specification for a sphere of mixture 3 having a radius of 1.5 cm is: RES=3 SPHERE 1.5

MP-52 *** WARNING *** IN MORE DATA, DANCOFF INFORMATION (DAN( )=) WAS SUPPLIED FOR MIXTURE _____. THIS VALUE WILL BE USED INSTEAD OF CALCULATING THE DANCOFF FROM THE CELL DESCRIPTION.

This message from subroutine MOREDT is printed to alert the user that the Dancoff information calculated from the unit cell (Sects. C4.4.6 and C4.4.7) specification is being overridden by the value that was entered in MORE DATA (Sect. C4.4.8).

MP-54 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the volume fraction data from subroutine VERIFY. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-55 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the mixing table data required for subroutine BONAMI. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-56 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the mixture number, outer radii, temperature, sigma-H, and zone identifiers for each BONAMI zone. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-57 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the BONAMI control parameters. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-58 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the cross-section data required by subroutines EPSIG and XSMESH. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-59 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the data required by subroutine XSDRN. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-60 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutine C4DATA indicates that the allocated computer storage will not hold the data required by subroutine ICE. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem.

MP-61 *** ERROR *** THE CROSS-SECTION LIBRARY NAME ENTERED IN THE MATERIAL INFORMATION PROCESSOR DATA FOR THIS CSAS PROBLEM IS INCORRECT. SEE TABLE M8.2.2 OF THE SCALE MANUAL.

This message from subroutine C4DATA indicates that an invalid CROSS-SECTION LIBRARY NAME (see item 2 of Sect. M7.4.3) was entered. The name was misspelled, out of order, or improperly specified.

MP-62 ***ERROR*** A MIXTURE NUMBER IS OUT OF RANGE. ENTRY _____ IN THE MIXING TABLE IS _____. IT SHOULD FALL BETWEEN 1 AND _____, THE LARGEST NUMBER USED IN THE STANDARD COMPOSITION DATA.

This message is from subroutine EPSIG. Because the largest mixture number is determined by the code as the input data are read, this message may be the result of a code error introduced when changes were made to the code.

MP-63 ***ERROR*** A POINTER INTO THE NUCLIDE DATA IS OUT OF RANGE. ENTRY ___ IN THE MIXING TABLE IS _____. IT SHOULD FALL BETWEEN 1 AND _____, THE NUMBER OF NUCLIDES IN THE STANDARD COMPOSITION LIBRARY.

This message is from subroutine EPSIG. It may result from a code error introduced when changes were made to the code.

MP-64 TAPE COPY NEEDS _____ WORDS, BUT ONLY HAS _____ WORDS.

This message from subroutine SHORTX indicates that the allocated computer storage is insufficient to create the short cross-section library utilized by the Materials Information Processor. Increase the region size for the "go step" and resubmit the problem. A STOP 200 is executed when this message is printed.

MP-65 ***** ERROR ***** THE FOLLOWING NUCLIDES WERE NOT FOUND ON THE MASTER LIBRARY:

This message from subroutine SHORTX indicates that the user specified a standard composition that contains a nuclide that is not available on the specified master library. For example, nuclide ID 25304, which is stainless-steel-weighted manganese, is not available on any of the libraries but is listed in the Standard Composition Library. 25055 could be used instead.

MP-66 ***ERROR*** THE MIX. NO. (MIXZ=_____) ASSIGNED TO ZONE IZ=_____ WAS OUTSIDE THE RANGE 0 TO MXX=_____.

This message from subroutine VERIFY indicates that the mixture number is out of range. A code error is the likely cause of this error.

MP-67 **WARNING** MIXTURE _____ WAS ASSIGNED TO ZONES _____ AND _____. THIS MAY BE CORRECT IF THE MIXTURE HAS NO RESONANCE NUCLIDES AND HAS THERMAL SCATTERING DATA AT ONLY ONE TEMPERATURE. USUALLY, UNIQUE MIXTURE NUMBERS SHOULD BE USED IN EACH ZONE, EVEN THOUGH THE MIXTURE SPECIFICATIONS MAY BE IDENTICAL. THIS ALLOWS BONAMI AND NITAWL TO PRODUCE SEPARATE CROSS SECTIONS BASED ON THE APPROPRIATE NUMBER OF EXTERNAL MODERATORS AND THE ACTUAL MEAN CHORD LENGTH FOR EACH SPECIFIED ZONE AS WELL AS THE ACTUAL TEMPERATURE FOR THAT ZONE.

This self-explanatory message is from subroutine VERIFY. The user should verify that the multiple use of the stated mixture number was intentional and correct.

MP-68 ERRONEOUS MIXING TABLE LENGTH FOR XSDRN.

This message from subroutine XSDRN is indicative of a code error. The computed mixing table length, MS, passed to subroutine XSDRN, does not match the counted length in subroutine XSDRN.

MP-69 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

This message from subroutine XSMESH indicates that the allocated computer storage will not hold the interval boundaries and zone number for each interval. The first number printed is the amount of storage, in words, needed to hold this data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage required to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. Specification (by the control module) of too many mesh intervals in a given zone is the most frequent cause of failure. In MULTIREGION calculations where one has a large zone containing a strong absorber (such as a tank of uranyl-fluoride solution), it may be necessary to reduce the number of mesh intervals by increasing the size factor (SZE) in the optional parameter data (Sect. C4.4.8). Making this factor large enough (SZF=10, 15, 20, 30, etc.) will generally allow any problem to run in the space allocated. Once the problem runs, one should check the number density of all

strong absorbers to see if they are realistic. Occasionally a user will accidentally specify an unrealistic concentration of a strong absorber in one or more zones. Such a mistake dramatically increases the number of mesh intervals the code thinks it needs.

MP-70 ***ERROR*** MORE THAN ONE ZONE WAS ENCOUNTERED FOR THIS INFINITE HOMOGENEOUS MEDIA PROBLEM.

This self-explanatory message is from subroutine XSMESH. Correct the input data and resubmit the problem.

MP-71 ***WARNING*** THE TEMPERATURE FOR STANDARD COMPOSITION _____ WAS SPECIFIED AS _____ DEGREE CELSIUS.
DENSITY DATA AT 25 DEGREES CELSIUS WILL BE USED FOR THIS SOLUTION.

This message from subroutine SLNS is printed if SOLNUO2F2 or SOLNPU(NO3)4 were specified in the standard composition data with a temperature outside the range of 15 to 30°C. The Standard Composition Library does not contain data for these solutions outside that temperture range.

MP-72 *** ERROR *** KEYWORD SPG= TO SPECIFY THE SPECIFIC GRAVITY OF THE SOLUTION WAS EXPECTED. KEYWORD _____ WAS READ INSTEAD.

This message from subroutine STDCMP indicates an error in the specification of solution data in the standard composition specification. If the specific gravity of a solution is to be entered, it is the fourth entry after the solution name. Check the solution input data carefully.

MP-73 ***ERROR*** EXTERNAL MODERATOR INDEX IS INCORRECT IN ZONE _____ OF THE MULTIREGION DATA. ENTER NOEXTERMOD, ONE EXTERMOD, OR TWOEXTERMOD INSTEAD OF (_____). CHECK SPELLING.

This self-explanatory message is printed from subroutine MULTRG and subroutine RESDA. The user has misspelled the word defining the external moderator index of the specified zone or the MULTIREGION data are out of order. See Sect. M7.4.4.7.

MP-74 *** ERROR *** FIRST MODERATOR HAS NEGATIVE THICKNESS

This message from subroutine DANCOF indicates that the dimensions specified for an ASYMSLABCELL are inconsistent. The array pitch (PITCH) is smaller than the sum of the second moderator thickness (TKMOD2) and *MAX* where *MAX* is the outside diameter of the clad (CLADOD) if entered; otherwise, *MAX* is the outside diameter of the fuel (FUELOD). Correct the data and resubmit the problem. See Sect. M7.4.6 and Fig. M7.5.6.2 for assistance.

MP-75 *** ERROR *** KEYWORD DEN= OR SPG= TO SPECIFY THE DENSITY OF THE BASIC STANDARD COMPOSITION WAS EXPECTED. KEYWORD _____ WAS READ INSTEAD.

This message from subroutine STDCMP indicates an error in the specification of the density in the basic standard composition data. If the density of the material is to be entered, it is the second entry after the standard composition name. The density is optional data. If the density is entered, it is multiplied by the volume fraction to obtain the density actually used for this composition.

MP-76 *** ERROR *** THE LOWER BOUND OF XSDRN INTERVAL _____ IS _____ WHICH MUST BE LESS THAN THE UPPER BOUND OF _____.

This message from subroutine XSMESH indicates that the specified XSDRN mesh interval is incorrect. Each mesh interval must have a finite positive thickness. This message can be caused by an error in the unit cell data. Either a zero-thick region was specified or the unit cell dimensions were incorrectly specified. Carefully check the unit cell dimensions. If a LATTICECELL annular cell is specified, verify that the FUELOD is at least as large as TKMOP2+2(CLADOD-FUELOD).

MP-77 A NEGATIVE DIMENSION WAS ENCOUNTERED IN THE UNIT CELL DATA. CHECK AND CORRECT THE GEOMETRY DIMENSION.

This message from subroutine LATCEL is printed if a negative number is read for a cell dimension. Check the printed problem geometry and correct the input data (Sect. M7.4.6).

MP-78 THE FUEL THICKNESS IS NEGATIVE. THE ANNULAR CELL DIMENSIONS FOR TKMOD2, CLADOD, AND FUELOD ARE INCONSISTENT.

This message from subroutine LATCEL indicates an error in the description of a cylindrical or spherical annular cell. The cell description must provide a finite fuel thickness. The ID of the fuel is calculated using the diameter of the second moderator, TKMOD2, and the OD of the clad, CLADOD. If the calculated ID of the fuel is greater than or equal to the specified OD of the fuel, there is no fuel in the cell and this message is printed. The thickness of the gap and clad is ½(CLADOD–FUELOD), so the ID of the fuel is TKMOD2+CLADOD–FUELOD. See Sect. M7.4.6 for data input instructions.

MP-79 *** ERROR *** THE ORIGIN MUST BE 0.0 FOR SPHERICAL OR CYLINDRICAL GEOMETRY.

This message from subroutine MULTRG is printed if the origin, ORGN of Table M7.4.8, Sect. M.4.7, is nonzero for a cylinder or sphere. Either the MULTIREGION unit cell data are out of order or a nonzero number has been entered for ORGN. Correct the data and resubmit the problem.

MP-80 *** ERROR *** NOT ENOUGH STORAGE IN CLAPSE – FIRST NUMBER IS THE AMOUNT NEEDED, SECOND IS THE AMOUNT AVAILABLE.

PERTINENT CONSTANTS

This message from subroutine CLAPSE indicates that the allocated computer storage is insufficient to allow collapsing the thermal cross sections to one group for shielding calculations. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated. A STOP 201 is executed when this message is printed.

MP-81 *** ERROR *** DANCOFF FACTOR MUST BE BETWEEN 0.0 AND 1.0.

This message from subroutine MOREDT is printed if DAN(n)= is specified in MORE DATA with a value greater than 1.0 or less than 0.0. Dancoff factors must lie between 0 and 1. The problem will not be run if message MP-81 is printed. Correct the data and resubmit the problem. See Sect. M7.4.7 for assistance.

MP-82 THE FIRST MODERATOR THICKNESS IS NEGATIVE. THE ASYMMETRIC SLAB CELL DIMENSIONS FOR TKMOD2, CLADOD, AND PITCH ARE INCONSISTENT

This message from subroutine LATCEL indicates an error in the description of an asymmetric slab cell. The thickness of the first moderator is not specified in the input data and is calculated as PITCH–TKMOD2/2–CLADOD. If the thickness of the first moderator is negative, this message is printed.

MP-83 *** ERROR *** AN INPUT DATA ERROR HAS BEEN ENCOUNTERED IN THE MATERIAL INFORMATION PROCESSOR DATA ENTERED FOR THIS PROBLEM.

This message from subroutine C4DATA is printed if the subroutine library routine LRDERR returns a value of "TRUE," indicating that a reading error was encountered in the Material Information Processor input data. Locate the unnumbered message stating "***** ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE *****." Correct the data and resubmit the problem.

MP-84 *** WARNING *** FOR MIXTURE _____ THE DANCOFF FACTOR OF _____ IS OUTSIDE THE RANGE OF 0 TO 1. IT WILL BE RESET TO THE CLOSER BOUND.

This message from subroutine RESDA is printed when the DANCOFF factor is less than 10^{-4} outside the allowed range of 0 to 1. This is usually due to roundoff in calculating the Dancoff factor.

MP-85 *** ERROR *** FOR MIXTURE _____ THE DANCOFF FACTOR OF _____ IS OUTSIDE THE RANGE OF 0 TO 1. IT WILL BE RESET TO THE CLOSER BOUND. THE PROBLEM WILL NOT BE EXECUTED.

This message from subroutine RESDA is printed when the Dancoff factor is more than 10^{-4} outside the allowed range of 0 to 1. Check the input data to be sure that the specified Dancoff factor is between 0 and 1. See Sect. M7.4.8 or C4.4.8 for input specifications for the Dancoff factor. If the Dancoff factor was not specified in the optional parameter data, the message is due to a code error.

C4.7.2 MESSAGES FROM CRITICALITY SAFETY SEQUENCE NO. 4

The following messages originate in the part of CSAS4 that reads, checks, and prepares data for KENO V.a and the search module MODIFY.

CS-16 ***WARNING*** READ FLAG NOT FOUND. ASSUME KENO V PARAMETER DATA FOLLOWS.

This message from subroutine CPARAM indicates that the word READ is not the first word of KENO V.a data following the KENO V.a title. If parameter data is to be entered, the code expects the words READ PARAMETERS to precede the parameter input data. If the word READ is not the first word, the code assumes the data are parameter input data.

CS-21 A UNIT NUMBER WAS ENTERED FOR THE CROSS-SECTION LIBRARY. (LIB= IN PARAMETER DATA.) THE DEFAULT VALUE SHOULD BE USED IN ORDER TO UTILIZE THE CROSS SECTIONS GENERATED BY CSAS. MAKE CERTAIN THE CORRECT CROSS-SECTION LIBRARY IS BEING USED.

This message is from subroutine CPARAM. It indicates that a value has been entered for the cross-section library in the KENO V.a parameter data. The cross-section library created by the analytical sequence should be used. MAKE CERTAIN THAT THE CORRECT CROSS SECTIONS ARE BEING USED.

CS-50 *** ERROR *** SEARCH COMMAND NUMBER ____ IS UNABLE TO PERFORM A PITCH SEARCH BECAUSE THE DIMENSIONS OF REGION _____ OF UNIT _____ ARE NOT EXPLICITLY DEFINED.

This message from subroutine PCHSRH indicates that the specified search command is not valid for the specified region. An ARRAY or CORE region cannot be altered; nor can a REPLICATE or REFLECTOR region immediately following an ARRAY or CORE region.

CS-55 *** ERRORS WERE ENCOUNTERED IN PROCESSING THE CSAS-KENO5 DATA. EXECUTION IS IMPOSSIBLE. ***

This message from subroutine SASSY is printed if errors were found in the KENO V.a input data for CSAS. If a search is being made, data reading will continue until all the data have been entered or a fatal error terminates the data reading. When the data reading and checking have been completed, the problem will terminate without executing. Check the printout to locate the errors responsible for this message.

CS-62 *** ERROR *** MIXTURE _____ IN THE GEOMETRY WAS NOT CREATED IN THE STANDARD COMPOSITIONS SPECIFICATION DATA.

This message from subroutine MIXCHK indicates that a mixture specified in the KENO V.a geometry was not created in the standard composition data. If mixture 500 (a cell-weighted, homogenized mixture) is to be used in the KENO V.a geometry data, CSAS2X or CSAS4X must be specified to create it.

CS-65 *** ERROR *** INSUFFICIENT SPACE ALLOCATION. C4DATA WAS NOT CALLED.

This message from the main program, CSAS, is printed if the space requested in the job control language is not enough to hold the program. There is not enough space available to load the material input processor and data preprocessor. Increase the amount of space requested in the job control language and resubmit the problem. A STOP 207 is executed when this message is printed.

CS-66 *** ERROR *** INSUFFICIENT SPACE ALLOCATION. SASSY WAS NOT CALLED.

This message from the main program, CSAS, is printed if the space requested in the job control language is not enough to hold the program. There is not enough space available to load the KENO V.a input processor. Increase the amount of space requested in the job control language and resubmit the problem. A STOP 208 is executed when this message is printed.

CS-67 *** ERROR *** INSUFFICIENT SPACE ALLOCATION. RDOPT WAS NOT CALLED.

This message from the main program, CSAS, is printed if the space requested in the job control language is not enough to hold the program. There is not enough space available to load the processor for

the search data. Increase the amount of space requested in the job control language and resubmit the problem. A STOP 209 is executed when this message is printed.

CS-68 *** ERROR *** AN INPUT DATA ERROR HAS BEEN ENCOUNTERED IN THE ____ DATA ENTERED FOR THIS PROBLEM.

This message from the main program, CSAS, is printed if the subroutine library routine LRDERR returns a value of "TRUE," indicating that a reading error has been encountered in the "KENO PARAMETER" data or the CSAS "SEARCH" data. The appropriate data type is printed in the message. Locate the unnumbered message stating "***** ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE *****." Correct the data and resubmit the problem.

CS-69 ***ERROR*** MIXTURE _____ IS AN INAPPROPRIATE MIXTURE NUMBER FOR USE IN THE KENO GEOMETRY DATA BECAUSE IT IS A COMPONENT OF THE CELL-WEIGHTED MIXTURE CREATED BY XSDRNPM.

This message from subroutine CMXCHK indicates that a mixture that is a component of a cell-weighted mixture has been used in the KENO V.a geometry data.

CS-70 ***** ERROR ***** SEARCH OR OPTIMIZATION DATA MUST BE ENTERED FOR CSAS4, CSAS4X, AND CSAS3. NO SEARCH DATA WAS ENTERED.

This message from subroutine RDOPT is self-explanatory. If the user does not desire to run a search, another sequence such as CSAS25, CSAS2X, or CSAS1X should be chosen.

CS-71 *** ERROR *** _____ IS NOT A VALID SEARCH TYPE.

This message is from subroutine RDOPT. The allowed search types include OPTIMIZATION, DIMENSION, and CONCENTRATION. The first four characters of the search data after the words READ SEARCH must be OPTI, OPT, OPTM, DIM, DIME, DMSN, CON, or CONC. The data may be misspelled or out of order.

CS-72 *** ERROR *** THE SEARCH TYPE IS INVALID. I=_____.

This message is from subroutine RDOPT. The numerical index, I, should be 1 for an optimum pitch search, 2 for a dimension search, and 3 for a concentration search. If it is none of these, the search type has been incorrectly specified or a code error has been introduced.

CS-73 ***** AN END OF FILE WAS ENCOUNTERED BEFORE ALL THE SEARCH DATA WAS READ.

This self-explanatory message is from subroutine RDOPT. Check the input data to be sure nothing was omitted or misspelled.

CS-74 ***** AN END SEARCH FLAG WAS READ BEFORE ALL THE SEARCH DATA WAS READ.

This self-explanatory message is from subroutine RDOPT. Check the input data for omissions and correct order.

CS-75 *** ERROR *** READ SEARCH FLAG WAS NOT FOUND. _____ WAS READ INSTEAD.

This self-explanatory message is from subroutine RDOPT. READ SEARCH was expected but was not found. Check the input data for omissions and correct order.

CS-76 *** ERROR *** END SEARCH FLAG WAS NOT FOUND. _____ WAS READ INSTEAD.

This self-explanatory message from subroutine RDOPT indicates that an end of file was encountered when looking for READ SEARCH. Check the input data for omissions, correct order, and spelling.

CS-77 *** ERROR *** AN END OF FILE WAS FOUND WHEN THE READ SEARCH FLAG WAS EXPECTED.

This self-explanatory message is from subroutine RDOPT. Check the input data for omissions, correct order, and spelling.

CS-78 *** ERROR *** _____ IS NOT A VALID OPTIMIZATION SEARCH TYPE.

This message is from subroutines FIXTYP and OPTYPE. It indicates that an invalid search type was read. The valid search names include OPTIMUM PITCH, OPTIMUM CONCENTRATION, and OPTIMUM DIMENSION. Either the data was entered improperly or a code error has been introduced. A STOP 215 is executed when this message is printed.

CS-79 *** ERROR *** THE SEARCH TYPE IS INVALID. I=_____.

This message from subroutines FIXTYP and OPTYPE indicates that the search type was misspelled or a code error has been introduced. A STOP 216 is executed when this message is printed.

CS-80 *** ERROR *** SEARCH DATA HAS BEEN DESTROYED. I=_____ ICMND=_____ IPNUM=_____ II=_____ IGEOM=_____

This message from subroutines CNCSRH or DIMSRH indicates that the search data cannot be interpreted. This is probably due to a code error.

CS-81 THE SEARCH WAS PREMATURELY TERMINATED BECAUSE ONLY _____ GENERATIONS WERE COMPLETED IN THE LAST KENO PASS. AT LEAST _____ GENERATIONS (NSK= , IN THE KENO PARAMETER DATA) ARE REQUIRED TO SUSTAIN A SEARCH.

This self-explanatory message is from subroutine LODATA. Alter the data and/or the job control language to specify enough time and I/Os to allow completion of a sufficient number of generations in each pass. A STOP 212 is executed when this message is printed.

CS-82 *** AN ERROR WAS ENCOUNTERED IN ONE OF THE FUNCTIONAL MODULES.

This message from MODIFY, the main program of the search package, indicates that an error was encountered during execution of BONAMI, NITAWL, XSDRN, or KENO V.a. Check the printout to locate and correct the error.

CS-83 ***** NO FEASIBLE SOLUTION WAS FOUND IN THE SEARCH PACKAGE. EXECUTION IS TERMINATED. *****

This message from MODIFY, the main program of the search package, is self-explanatory. The code was unable to reach a feasible solution for the requested type of search.

CS-84 **** ERROR **** POINTER INDEX IS OUT OF RANGE. MODIFIED KENO V DATA CANNOT BE WRITTEN. NDX=_____.

This message from subroutine RERITE is probably due to a code error. A STOP 213 is executed when this message is printed.

CS-85 *** ERROR *** ALL OF THE ROOTS FOR K=_____ LIE OUTSIDE THE PARAMETER CONSTRAINTS.

This self-explanatory message from subroutine LODATA indicates that a solution does not exist for the specified desired value of k-effective.

CS-86 FIRST TWO NUMBERS ARE WORDS OF STORAGE NEEDED AND ALLOCATED. THIRD IS REQUIRED ADDITIONAL WORDS.

PERTINENT CONSTANTS

This message from subroutines FIXTYP and OPTYP indicates that the allocated computer storage will not hold the information required for a search. The first number printed is the amount of storage, in words, needed to hold these data. The second number is the amount of computer storage that was allocated, and the third number is the minimum additional words of storage necessary to hold the data to this point. Subsequent portions of the program may require even more storage. Increase the region size for the "go step" in the job control language and resubmit the problem. A STOP 211 is executed in conjunction with this message.

CS-87 *** ERROR *** INSUFFICIENT SPACE ALLOCATION. LODATA WAS NOT CALLED.

This message from subroutine MODIFY indicates that the allocated computer storage is not large enough to load the search data. The message is accompanied by a STOP 220. Increase the requested computer storage in the job control language.

CS-88 *** NOT ENOUGH STORAGE TO LOAD THE KENO V MIXING TABLE.

This message from subroutine MXTBLE is printed if the allocated computer storage will not accommodate the KENO V.a mixing table data. Increase the requested computer storage in the job control language.

CS-89 *** ERROR *** _____ IS AN INVALID DIMENSION SEARCH COMMAND.

This message from subroutine DMSN indicates that the dimension search data are out of order, a search command is spelled incorrectly, or the search data are specified incorrectly.

CS-90 *** ERROR *** _____ IS AN INVALID SEARCH PARAMETER.

This message printed from subroutines FIXCNC, FIXDIM, FIXPCH, OPTCNC, OPTDMN, or OPTPCH indicates that a parameter entered in the search type specification data is not valid (see Sect. C4.4.9.1 and Table C4.4.15). The data could be misspelled or out of order. Omission of the keyword MORE before entering the individual search commands (Sect. C4.4.9.2) can cause this error.

CS-91 *** ERROR *** _____ IS AN INVALID CONCENTRATION SEARCH COMMAND.

This message from subroutine CNCN is caused by a misspelled or illegal search command when attempting to do a concentration search.

CS-92 *** ERROR *** ITY IS NOT PITCH(1), DIMENSION(2), OR CONCENTRATION(3). ITY IS PRINTED BELOW.

PERTINENT CONSTANTS

This message from subroutine LODATA indicates that the search data was incorrect when it was reloaded. This error is probably due to a code error.

CS-93 *** ERROR *** NOPT IS NOT MINIMUM (-1), CRITICAL(0), OR MAXIMUM(1). NOPT IS PRINTED BELOW.

PERTINENT CONSTANTS

This message from subroutine LODATA indicates that the search data were incorrect when they were reloaded. This error is probably due to a code error.

CS-94 *** ERROR *** REG= _____ IS AN INVALID SEARCH DATA ENTRY. THE REGION NUMBER MUST BE GREATER THAN ZERO AND NO LARGER THAN THE NUMBER OF REGIONS IN THE UNIT.

This message from subroutine DMSN indicates that the region to be altered is incorrectly specified. For example, if the unit being altered contains five geometry regions, the value specified for REG= can be as small as 1 and as large as 5.

CS-95 *** ERROR *** AN ERROR WAS ENCOUNTERED IN THE SEARCH DATA. THE LAST REGION NUMBER MUST BE AT LEAST AS LARGE AS THE FIRST REGION NUMBER. CHECK THE SEARCH DATA PRINTED BELOW.
keyword UNIT ____ REGIONS ____ TO ____ PARAMETER=____
SEARCH CONSTANTS ARE _____ _____ _____ _____ _____ _____

This message from subroutine DMSN indicates that the search data specified an invalid region number for the final region to be altered. Check the printed data and correct as appropriate.

CS-96 *** ERROR *** AN ERROR WAS ENCOUNTERED IN THE SEARCH DATA. THE REGION NUMBERS MUST BE GREATER THAN ZERO AND NO LARGER THAN THE NUMBER OF REGIONS IN THE UNIT. CHECK THE SEARCH DATA PRINTED BELOW.
keyword UNIT _____ REGIONS _____ TO _____ PARAMETER=_____
SEARCH CONSTANTS ARE _____ _____ _____ _____ _____ _____

This message from subroutine DMSN indicates that one of the specified region numbers is incorrect. Check the printed data and correct as appropriate.

CS-97 *** ERROR *** NO VALID SEARCH COMMANDS WERE FOUND IN THE DATA.

This message is accompanied by a STOP 235 and is printed from subroutines PCHSRH, CNCSRH, and DIMSRH. A common cause of this error is the omission of the MORE command before the individual search commands are entered. See Sects. C4.4.10.1 and C4.4.10.2.

CS-99 THIS PROBLEM WILL NOT BE RUN BECAUSE PARM=CHECK WAS ENTERED IN THE ANALYTICAL SEQUENCE SPECIFICATION.

This message from subroutine CSAS indicates that the problem data were read and checked and no errors were found. To execute the problem, remove the PARM=CHECK or PARM=CHK from the analytical sequence indicator data entry.

CS-100 THIS PROBLEM WILL NOT BE RUN BECAUSE ERRORS WERE ENCOUNTERED IN THE INPUT DATA.

This message from subroutine CSAS is self-explanatory. Examine the printout to locate the error or errors in the input data. Correct them and resubmit the problem.

C4.7.3. STOP CODES

The STOP codes that are utilized in CSAS3 and CSAS4 are listed in tabular form, indicating the subroutine where they occur and the associated error message. A STOP is executed when a fatal error is recognized. Locate the associated message number to determine the appropriate corrective measures. A traceback may be generated whenever subroutine SOTP is called to print a message. If no traceback is indicated in the STOP CODE table, a STOP is printed at the completion of the associated message.

Stop No.	Subroutine	Traceback	Associated Message
20			See Sect. C4.7.5
200	SHORTX	No	MP-64
201	CLAPSE	No	MP-80
203	MXTBLE	No	CS-88
207	CSAS	Yes	CS-65
208	CSAS	Yes	CS-66
209	CSAS	Yes	CS-67
211	OPTYP	No	CS-86
	FIXTYP	No	CS-86
212	LODATA	No	CS-81
213	RERITE	No	CS-84
214	CSAS	Yes	CS-68
215	OPTYP	No	CS-78
	FIXTYP	No	CS-78
216	OPTYP	No	CS-79
	FIXTYP	No	CS-79
220	MODIFY	No	CS-87
225	LODATA	Yes	CS-92
230	LODATA	Yes	CS-93
235	DIMSRH	Yes	CS-97
	OPTSRH	Yes	CS-97
	PCHSRH	Yes	CS-97
300	KNIGHT	Yes	MP-1
310	KNIGHT	Yes	MP-2
320	KNIGHT	Yes	MP-3
330	SETUPA	Yes	MP-4
340	MTABLE	Yes	MP-23
350	MIXTAB	Yes	MP-24
360	MIXTAB	Yes	MP-25
370	MIXTAB	Yes	MP-26
380	REORDR	No	MP-27
385	REORDR	No	MP-40
390	SETUPB	Yes	MP-19
395	IDENTS	No	MP-28
	SLNS	No	MP-28
396	CSPARM	No	MP-45

C4.7.4 MESSAGES ASSOCIATED WITH STOP 20 IN CSAS

The following messages from Subroutine Library routines will result in a STOP 20 in the material information processor and CSAS:

LMP001 DA ERROR - INVALID UNIT NUMBER. THE LOGICAL UNIT NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that an invalid unit number was specified as a direct-access device. In CSAS this message is indicative of a code error.

LMP002 DA ERROR - FORTRAN USING THIS UNIT. THE LOGICAL UNIT NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that the specified unit number is open as a sequential dataset rather than a direct-access dataset. In CSAS, this error may be caused by entering a direct-access unit number for FRD= or FWR= in MORE DATA.

LMP003 DA ERROR - DCB NOT OPEN. THE LOGICAL UNIT NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that the program attempted to read or write on a direct-access device but that the data control block was not open. In CSAS this message is indicative of a code error.

LMP004 DA ERROR - UNABLE TO OPEN DCB. THE LOGICAL UNIT NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that the program is unable to open the data control block for the direct-access device. This message indicates that the job control language did not include proper specification of the above-named unit.

LMP005 DA ERROR - RELATIVE BLOCK NOT IN DATA SET. RELATIVE BLOCK NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that the number of direct-access blocks is too small for the problem. Increase the number of direct-access blocks in MORE DATA by entering the parameter DAB=nnn where nnn is larger. For example, if the relative block number is 201, try increasing the number of direct-access blocks to 300 or more. For CSAS25, CSAS2X, CSAS4, and CSAS4X, it may also be necessary to set NB8=nnn in the KENO parameter data.

LMP006 DA ERROR - INVALID BLOCK LENGTH. THE BLOCK LENGTH IS _____.

This message from the Subroutine Library direct-access routines indicates that the length of the direct-access blocks is invalid. A valid block length must be positive. In CSAS this message is indicative of a code error.

LMP007 DA ERROR - DCB ALREADY OPEN. THE LOGICAL UNIT NUMBER IS _____.

This message from the Subroutine Library direct-access routines indicates that the data control block for the above-named unit was previously opened and not closed.

LMP008 DA ERROR – PERMANENT I/O ERROR.

This message from the Subroutine Library direct-access routines indicates that a permanent I/O error has occurred.

C4.7.5 UNNUMBERED MESSAGES

Occasionally the code may terminate without printing a message that can be located via the message number. Some of these messages are:

***** END OF FILE READ ON UNIT n *****

This message is from subroutine ENFILE in the Subroutine Library. Unit n is the device from which data is being read. This message can be caused by lack of a double blank between the END for the last standard composition and the END COMP. It can also be caused by omitting the END COMP or misspelling COMP in the END COMP entry. Other causes include incomplete or missing data. A traceback accompanies this message. Correct the data and resubmit the problem.

***** ERROR IN INPUT. CARD IMAGE PRINTED ON NEXT LINE *****
card image is printed here
ON THE ABOVE CARD, CHARACTER NUMBER m (IMAGE=c) IS NOT VALID.

This message is from the Subroutine Library free-form reading routine DREAD. The character number, m, and the character image, c, printed in the message are recognized as being invalid for the type of data being read. For example, character data were encountered when numerical data were expected. This message can be caused by missing or incomplete data and by omitting double blanks after a labeled or unlabeled END. A traceback accompanies this message. Correct the data and resubmit the problem.

APPENDICES

C4.A ALPHABETICAL SUBROUTINE INDEX AND CROSS REFERENCE

C4.B SAMPLE PROBLEMS

C4.C SAMPLE OUTPUT

C4.A ALPHABETICAL INDEX OF SUBROUTINES

This section provides a convenient alphabetical index of the subroutines and functions and common blocks used in CSAS.

Table C4.A.1 provides an alphabetical listing of the subroutines and functions that comprise CSAS. The first column lists the subroutine name, the second column lists the subroutine that calls it, and the third column contains a list of the subroutines it calls. KENO V.a subroutines utilized by CSAS are contained in brackets <>; Material Information Processor subroutines used by CSAS are contained in braces {}, and FORTRAN-supplied library routines are contained in parentheses ().

Table C4.A.2 provides an alphabetical listing of the subroutines and functions in the control module MODIFY. MODIFY allows the user to perform searches using KENO V.a.

Table C4.A.3 provides an alphabetical index of the common blocks used in CSAS.

Table C4.A.4 provides an alphabetical index of the common blocks used in MODIFY.

Table C4.A.1 Alphabetical index of CSAS routines

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{ADAN}	{DAN}	(ACOS) (ASIN) (COS) (SIN) (SQRT) {GAUSS} {GDAN}
<ADJUST>	<HOLCHK>	MOVE
(ACOS)	{ADAN} {DAN} {FINNER} {GDAN} {OUTER} {SPHDAN}	
(ASIN)	{ADAN} {GDAN} {OUTER}	
(COS)	{ADAN} {DAN} {FINNER} {GDAN} {OUTER}	
(EXP)	{DANCOF} {DANDAD} {FINNER}	
(SIN)	{ADAN} {FINNER} {GDAN} {OUTER}	
(SQRT)	{ADAN} {BALL} {DAN} {FINNER {GDAN} {OUTER} {POKE}	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
(ASIN)	<VOLUME>	
(EXP)	{NFLUX}	
(SQRT)	{BONDA}	
	<CORSIZ>	
	<CRMAX>	
	<CRMIN>	
	{DANCOF}	
	{EPSIG}	
	<HOLHOL>	
	{NFLUX}	
	<RDPLOT>	
	<SRMAX>	
	<SRMIN>	
	<VOLUME>	
	<XRMIN>	
	<XXLIM>	
	<XXMIN>	
{AGAUSS}	{DAN}	
	{SPHDAN}	
<ALBRD>	<DIFALB>	<ALBUSE>
<ALBUSE>	<ALBRD>	INQUIR
		IO
		RITE
ALLOWC	{MOREDT}	
ALOCAT	CSAS	
<ARALBA>	<JOMITY>	<PRTLBA>
	SASSY	
<ARASIZ>	<CORSIZ>	<LSCAN>
<ARAYIN>	<DATAIN>	AREAD
		<BOX>
		CLEAR
		<HLFWRD>
		IREAD
		<RCHRS>

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		<RDBOX>
		STOP
		YREAD
{ARCHK}	{DAN}	
AREAD	<ARAYIN>	
	CNCN	
	CPARAM	
	{CSPARM}	
	<DATAIN>	
	DMSN	
	FIXCNC	
	FIXDIM	
	FIXPCH	
	FIXTYP	
	<KENOG>	
	{LATCEL}	
	<MIXIT>	
	{MOREDT}	
	{MULTRG}	
	OPTCNC	
	OPTDMN	
	OPTPCH	
	OPTYP	
	<RCHRS>	
	<RDBIAS>	
	RDOPT	
	<RDORGN>	
	<RDPLOT>	
	<RDREF>	
	<RDSTRT>	
	{SETUPA}	
	{SETUPB}	
	{STDCMP}	
{ARRAY3}	{MIXTAB}	
{AVGB}	{BOND}	
{AVGY}	{TWODYS}	MGCWRD
		STOP

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{AVG1}	{CLAPSE}	
{AVG2}	{TWODXS}	MGCWRD
{AXSDRN}	{C4DATA}	
{BALL}	{DANDAD}	(SQRT) {SPHDAN}
{BINFIL}	{ICE} {XSDRN}	
{BINRCF}	{BONAMI} {ICE} {NITAWL} {XSDRN}	
{BINRCX}	{BONAMI} {ICE} {NITAWL} {XSDRN}	
BIRITE	CPARAM	
{BONAMI}	{C4DATA}	{BINRCF} {BINRCX} {LCHKMX}
{BOND}	{CLAPSE}	{AVGB} {FOLD} IO {UNFOLD}
{BONDA}	{RESDA}	(SQRT)
<BOX>	<ARAYIN>	
<BOXC>	<LOADIT>	
{CALCMS}	{C4DATA}	{LCHKMX}
CELLMX	{C4DATA}	{LCHKMX}

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{CINIT}	{C4DATA}	CLEAR
		INQUIR
		OPENDA
		RITE
{CLAPSE}	{C4DATA}	{AVG1}
		{BOND}
		CLEAR
		COPY
	{DEAN}	
		IO
		IO4
		STOP
		{TWODXS}
		{TWODYS}
CLEAR	<ARAYIN>	
	{CINIT}	
	{CLAPSE}	
	CNCN	
	CPARAM	
	CSAS	
	{C4DATA}	
	<DATAIN>	
	DMSN	
	<GEOMIN>	
	<HOLE>	
	<HUNTER>	
	<LODARA>	
	<LODWTS>	
	<MESH>	
	{NITAWL}	
	<PRTPLT>	
	<RDALB>	
	<RDICE>	
	RDOPT	
	<RDPLOT>	
	<RDSTRT>	
	<RELATE>	
	{RESDA}	
	<RGUSED>	
	<RTARA>	
	<SAVST6>	
	{SETUPB}	
	<SORTA>	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
	{TWODXS}	
	{TWODYS}	
	<UNTCRS>	
	<VOLUME>	
	{XSDRN}	
CLOSDA	CSAS	
	{KNIGHT}	
	{SHORTX}	
CMXCHK	SASSY	{LCHKMX}
CNCN	FIXTYP	AREAD
	OPTYP	CLEAR
		FREAD
		INQUIR
		IREAD
		RITE
CNCSRH	FIXTYP	PRTSRH
	OPTYP	RITE
		STOP
COPY	{CLAPSE}	
	{SHORTX}	
	{TWODXS}	
	{TWODYS}	
<CORSIZ>	<JOMITY>	(SQRT)
		<ARASIZ>
CPARAM	CSAS	AREAD
		BIRITE
		CLEAR
		FREAD
		IREAD
		LIBEQL
		OPNFIL
		RNDIN
		RNDOUT
		TIMFAC
		ZREAD
CREAD	<RDREF>	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
<CRMAX>	<HOLEXT>	(SQRT)
	<JOMCHK>	<CRSPRD>
		<DOTPRD>
		STOP
		<VECADD>
		<VECNRM>
<CRMIN>	<HOLHOL>	(SQRT)
		<CRSPRD>
		<DOTPRD>
		STOP
	<VECADD>	
		<VECNRM>
<CRSPRD>	<CRMAX>	
	<CRMIN>	
	<SRMAX>	
	<SRMIN>	
CSAS		ALOCAT
		CLEAR
		CLOSDA
		CPARAM
		{C4DATA}
		GETMS
		INDEX
		IOLEFT
		<IOSDUN>
		OPNFIL
		PARTBL
		RDOPT
		RESETM
		SASSY
		SCANON
		STOP
{CSPARM}	{SETUPA}	AREAD
		LCOMPR
		{SMMTBA}
{C4DATA}	CSAS	{AXSDRN}
		{BONAMI}
		{CALCMS}
		CELLMX
		{CINIT}

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		{CLAPSE}
		CLEAR
		{EPSIG}
		{ICE}
		{KNIGHT}
		{MIPCHK}
		{NITAWL}
		{PRELPS}
		{SHORTX}
		{SMMTBA}
		STOP
		{VERIFY}
		{XSDRN}
		{XSMESH}
{DAN}	{DANDAD}	{ADAN}
		(ACOS)
		(COS)
		(SQRT)
		{AGAUSS}
		{ARCHK}
		ERRSET
{DANCOF}	{RESDA}	(EXP)
		(SQRT)
		{DANDAD}
		E3
		SHELC
		STOP
{DANDAD}	{DANCOF}	(EXP)
		{BALL}
		{DAN}
		{SDAN}
<DATAIN>	SASSY	<ARAYIN>
		AREAD
		CLEAR
		<EXTRA>
		<FLDATA>
		<GEOMIN>
		<IDX1D>
		IOWRT
		<MIXIT>
		<RDBIAS>

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		<RDPLOT>
		<RDREF>
		<RDRST>
		<RDSTRT>
		<RT>
		<RTARA>
		<SAVST6>
		STOP
		<WRTPLT>
{DEAN}	{CLAPSE}	{KAUL}
<DIFALB>	<FLDATA>	<ALBRD>
DIMSRH	FIXTYP	PRTSRH
	OPTYP	RITE
		STOP
DMSN	FIXTYP	AREAD
	OPTYP	CLEAR
		FREAD
		INQUIR
		IREAD
		RITE
<DOTPRD>	<CRMAX>	
	<CRMIN>	
	<SRMAX>	
	<SRMIN>	
	<XRMIN>	
DTASET	{SHORTX}	
{EPSIG}	{C4DATA}	(SQRT)
ERRSET	{DAN}	
<EXTRA>	<DATAIN>	
E3	{DANCOF}	
	{SDAN}	
{FAX}	{STDCMP}	FREAD
		IREAD

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{FAXPRT}	{STDCMP}	
<FINDBX>	<LOCATE>	
{FINNER}	{OUTER}	(ACOS) (COS) (EXP) (SIN) (SQRT)
{FIX}	{STDCMP}	
FIXCNC	FIXTYP	AREAD FREAD IREAD
FIXDIM	FIXTYP	AREAD FREAD IREAD
FIXPCH	FIXTYP	AREAD FREAD IREAD REED
FIXTYP	RDOPT	AREAD CNCN CNCSRH DIMSRH DMSN FIXCNC FIXDIM FIXPCH PCHSRH REED STOP
<FLDATA>	<DATAIN>	<DIFALB> REED <RGUSED> RITE <SORTA> <SORTR>

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		STOP
		<WATES>
{FOLD}	{BOND}	
{FOX}	{STDCMP}	
FREAD	CNCN	
	CPARAM	
	DMSN	
	{FAX}	
	FIXCNC	
	FIXDIM	
	FIXPCH	
	{LATCEL}	
	<MIXIT>	
	{MOREDT}	
	{MULTRG}	
	OPTCNC	
	OPTDMN	
	OPTPCH	
	<RDBIAS>	
	<RDORGN>	
	<RDPLOT>	
	<RDSTRT>	
	{SETUPA}	
	{STDCMP}	
	<XXIN>	
{GAUSS}	{ADAN}	
	{OUTER}	
{GDAN}	{ADAN}	(ACOS)
		(ASIN)
		(COS)
		(SIN)
		(SQRT)
		KI3
<GEOMIN>	<DATAIN>	CLEAR
		<KENOG>
		<READGM>
		STOP

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
GETMS	CSAS	
GETPTR	<RCHRS>	
{GFLUX}	{PRELPS}	
<GOCURS>	<VOLUME>	<HUNTER>
<GTVOLS>	<VOLUME>	
<HLFWRD>	<ARAYIN>	
{HOGGIE}	{TWODYS}	STOP
<HOLCHK>	<JOMCHK>	<ADJUST> <HOLEXT> <HOLHOL>
<HOLE>	<LODARA>	CLEAR STOP
<HOLEXT>	<HOLCHK>	<CRMAX> <SRMAX> <XXLIM>
<HOLHOL>	<HOLCHK>	(SQRT) <CRMIN> <SRMIN> <XRMIN> <XXMIN>
<HUNTER>	<GOCURS> <VOLUME>	CLEAR MOVE
{ICE}	{C4DATA}	{BINFIL} {BINRCF} {BINRCX} {VOLFRC}
{IDENTS}	{MTABLE}	{ISCAN} {NOFRAC}
<IDX1D>	<DATAIN>	IREAD

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
INDEX	CSAS	
	<RTADJ>	
INQUIR	<ALBUSE>	
	{CINIT}	
	CNCN	
	DMSN	
	<MIXIT>	
	MXTBLE	
	<PRTPLT>	
	<RDALB>	
	<RDARA>	
	<RDICE>	
	RDOPT	
	<RDRST>	
	<RDWTS>	
	<RT>	
	<RTARA>	
	<SAVST6>	
	<WAITIN>	
	<WATES>	
	<WRTALB>	
	<WRTICE>	
	<WRTPLT>	
	<WRTRST>	
IO	<ALBUSE>	
	{BOND}	
	{CLAPSE}	
	<RDALB>	
	<RDARA>	
	<RDBIAS>	
	<RDICE>	
	<RDPLOT>	
	<RDRST>	
	<RDSTRT>	
	<RDWTS>	
	<SAVST6>	
	{TWODXS}	
	{TWODYS}	
	<WAITIN>	
	<WATES>	
	<WRTALB>	
	<WRTARA>	
	<WRTICE>	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
	<WRTPLT>	
	<WRTRST>	
	<WRTWTS>	
IOLEFT	CSAS	
	<IOSDUN>	
<IOSDUN>	CSAS	IOLEFT
	<JOMITY>	
	SASSY	
IOWRT	<DATAIN>	
	{SHORTX}	
IO4	{CLAPSE}	
	{TWODXS}	
	{TWODYS}	
IREAD	<ARAYIN>	
	CNCN	
	CPARAM	
	DMSN	
	{FAX}	
	FIXCNC	
	FIXDIM	
	FIXPCH	
	<IDX1D>	
	<KENOG>	
	{LATCEL}	
	<MIXIT>	
	{MOREDT}	
	{MULTRG}	
	OPTCNC	
	OPTDMN	
	OPTPCH	
	<RDBIAS>	
	<RDBOX>	
	<RDPLOT>	
	<RDSTRT>	
	{SETUPA}	
	{SETUPB}	
	{STDCMP}	
	{XSMESH}	
	<XXIN>	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{ISCAN}	{IDENTS}	
	{NITAWL}	
	{REORDR}	
	{SLNS}	
	{STDCMP}	
<JOMCHK>	<JOMITY>	<CRMAX>
		<HOLCHK>
		<SRMAX>
		<XXLIM>
<JOMITY>	SASSY	<ARALBA>
		<CORSIZ>
		<IOSDUN>
		<JOMCHK>
		<LOADIT>
		<PRTJOM>
		<VOLUME>
{KAUL}	{DEAN}	
<KENOG>	<GEOMIN>	AREAD
		IREAD
		<RCHRS>
		<RDORGN>
		<XXIN>
		XXINA
KI3	{GDAN}	
{KNIGHT}	{C4DATA}	CLOSDA
		MESAGE
		OPENDA
		REED
		{SETUPA}
		STOP
{LATCEL}	{SETUPB}	AREAD
		FREAD
		IREAD
		LCOMPR
		{MIXERR}
		SCANOF
		SCANON

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{LCHKMX}	{BONAMI}	
	{CALCMS}	
	CELLMX	
	CMXCHK	
	MIXCHK	
	{XSDRN}	
LCOMPR	{CSPARM}	
	{LATCEL}	
	{MULTRG}	
	{RESDA}	
	{SETUPA}	
	{SETUPB}	
	{SMMTBA}	
LEN	<RCHRS>	
LIBEQL	CPARAM	
<LOADIT>	<JOMITY>	<BOXC>
		<LODALB>
		<LODARA>
		<PRTARA>
		REED
<LOCATE>	<MESH>	<FINDBX>
		<LOCBOX>
		MOVE
		<POSIT>
<LOCBOX>	<LOCATE>	
	<LODARA>	
	<SORTA>	
<LODALB>	<LOADIT>	REED
<LODARA>	<LOADIT>	CLEAR
		<HOLE>
		<LOCBOX>
		REED
<LODRGC>	<RGUSED>	
<LODWTS>	SASSY	CLEAR
		<PRTWTS>

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		RD REED
{LOGID}	{SHORTX}	
LREAD	<MIXIT> {MULTRG} {SETUPA} {STDCMP}	
<LSCAN>	<ARASIZ> <RGUSED>	
MESAGE	{KNIGHT}	
<MESH>	<PRINT>	CLEAR <LOCATE>
MGCWRD	{AVGY} {AVG2}	
{MIPCHK}	{C4DATA}	WOT8
MIXCHK	MXTBLE	{LCHKMX}
{MIXERR}	{LATCEL} {MOREDT} {MULTRG}	
<MIXIT>	<DATAIN>	AREAD FREAD INQUIR IREAD LREAD <RDMIXT> RITE STOP
{MIXTAB}	{SETUPB}	{ARRAY3} {MODIFY} {MTABLE} {REORDR} STOP

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{MODIFY}	{MIXTAB}	
{MOREDT}	{SETUPB}	ALLOWC
		AREAD
		FREAD
		IREAD
		{MIXERR}
		RESETC
		SCANOF
		SCANON
MOVE	<ADJUST>	
	<HUNTER>	
	<LOCATE>	
	SASSY	
	<SAVST6>	
	{TWODYS}	
	<VOLUME>	
	<WATES>	
{MTABLE}	{MIXTAB}	{IDENTS}
		STOP
{MULTRG}	{SETUPB}	AREAD
		FREAD
		IREAD
		LCOMPR
		LREAD
		{MIXERR}
		SCANOF
		SCANON
MXTBLE	SASSY	INQUIR
		MIXCHK
		RITE
		STOP
		TABLE
{NFLUX}	{PRELPS}	(EXP)
		(SQRT)
{NITAWL}	{C4DATA}	{BINRCF}
		{BINRCX}

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		CLEAR
		{ISCAN}
{NOFRAC}	{IDENTS}	{WTINV}
OPENDA	{CINIT}	
	{KNIGHT}	
	{SHORTX}	
OPNFIL	CPARAM	
	CSAS	
	<RDSTRT>	
	{SHORTX}	
OPTCNC	OPTYP	AREAD
		FREAD
		IREAD
OPTDMN	OPTYP	AREAD
		FREAD
		IREAD
OPTPCH	OPTYP	AREAD
		FREAD
		IREAD
		REED
OPTYP	RDOPT	AREAD
		CNCN
		CNCSRH
		DIMSRH
		DMSN
		OPTCNC
		OPTDMN
		OPTPCH
		PCHSRH
		REED
		STOP
{OUTER}	{SPHDAN}	(ACOS)
		(ASIN)
		(COS)
		(SIN)
		(SQRT)

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		{FINNER}
		{GAUSS}
PARTBL	CSAS	RNDOUT
{PATCH}	{TWODXS}	
	{TWODYS}	
PCHSRH	FIXTYP	PRTSRH
	OPTYP	RITE
		STOP
		<XXLIM>
<POINT>	SASSY	
{POKE}	{SETUPB}	(SQRT)
<POSIT>	<LOCATE>	
PRATBL	SASSY	<RTADJ>
{PRELPS}	{C4DATA}	{GFLUX}
		{NFLUX}
<PRINT>	<PRTPLT>	<MESH>
<PRTARA>	<LOADIT>	
	SASSY	
<PRTJOM>	<JOMITY>	
	SASSY	
<PRTLBA>	<ARALBA>	
<PRTPLT>	SASSY	CLEAR
		INQUIR
		<PRINT>
		REED
		<RELATE>
		<UNTCRS>
PRTSRH	CNCSRH	
	DIMSRH	
	PCHSRH	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
<PRTWTS>	<LODWTS>	
<RCHRS>	<ARAYIN>	AREAD
	<KENOG>	GETPTR
	<RDPLOT>	LEN
		RCRDLN
		RSTPTR
		STOP
RCRDLN	<RCHRS>	
RD	<LODWTS>	
<RDALB>	<RDRST>	CLEAR
		INQUIR
		IO
		RITE
<RDARA>	<RDRST>	INQUIR
		IO
		RITE
<RDBIAS>	<DATAIN>	AREAD
		FREAD
		IO
		IREAD
		<WAITIN>
<RDBOX>	<ARAYIN>	IREAD
<RDICE>	<RDRST>	CLEAR
		INQUIR
		IO
		RITE
<RDMIXT>	<MIXIT>	
RDOPT	CSAS	AREAD
		CLEAR
		FIXTYP
		INQUIR
		OPTYP
		RITE

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
<RDORGN>	<KENOG>	AREAD
		FREAD
<RDPLOT>	<DATAIN>	(SQRT)
		AREAD
		CLEAR
		FREAD
		IO
		IREAD
		<RCHRS>
<RDREF>	<DATAIN>	AREAD
		CREAD
<RDRST>	<DATAIN>	INQUIR
		IO
		<RDALB>
		<RDARA>
		<RDICE>
		<RDWTS>
		RITE
<RDSTRT>	<DATAIN>	AREAD
		CLEAR
		FREAD
		IO
		IREAD
		OPNFIL
<RDWTS>	<RDRST>	INQUIR
		IO
		RITE
<READGM>	<GEOMIN>	
REED	FIXPCH	
	FIXTYP	
	<FLDATA>	
	{KNIGHT}	
	<LOADIT>	
	<LODALB>	
	<LODARA>	
	<LODWTS>	
	OPTPCH	
	OPTYP	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
	<PRTPLT>	
	{SHORTX}	
	<SORTA>	
	{STDCMP}	
	<WATES>	
	<WRTALB>	
	<WRTARA>	
	<WRTICE>	
	<WRTRST>	
	<WRTWTS>	
<RELATE>	<PRTPLT>	CLEAR
{REORDR}	{MIXTAB}	{ISCAN}
{RESDA}	{SETUPB}	{BONDA}
		CLEAR
		{DANCOF}
		LCOMPR
RESETC	{MOREDT}	
RESETM	CSAS	
<RGUSED>	<FLDATA>	CLEAR
		<LODRGC>
		<LSCAN>
RITE	<ALBUSE>	
	{CINIT}	
	CNCN	
	CNCSRH	
	DIMSRH	
	DMSN	
	<FLDATA>	
	<MIXIT>	
	MXTBLE	
	PCHSRH	
	<RDALB>	
	<RDARA>	
	<RDICE>	
	RDOPT	
	<RDRST>	
	<RDWTS>	
	<RT>	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
	<RTARA>	
	<SAVST6>	
	<WAITIN>	
	<WATES>	
	<WRTPLT>	
RNDIN	CPARAM	
RNDOUT	CPARAM	
	PARTBL	
	<WRTRST>	
RSTPTR	<RCHRS>	
<RT>	<DATAIN>	INQUIR
		RITE
<RTADJ>	PRATBL	INDEX
<RTARA>	<DATAIN>	CLEAR
		INQUIR
		RITE
SASSY	CSAS	<ARALBA>
		CMXCHK
		<DATAIN>
		<IOSDUN>
		<JOMITY>
		<LODWTS>
		MOVE
		MXTBLE
		<POINT>
		PRATBL
		<PRTARA>
		<PRTJOM>
		<PRTPLT>
		STOP
		<WRTRST>
<SAVST6>	<DATAIN>	CLEAR
		INQUIR
		IO
		MOVE

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		RITE
		STOP
SCANOF	{LATCEL}	
	{MOREDT}	
	{MULTRG}	
	{STDCMP}	
SCANON	CSAS	
	{LATCEL}	
	{MOREDT}	
	{MULTRG}	
	{SETUPA}	
{SDAN}	{DANDAD}	E3
{SETUPA}	{KNIGHT}	AREAD
		{CSPARM}
		FREAD
		IREAD
		LCOMPR
		LREAD
		SCANON
		{SETUPB}
		STOP
{SETUPB}	{SETUPA}	AREAD
		CLEAR
		IREAD
		{LATCEL}
		LCOMPR
		{MIXTAB}
		{MOREDT}
		{MULTRG}
		{POKE}
		{RESDA}
		{STDCMP}
		STOP
SHELC	{DANCOF}	
{SHORTX}	{C4DATA}	CLOSDA
		COPY
		DTASET
		IOWRT

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		{LOGID}
		OPENDA
		OPNFIL
		REED
{SLNAME}	{STDCMP}	
{SLNS}	{STDCMP}	{ISCAN}
{SMMTBA}	{CSPARM}	LCOMPR
	{C4DATA}	
<SORTA>	<FLDATA>	CLEAR
		<HOLE>
		<LOCBOX>
		REED
		STOP
<SORTR>	<FLDATA>	
{SPHDAN}	{BALL}	(ACOS)
		{AGAUSS}
		{OUTER}
<SRMAX>	<HOLEXT>	(SQRT)
	<JOMCHK>	<CRSPRD>
		<DOTPRD>
		STOP
		<VECADD>
		<VECNRM>
<SRMIN>	<HOLHOL>	(SQRT)
		<CRSPRD>
		<DOTPRD>
		STOP
		<VECADD>
		<VECNRM>
{STDCMP}	{SETUPB}	AREAD
		{FAX}
		{FAXPRT}
		{FIX}
		{FOX}
		FREAD
		IREAD

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		{ISCAN}
		LREAD
		REED
		SCANOF
		{SLNAME}
		{SLNS}
STOP	<ARAYIN>	
	{AVGY}	
	{CLAPSE}	
	CNCSRH	
	<CRMAX>	
	<CRMIN>	
	CSAS	
	{C4DATA}	
	{DANCOF}	
	<DATAIN>	
	DIMSRH	
	FIXTYP	
	<FLDATA>	
	<GEOMIN>	
	{HOGGIE}	
	<HOLE>	
	{KNIGHT}	
	<MIXIT>	
	{MIXTAB}	
	{MTABLE}	
	MXTBLE	
	OPTYP	
	PCHSRH	
	<RCHRS>	
	SASSY	
	<SAVST6>	
	{SETUPA}	
	{SETUPB}	
	<SORTA>	
	<SRMAX>	
	<SRMIN>	
	{TWODYS}	
	<WATES>	
	{XSDRN}	
	{XSMESH}	
TABLE	MXTBLE	

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
TIMFAC	CPARAM	
{TWODXS}	{CLAPSE}	{AVG2}
		CLEAR
		COPY
		IO
		IO4
		{PATCH}
{TWODYS}	{CLAPSE}	{AVGY}
		CLEAR
		COPY
		{HOGGIE}
		IO
		IO4
		MOVE
		{PATCH}
		STOP
{UNFOLD}	{BOND}	
<UNTCRS>	<PRTPLT>	CLEAR
<VECADD>	<CRMAX>	
	<CRMIN>	
	<SRMAX>	
	<SRMIN>	
	<XRMIN>	
<VECNRM>	<CRMAX>	
	<CRMIN>	
	<SRMAX>	
	<SRMIN>	
{VERIFY}	{C4DATA}	
		{VOLJB}
{VOLFRC}	{ICE}	
{VOLJB}	{VERIFY}	
<VOLUME>	<JOMITY>	(ASIN)
		(SQRT)
		CLEAR
		<GOCURS>

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
		<GTVOLS>
		<HUNTER>
	MOVE	
<WAITIN>	<RDBIAS>	INQUIR
		IO
		RITE
<WATES>	<FLDATA>	INQUIR
		IO
		MOVE
		REED
		RITE
		STOP
WOT8	{MIPCHK}	
<WRTALB>	<WRTRST>	INQUIR
		IO
		REED
<WRTARA>	<WRTRST>	
		IO
		REED
<WRTICE>	<WRTRST>	INQUIR
		IO
		REED
<WRTPLT>	<DATAIN>	INQUIR
		IO
		RITE
<WRTRST>	SASSY	INQUIR
		IO
		REED
		RNDOUT
		<WRTALB>
		<WRTARA>
		<WRTICE>
		<WRTWTS>
<WRTWTS>	<WRTRST>	IO
		REED

Table C4.A.1 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
{WTINV}	{NOFRAC}	
<XRMIN>	<HOLHOL>	(SQRT) <DOTPRD> <VECADD>
{XSDRN}	{C4DATA}	{BINFIL} {BINRCF} {BINRCX} CLEAR {LCHKMX} STOP
{XSMESH}	{C4DATA}	IREAD STOP
<XXIN>	<KENOG>	FREAD IREAD
XXINA	<KENOG>	
<XXLIM>	<HOLEXT> <JOMCHK> PCHSRH	(SQRT)
<XXMIN>	<HOLHOL>	(SQRT)
YREAD	<ARAYIN>	
ZREAD	CPARAM	

Table C4.A.2 Alphabetical index of MODIFY routines

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
(ACOS)	FIXEDK RCUBIC	
ALOCAT	MODIFY	
ALTER	LODATA	CLEAR XXLIM
AVGKEF	LODATA	(SQRT)
CLEAR	ALTER	
CLOSDA	MODIFY	
(COS)	FIXEDK RCUBIC	
CUBFIT	FIXEDK MAXMIN OPTMIZ	DECOMP SOLVE
DECOMP	CUBFIT	
DENSTY	LODATA	
(DSQRT)	OPTMIZ	
FIXEDK	OPTMIZ	(ACOS) (COS) (SQRT) CUBFIT
GETMS	MODIFY	
INQUIR	WRTALB	
IO	RERITE WRTALB WRTARA WRTWTS	
IOLEFT	MODIFY	
ISCAN	MAXMIN	

Table C4.A.2 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
LISTQA	MODIFY	
LODATA	LODCOM	ALTER
		AVGKEF
		DENSTY
		MOVE
		OPTMIZ
		PRTJOM
		PRTMIX
		PRTSRH
		REED
		RERITE
		RESTRT
		RITE
		STOP
LODCOM	MODIFY	LODATA
		MOVE
MAXMIN	OPTMIZ	(SQRT)
		CUBFIT
		ISCAN
MODBLK		
MODIFY		ALOCAT
		CLOSDA
		GETMS
		IOLEFT
		LISTQA
		LODCOM
		OPENDA
		OPNFIL
		REED
		RESETM
		RITE
		STOP
MOVE	LODATA	
	LODCOM	
OPENDA	MODIFY	
OPNFIL	MODIFY	

Table C4.A.2 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
OPTMIZ	LODATA	(SQRT) CUBFIT DSQRT FIXEDK MAXMIN RCUBIC
PRTJOM	LODATA	
PRTMIX	LODATA	
PRTSRH	LODATA	
RCUBIC	OPTMIZ	(ACOS) (COS) (SQRT)
REED	LODATA MODIFY RERITE WRTALB WRTARA WRTWTS	
RERITE	LODATA	IO REED WRTALB WRTARA WRTWTS
RESETM	MODIFY	
RESTRT	LODATA	
RITE	LODATA MODIFY	
SOLVE	CUBFIT	
(SQRT)	AVGKEF FIXEDK MAXMIN OPTMIZ	

Table C4.A.2 (continued)

SUBROUTINE NAME	CALLING SUBROUTINE	CALLED SUBROUTINE
	RCUBIC	
	XXLIM	
STOP	LODATA	
	MODIFY	
WRTALB	RERITE	INQUIR
		IO
		REED
WRTARA	RERITE	IO
		REED
WRTWTS	RERITE	IO
		REED
XXLIM	ALTER	(SQRT)

Table C4.A.3 Commons used in CSAS

COMMON NAME	SUBROUTINE
ALBDAT	ALBRD
	ALBUSE
	CPARAM
	DATAIN
	DIFALB
	FLDATA
	LOADIT
	PARTBL
	POINT
	PRATBL
	RDALB
	RDREF
	RDRST
	SASSY
	WRTALB
	WRTRST
ALBNAM	ALBRD
	ALBUSE
	CPARAM
	DATAIN
	DIFALB
	FLDATA
	LOADIT
	PARTBL
	POINT
	PRATBL
	RDALB
	RDREF
	RDRST
	SASSY
	WRTALB
	WRTRST
BLKLNC	CINIT
	CPARAM
	MOREDT
	PARTBL
	SETUPB
	STDCMP
CCDATA	CSAS
	C4DATA
	SASSY

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
CDATA	CSAS
	C4DATA
	SASSY
CELMIX	CELLMX
	CMXCHK
CLAD	DANDAD
	GDAN
	SDAN
COMPOZ	KNIGHT
	MTABLE
CONMOD	KNIGHT
CUNIT	ARCHK
	CSAS
	CSPARM
	FAXPRT
	IDENTS
	KNIGHT
	LATCEL
	MIXTAB
	MOREDT
	MTABLE
	MULTRG
	NOFRAC
	POKE
	REORDR
	SETUPA
	SETUPB
	SHORTX
	SLNAME
	SLNS
	STDCMP
DEAL	C4DATA
	DANCOF
	LATCEL
	MULTRG
	POKE
	RESDA
	SETUPB

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
DIMEN	ARASIZ
	ARAYIN
	BOX
	BOXC
	CNCN
	CORSIZ
	CPARAM
	C4DATA
	DATAIN
	DMSN
	FINDBX
	FIXTYP
	FLDATA
	GEOMIN
	HOLCHK
	JOMCHK
	JOMITY
	KENOG
	LOCATE
	LOCBOX
	LODARA
	MESH
	MIXIT
	MXTBLE
	OPTYP
	PARTBL
	POINT
	POSIT
	PRATBL
	PRINT
	PRTJOM
	PRTPLT
	RDBIAS
	RDBOX
	RDICE
	RDREF
	RDRST
	RDSTRT
	READGM
	RGUSED
	RTARA
	SASSY
	SORTA
	SORTR
	VOLUME

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	WRTICE
	WRTRST
DRTACS	ALBUSE
	CINIT
	CNCN
	CNCSRH
	CSAS
	DATAIN
	DIMSRH
	DMSN
	FIXPCH
	FIXTYP
	FLDATA
	LOADIT
	LODARA
	LODWTS
	MIXIT
	MXTBLE
	OPTPCH
	OPTYP
	PCHSRH
	PRTPLT
	RDALB
	RDARA
	RDICE
	RDOPT
	RDRST
	RDWTS
	RT
	RTARA
	SASSY
	SAVST6
	SHORTX
	SORTA
	WAITIN
	WATES
	WRTALB
	WRTICE
	WRTPLT
	WRTRST
	WRTWTS

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
ERRFLG	ARAYIN
	PRTLBA
	SASSY
FLG	ARCHK
	CNCSRH
	CSAS
	C4DATA
	DANCOF
	DIMSRH
	FAX
	FIXCNC
	FIXDIM
	FIXPCH
	FIXTYP
	LATCEL
	MOREDT
	MULTRG
	OPTCNC
	OPTDMN
	OPTPCH
	OPTYP
	PCHSRH
	RDOPT
	SETUPA
	SETUPB
	SHORTX
	SLNS
	STDCMP
	VERIFY
	XSMESH
GIN	ADAN
	BALL
	DAN
	DANDAD
	FINNER
	GDAN
	OUTER
	SPHDAN
ICECOM	ICE
	MOREDT
	SETUPB

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
IOS	CSAS
	SASSY
LIBA	C4DATA
	EPSIG
	FIX
	FOX
	KNIGHT
	LATCEL
	MIPCHK
	MIXTAB
	MODIFY
	MULTRG
	RESDA
	SETUPA
	SETUPB
	SHORTX
	STDCMP
LIBC	C4DATA
	EPSIG
	FIX
	FOX
	KNIGHT
	LATCEL
	MIPCHK
	MIXTAB
	MODIFY
	MULTRG
	RESDA
	SETUPA
	SETUPB
	SHORTX
	STDCMP
LOGIC	ALBRD
	ARASIZ
	ARAYIN
	CORSIZ
	CPARAM
	CSAS
	DATAIN
	FLDATA

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	IDX1D
	JOMCHK
	JOMITY
	KENOG
	LOCATE
	MESH
	PARTBL
	POINT
	POSIT
	PRTJOM
	PRTPLT
	RDBIAS
	RDBOX
	RDREF
	RDRST
	READGM
	RTARA
	SASSY
	SORTA
	SORTR
	VOLUME
	WATES
	WRTRST
LOWBND	CORSIZ
	GOCURS
	HUNTER
	JOMCHK
	LOCATE
	LODARA
	MESH
	POINT
	PRINT
	PRTJOM
	PRTPLT
	VOLUME
LPNT	CINIT
	RDOPT
	SASSY
MATRX	FLDATA
	PRATBL
	SORTA

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
NUTRON	FINDBX
	FLDATA
	LOCATE
	MESH
PARM	C4DATA
	MOREDT
	SETUPA
	SETUPB
PASS	C4DATA
	DANCOF
	KNIGHT
	LATCEL
	MIPCHK
	MIXTAB
	MODIFY
	MOREDT
	MULTRG
	POKE
	RESDA
	SASSY
	SETUPA
	SETUPB
	VERIFY
	XSDRN
PASS2	C4DATA
	KNIGHT
	MIXTAB
	MOREDT
	SETUPA
	SETUPB
	XSDRN
PICT	MESH
	PRINT
	PRTPLT
	RDPLOT
	RELATE
PICTTL	MESH
	PRINT
	PRTPLT

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	RDPLOT
	RELATE
POINTA	C4DATA
	SETUPB
POINTB	C4DATA
	SETUPA
POINTC	C4DATA
	SETUPA
POINTR	DATAIN
	JOMITY
	LOADIT
	POINT
	SASSY
REC1	CNCN
	CSAS
	DMSN
	FIXPCH
	FIXTYP
	OPTPCH
	OPTYP
	PRTSRH
	RDOPT
	SASSY
RUNTYP	BIRITE
	CPARAM
	CSAS
	DATAIN
	PARTBL
STDATA	DATAIN
	RDRST
	RDSTRT
	SASSY
	WRTRST
TITL	ARASIZ
	CORSIZ
	CPARAM
	DATAIN

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	GEOMIN
	HOLCHK
	HOLEXT
	HOLHOL
	JOMCHK
	KENOG
	PARTBL
	POINT
	PRATBL
	PRTJOM
	PRTLBA
	PRTPLT
	PRTSRH
	PRTWTS
	RDBOX
	RDPLOT
	READGM
	VOLUME
	WRTRST
UNIT	ALBRD
	ALBUSE
	ARASIZ
	ARAYIN
	BOX
	CINIT
	CNCN
	CNCSRH
	CORSIZ
	CPARAM
	CSAS
	DATAIN
	DIFALB
	DIMSRH
	DMSN
	FIXCNC
	FIXDIM
	FIXPCH
	FIXTYP
	FLDATA
	GEOMIN
	ICE
	IDX1D
	JOMCHK
	JOMITY

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	KENOG
	LOADIT
	LODARA
	LODWTS
	MIXIT
	MXTBLE
	OPTCNC
	OPTDMN
	OPTPCH
	OPTYP
	PARTBL
	PCHSRH
	POINT
	POSIT
	PRINT
	PRTARA
	PRTJOM
	PRTLBA
	PRTPLT
	PRTSRH
	RDALB
	RDBIAS
	RDBOX
	RDICE
	RDOPT
	RDPLOT
	RDREF
	RDRST
	RDSTRT
	RDWTS
	READGM
	RT
	RTARA
	SASSY
	SAVST6
	SHORTX
	SORTA
	SORTR
	VOLUME
	WAITIN
	WATES
	WRTALB
	WRTICE
	WRTRST

Table C4.A.3 (continued)

COMMON NAME	SUBROUTINE
	WRTWTS
UNITS	CSAS
	C4DATA
	SASSY
XSDRNC	MOREDT
	SETUPB
	XSDRN

Table C4.A.4 Commons used in MODIFY

COMMON NAME	SUBROUTINE
ALBDAT	LODCOM
	RERITE
	RESTRT
	WRTALB
ALBNAM	LODCOM
	RERITE
	RESTRT
	WRTALB
CCDATA	MODIFY
CDATA	MODIFY
CYCLE	LODATA
	LODCOM
	MODIFY
DIMEN	LODATA
	LODCOM
	PRTJOM
	RERITE
	RESTRT
DRTACS	LODATA
	LODCOM
	MODIFY
	RERITE
	RESTRT
	WRTALB
	WRTWTS
LOGIC	PRTJOM
	RERITE
	RESTRT
LOWBND	PRTJOM
LPNT	LODATA
	MODIFY
REC1	LODATA
	LODCOM
	MODIFY
	PRTSRH

Table C4.A.4 (continued)

COMMON NAME	SUBROUTINE
	RERITE
STDATA	LODCOM
	RERITE
	RESTRT
TITL	LODATA
	PRTJOM
	PRTMIX
	PRTSRH
	RESTRT
UNIT	LODATA
	LODCOM
	MODIFY
	PRTJOM
	PRTSRH
	RERITE
	WRTALB
	WRTWTS
UNITS	MODIFY

C4.B SAMPLE PROBLEMS

This section contains sample problems to demonstrate some of the options available in CSAS and its associated sequences. A brief problem description and the associated card input data are included for each problem. See Sect. C4.5 for additional examples.

SAMPLE PROBLEM 1 K-EFFECTIVE CALCULATION

The purpose of this problem is to calculate the k-effective of a system. This problem is the same as the KENO V.a sample problem 12 in Sect. F11.D except the cross-section library and KENO V.a mixing table are prepared by CSAS. The problem represents a critical experiment consisting of a composite array[1,2] of four highly enriched (93.2%) uranium metal cylinders having a density of 18.76 g/cc and four 5.0677-L Plexiglas containers filled with uranyl nitrate solution. The uranium metal cylinders have a radius of 5.748 cm and a height of 10.765 cm. The uranyl nitrate solution has a specific gravity of 1.555 and contains 415 g of uranium per liter. The ID of the Plexiglas bottle is 19.05 cm and the inside height is 17.78 cm. The Plexiglas is 0.635 cm thick. The center-to-center spacing between the metal units is 13.18 cm in the "y" direction and 13.45 cm in the "z" direction. The center-to-center spacing between the solution units is 21.75 cm in the "y" direction and 20.48 cm in the "z" direction. The spacing between the y-z plane that passes through the centers of the metal units and the y-z plane that passes through the centers of the solution units is 17.465 cm in the "x" direction.

The metal units in this experiment are designated in Table II of Ref. 1 as cylinder index 11 and reflector index 1. A photograph of the experiment is given in Fig. C4.B.1.

```
=CSAS25
SAMPLE PROBLEM 1  SET UP 4AQUEOUS 4 METAL IN CSAS25
HANSEN-ROACH   INFHOMMEDIUM
URANIUM        1 0.985 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
SOLNUO2(NO3)2  2 415 9.783-3 SPG=1.555 1.0 293 92235 92.6 92238 5.9
                                                92234 1.0  92236 0.5 END
PLEXIGLASS     3 END
END COMP
KENO V.A SAMPLE PROBLEM 19 4 AQUEOUS 4 METAL ARRAY OF ARRAYS (SAMP PROB 12)
READ PARAM  FLX=YES FDN=YES NUB=YES
END PARAM
READ GEOM
UNIT 1
COM='URANYL NITRATE SOLUTION IN A PLEXIGLAS CONTAINER'
CYLINDER  2 1 9.525 2P8.89
CYLINDER  3 1 10.16 2P9.525
CUBOID  0 1 4P10.875 2P10.24
UNIT 2
COM='URANIUM METAL CYLINDER'
CYLINDER  1 1 5.748 2P5.3825
CUBOID  0 1 4P6.59 2P6.225
UNIT 3
COM='1X2X2 ARRAY OF SOLUTION UNITS'
ARRAY 1 3*0.0
UNIT 4
COM='1X2X2 ARRAY OF METAL UNITS PADDED TO MATCH SOLUTION ARRAY'
ARRAY 2 3*0.0
REPLICATE 0 1 2*0.0 2*8.57 2*8.03 1
END GEOM
READ ARRAY ARA=1 NUX=1 NUY=2 NUZ=2 FILL F1 END FILL
ARA=2 NUX=1 NUY=2 NUZ=2 FILL F2 END FILL GBL=3 ARA=3 NUX=2 NUY=1 NUZ=1
COM='COMPOSITE ARRAY OF SOLUTION AND METAL UNITS'
FILL 4 3 END FILL
END ARRAY
END DATA
END
```

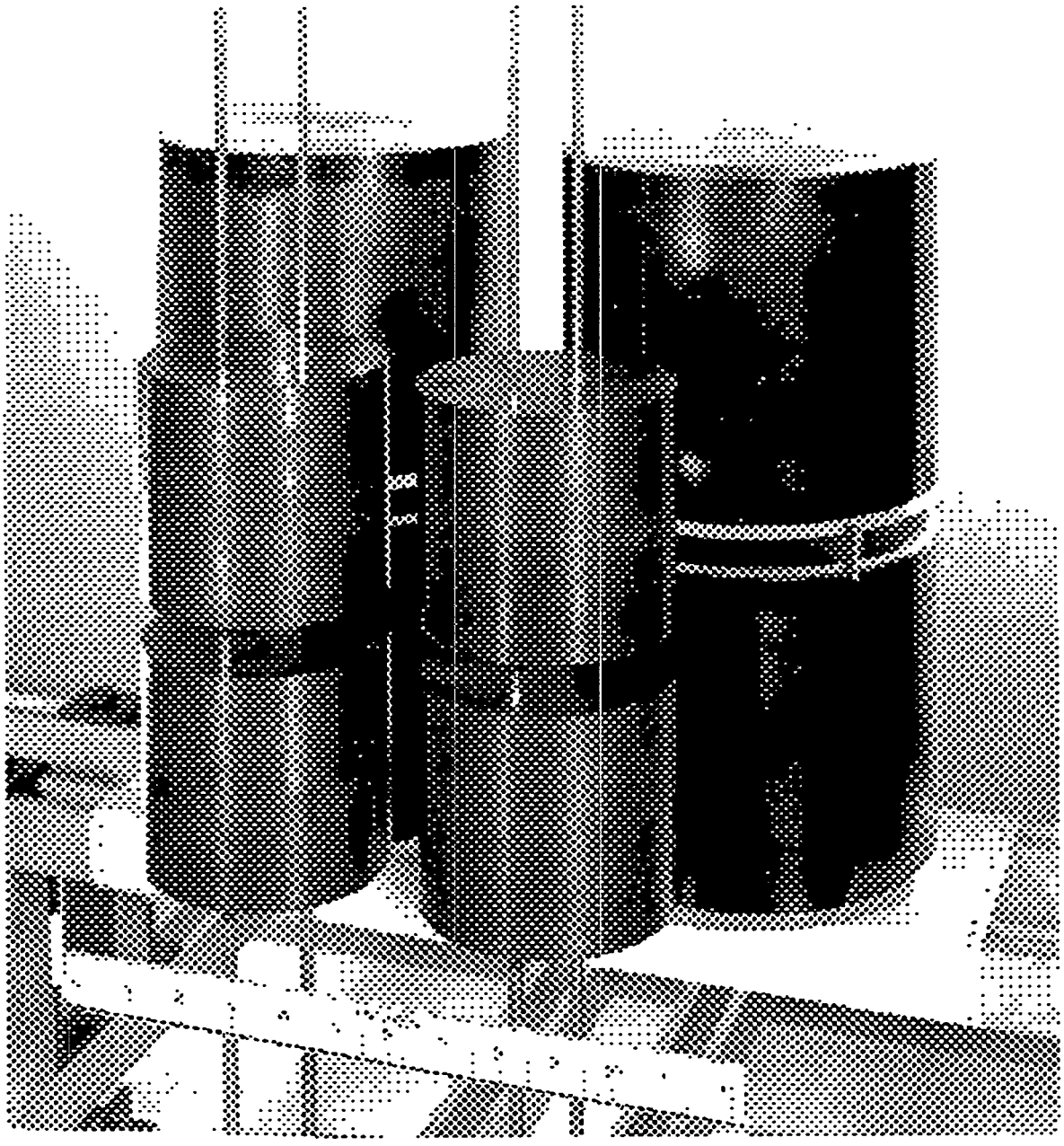


Figure C4.B.1 Critical assembly of four solution units and four metal units

SAMPLE PROBLEM 2 OPTIMUM PITCH SEARCH USING DETAILED GEOMETRY

This problem represents an attempt to optimize the reactivity of PWR-like fuel bundles in a storage pool. The storage array is an infinite planar array of flooded fuel bundles. Each bundle consists of a 17 × 17 × 1 array of 2.35%-enriched UO_2 pins, density 9.21 g/cc, clad with zirconium. The fuel is 0.823 cm in diameter, the clad diameter is 0.9627 cm, and the length of each pin is 366 cm. Each fuel bundle is encased in a boral sheath. There is a 1/4-in. gap flooded with water between the bundle and the sheath. The boral sheath is 3/8 in. thick. One inch of water separates the fuel bundle sheaths in the horizontal plane, and 15 cm of water is present on the top and bottom of the array.

The KENO V.a geometry represents each fuel pin in the bundle discreetly. The search should determine the optimum pitch within the fuel bundle. The gap between the bundle and the boral remains fixed, as does the thickness of the sheath and the spacing between sheaths.

```
=CSAS4
SAMPLE PROBLEM 2  PWR-LIKE FUEL BUNDLE
HANSEN-ROACH LATTICECELL
UO2  1 .84 293. 92235 2.35 92238 97.65 END
ZR  2 1 END
H2O  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
H2O  5 1 END
END COMP
SQUAREPITCH  1.2751 .823 1 3 .9627 2 END
STORAGE ARRAY OF PWR-LIKE FUEL BUNDLES IN POISON SHEATHS
READ PARAM  TME=7.0  NUB=YES FAR=YES GEN=53
END PARAM
READ ARRAY NUX=17 NUY=17 NUZ=1 END ARRAY
READ BOUNDS  XYF=MIRROR   END BOUNDS
READ GEOM
CYLINDER  1 1 .4115 183.0 -183.0
CYLINDER  2 1 .48135 183.1 -183.1
CUBOID  3 1 .63755 -.63755 .63755 -.63755 183.1 -183.1
CORE  0 1 0 0 0
REFLECTOR 5 1 4*.635 2Z 1
REFLECTOR 4 1 4*.9525 2Z 1
REFLECTOR 5 1 4*1.27 2Z 1
REFLECTOR 5 2 4Z 2*3.0 5
END GEOM
READ BIAS ID=500 2 6 END BIAS
END DATA
READ SEARCH  OPTIMUM PITCH  END SEARCH
END
```

SAMPLE PROBLEM 3 OPTIMUM PITCH SEARCH USING HOMOGENIZED GEOMETRY

This problem illustrates the use of CSAS4X to represent a fuel cask. It utilizes a cell-weighted mixture to represent a PWR-like fuel bundle. The cask contains a 2 × 2 × 1 array of fuel bundles. Each fuel bundle consists of a 17 × 17 × 1 array of zirconium clad, 2.35%-enriched UO_2 fuel pins with a density of 9.21 g/cc arranged in a square pitch. The pin diameter is 0.823 cm, and its length is 366 cm. The clad is 0.06985 cm thick, and the pitch is 1.275 cm. Each fuel bundle is contained in a 0.6625-cm-thick boral sheath. The bundles are separated by 1 cm of water, representing a flooded cask. The square aluminum cask is 10 cm thick on all faces and is reflected by 15 cm of water.

By using CSAS4X, a cell-weighted cross section is created to represent the fuel bundle. The KENO V.a geometry utilizes the cell-weighted mixture (500) and the overall dimensions of the fuel bundle to represent the entire fuel bundle as a single homogeneous region. The first reflector card represents the fuel cask, and the second reflector card represents the 15-cm reflector.

```
=CSAS4X
SAMPLE PROBLEM 3  SAMPLE FUEL CASK
HANSEN-ROACH LATTICECELL
UO2  1 .84 293. 92235 2.35 92238 97.65 END
ZR  2 1 END
H2O  3 1 END
B4C  4 0.367 END
AL  4 0.636 END
H2O  5 1 END
AL  6 1 END
END COMP
SQUAREPITCH  1.275 .823 1 3 .9627 2 END
SAMPLE SQUARE FUEL CASK
READ PARAM  TME=5.0  NUB=YES FAR=YES GEN=53
END PARAM
READ ARRAY NUX=2  NUY=2  NUZ=1 END ARRAY
READ GEOM
CUBOID 500 1 4P10.8375 2P183.0
CUBOID   4 1 4P11.5    2P183.0
CUBOID   5 1 4P12.0    2P183.0
CORE     0 1 3*0
REFLECTOR 6 1 6*10.0 1
REFLECTOR 5 2 6*3 5
END GEOM
READ BIAS ID=500 2 6 END BIAS
END DATA
READ SEARCH  OPTIMUM PITCH  END SEARCH
END
```

SAMPLE PROBLEM 4 SEARCH FOR A SPECIFIED VALUE OF K-EFFECTIVE

Find the pitch at which a 2 × 2 × 2 array of cylinders of highly enriched (93.2%) uranium metal with a density of 18.76 g/cc are critical. Each cylinder has a radius of 5.748 cm and a height of 10.765 cm. The surface-to-surface spacing between the units is the same in all directions. The initial guess for the critical surface-to-surface spacing was 3.0 cm. The experimentally critical surface-to-surface separation for this system, shown in Fig. C4.B.2, is 2.248 cm. The input data for this problem are given below.

```
=CSAS4
SAMPLE PROBLEM 4  SET UP 2C8 IN CSAS25
HANSEN-ROACH   INFHOMMEDIUM
URANIUM  1 0.985 293  92235 93.2 92238 5.6 92234 1.0 92236 0.2 END
END COMP
CRITICAL PITCH SEARCH FOR CASE 2C8 BARE
READ PARAMETERS  TME=1.0 FLX=YES FDN=YES FAR=YES
END PARAMETERS
READ GEOMETRY
CYLINDER 1 1 5.748 5.3825 -5.3825
CUBOID  0 1 4P7.248 2P6.8825
END GEOMETRY
READ ARRAY  NUX=2 NUY=2 NUZ=2  END ARRAY
END DATA
READ SEARCH   CRITICAL PITCH   MAXPITCH=15.5  MORE
ALTER  UNIT=1 REG=2 +Z=1.0 -Z=1.0
END SEARCH
END
```

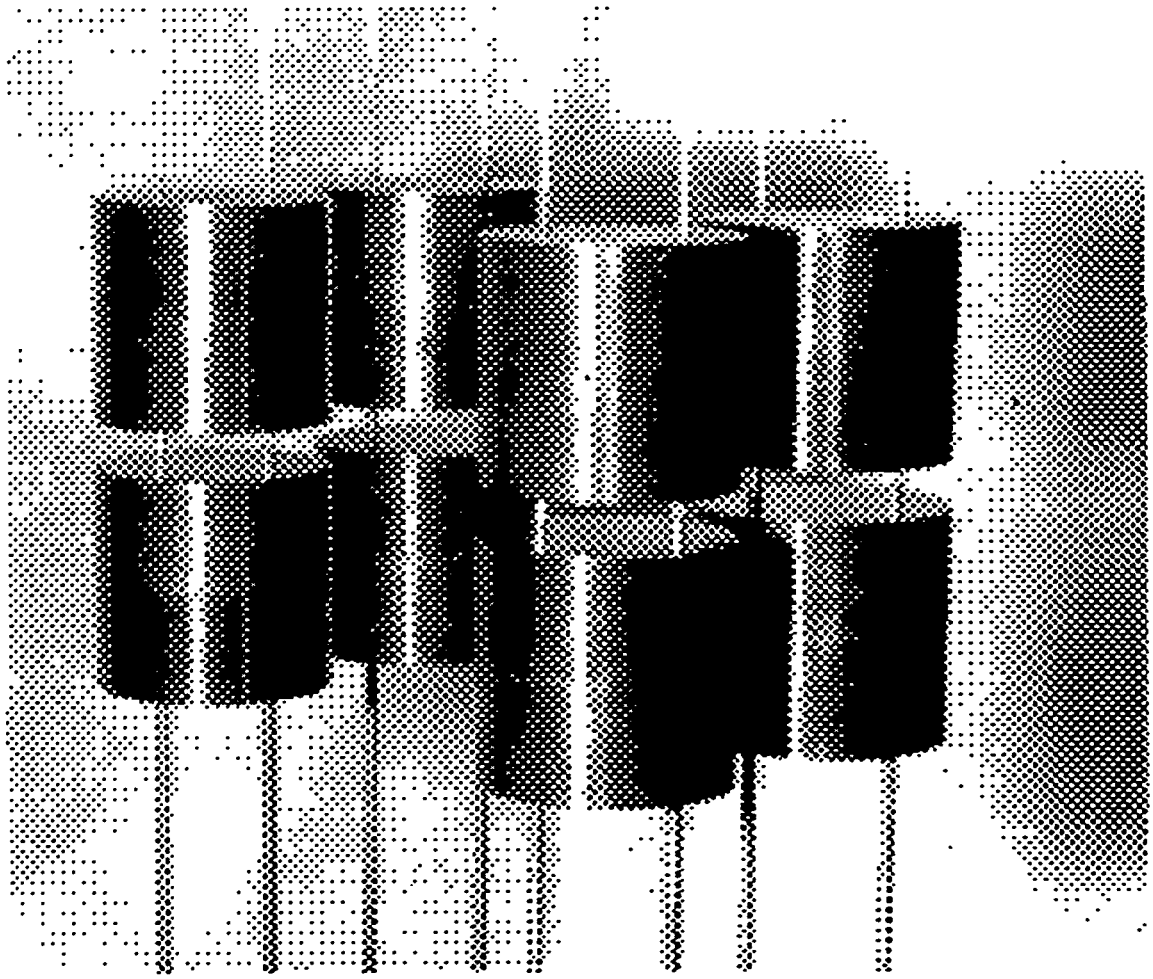


Figure C4.B.2 Critical assembly of eight highly enriched uranium metal cylinders

C4.B.1 REFERENCES

1. J. T. Thomas, "Critical Three-Dimensional Arrays of U(93.2)-Metal Cylinders," *Nucl. Sci. Eng.* 52, 350 (November 1973).

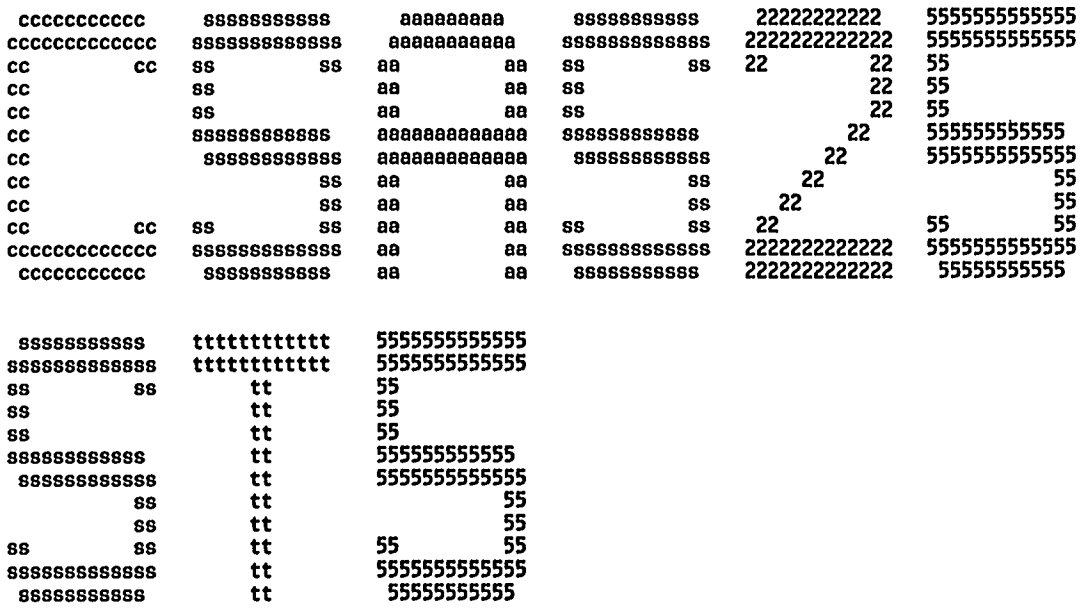
2. J. T. Thomas, *Critical Three-Dimensional Arrays of Neutron-Interacting Units, Part II*, ORNL/TM-868, Union Carbide Corp., Nucl. Div., Oak Ridge Natl. Lab., July 1964.

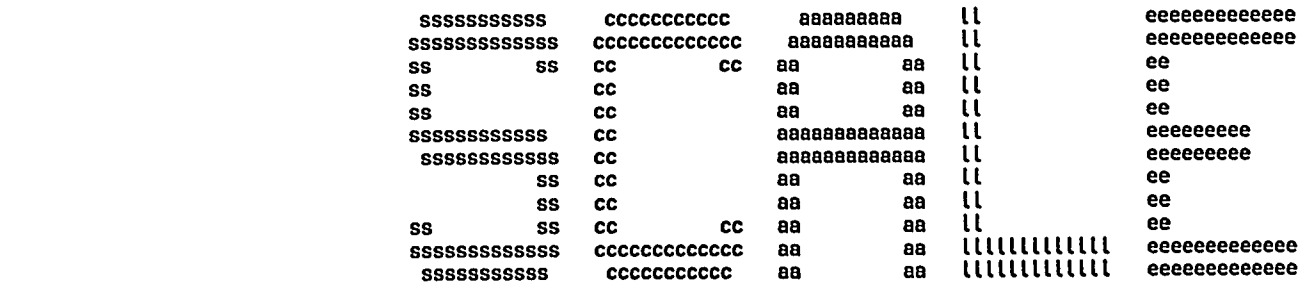
C4.C SAMPLE OUTPUT

This section contains the computer printout generated by the control module for each sample problem. Output from functional modules is not included in this section. See Sect. C4.6 for a generic explanation of the control module output.

Sample problem 1 does not perform a search, so the k-effective resulting from this calculation does not appear in the control module output. This problem is a description of a critical experiment, so the KENO V.a output should yield a k-effective of 1.0 within statistical accuracy.

Sample problems 2, 3, and 4 perform searches. The search data and search results are printed after the program verification table for MODIFY. The k-effective is printed as each search pass is completed. These k-effectives may vary because of differences in the random number sequences on different computers.


cccccccccc ssssssssss aaaaaaaaa ssssssssss 22222222222 5555555555555
ccccccccccccc sssssssssssss aaaaaaaaaaa sssssssssssss 2222222222222 5555555555555
cc cc ss ss aa aa ss ss 22 22 55
cc ss aa aa ss 22 55
cc ss aa aa ss 22 55
cc ssssssssssss aaaaaaaaaaaaa sssssssssssss 22 555555555555
cc sssssssssssss aaaaaaaaaaaaa sssssssssssss 22 5555555555555
cc ss aa aa ss 22 55
cc ss aa aa ss 22 55
cc cc ss ss aa aa ss ss 22 55 55
ccccccccccccc sssssssssssss aa aa sssssssssssss 2222222222222 5555555555555
ccccccccccc sssssssssss aa aa sssssssssss 2222222222222 55555555555
ssssssssss ttttttttttttt 5555555555555
sssssssssssss ttttttttttttt 5555555555555
ss ss tt 55
ss tt 55
ss tt 55
sssssssssssss tt 555555555555
ssssssssssss tt 5555555555555
ss tt 55
ss tt 55
ss ss tt 55 55
sssssssssssss tt 5555555555555
ssssssssss tt 55555555555
0000000 33333333333 // 11 44 // 99999999999 44
000000000 3333333333333 // 111 444 // 9999999999999 444
00 00 33 33 // 1111 4444 // 99 99 4444
00 00 33 // 11 44 44 // 99 99 44 44
00 00 33 // 11 44 44 // 99 99 44 44
00 00 333 // 11 44 44 // 9999999999999 44 44
00 00 333 // 11 44 44 // 999999999999 44 44
00 00 33 // 11 444444444444 // 99 444444444444
00 00 33 // 11 444444444444 // 99 444444444444
00 00 33 33 // 11 44 // 99 44
000000000 3333333333333 // 11111111 44 // 9999999999999 44
0000000 33333333333 // 11111111 44 // 999999999999 44
11 666666666666 33333333333 22222222222 33333333333 0000000
111 6666666666666 3333333333333 2222222222222 3333333333333 000000000
1111 66 ::: 33 33 22 22 ::: 33 33 00 00
11 66 ::: 33 22 ::: 33 00 00
11 66 ::: 33 22 ::: 33 00 00
11 666666666666 333 22 333 00 00
11 6666666666666 333 22 333 00 00
11 66 66 ::: 33 22 ::: 33 00 00
11 66 66 ::: 33 22 ::: 33 00 00
11 66 66 ::: 33 33 22 ::: 33 33 00 00
11111111 6666666666666 3333333333333 2222222222222 3333333333333 000000000
11111111 66666666666 33333333333 2222222222222 33333333333 0000000




```
*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                  program verification information                *****
*****                                                                     *****
*****                  code system:    scale  version:    4.2          *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  csas                                         *****
*****                                                                     *****
*****         creation date:  12/01/93                                    *****
*****                                                                     *****
*****              library:  /scale4.2p/exe                               *****
*****                                                                     *****
*****                                                                     *****
*****       production code:  csas                                        *****
*****                                                                     *****
*****              version:  2.2                                          *****
*****                                                                     *****
*****              jobname:  st5                                          *****
*****                                                                     *****
*****     date of execution:  03/14/94                                    *****
*****                                                                     *****
*****     time of execution:  16:32:30                                    *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

```
sample problem 1  set up 4aqueous 4 metal in csas25


**** problem parameters ****

lib hansen-roach library
mxx            3 mixtures
msc            3 composition specifications
izm            1 material zones
ge  infhommedium geometry
more           0 0/1 do not read/read optional parameter data
msln           1 fuel solutions


**** problem composition description ****

sc  uranium      standard composition
mx             1 mixture no.
vf         .9850 volume fraction
roth     19.0500 theoretical density
temp       293.0 deg kelvin
           92235  93.20%
           92238   5.60%
           92234   1.00%
           92236    .20%
end

sc  solnuo2(no3) standard composition
mx             2 mixture no.
fd       415.0000 solution fuel density
aml         .0098 acid molarity
vf        1.0000 volume fraction
temp       293.0 deg kelvin
spg       1.5550 specified specific gravity
           92235  92.60%
           92238   5.90%
           92234   1.00%
           92236    .50%
end

sc  plexiglass   standard composition
mx             3 mixture no.
vf        1.0000 volume fraction
roth      1.1800 theoretical density
end


**** problem geometry ****


**** infinite homogeneous medium ****
mfuel          1 mixture no. of the infinite homogeneous medium
```

```
sample problem 1  set up 4aqueous 4 metal  in csas25

********** data library information **********

      unit                                                volume
      number          data set name                       name        unit function
      ------          -------------                       ----        -------------

        89     /scale4.2p/datalib/scale.rev05.sclib                    standard composition library

        81     /scale4.2p/datalib/scale.rev02.xn16                     cross section library

        11     ft11f001                                                short cross section library

                              standard composition library data
                              ---------------------------------

      unit number  :  89

      dataset name :  /scale4.2p/datalib/scale.rev05.sclib

      library title:  scale-4 standard composition library
                      386 standard compositions, 332 nuclides
                      10 elements with variable isotopic distrbutions.

      creation date:   1/25/94

                                 cross section library data
                                 --------------------------

      unit number  :  81

      dataset name :  /scale4.2p/datalib/scale.rev02.xn16

      library title:  scale 4 - 16 neutron group criticality safety library
                        hansen-roach data with knight modifications and some endf/b 4 data
                          compiled for nrc        1/27/89
                            last updated         10/12/89
                              l.m.petrie         ornl
```

```
                    ........    0 io's were used before reading keno v data     ........

                    ........    0 io's were used reading the keno v parameter data     ........

                   *************** data reading completed ***************

                    ........    0 io's were used preparing the keno v input data     ........

                    ........    0 io's were used loading the keno v data     ........

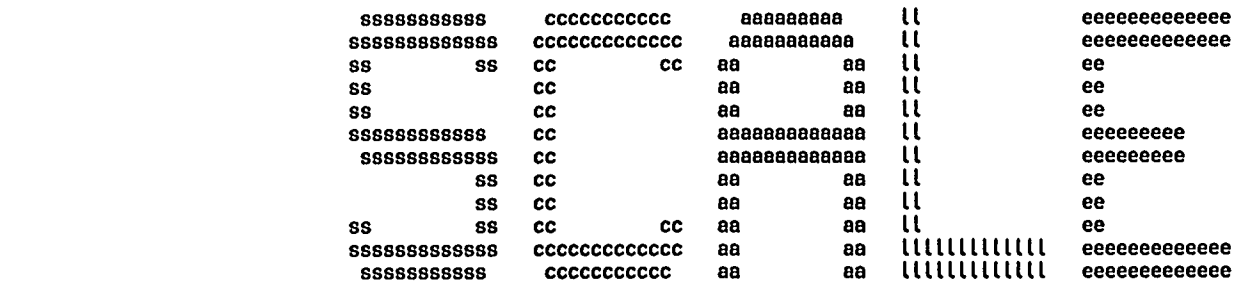
                    ........    0 io's were used loading the data     ........

                    ........    0 io's were used checking the keno v geometry data     ........
                    *****  restart data has been written on unit 95  *****

                    ........    0 io's were used writing the keno v - csas data     ........

                    ........    0 io's were used processing csas input data     ........

control module csas25    is complete.
```




```
*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                  program verification information                *****
*****                                                                     *****
*****                 code system:    scale  version:    4.2           *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  csas                                         *****
*****                                                                     *****
*****        creation date:  12/01/93                                     *****
*****                                                                     *****
*****              library:  /scale4.2p/exe                               *****
*****                                                                     *****
*****                                                                     *****
*****      production code:  csas                                         *****
*****                                                                     *****
*****              version:  2.2                                          *****
*****                                                                     *****
*****              jobname:  st5                                          *****
*****                                                                     *****
*****    date of execution:  03/14/94                                     *****
*****                                                                     *****
*****    time of execution:  16:33:08                                     *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

```
sample problem 2  pwr-like fuel bundle


**** problem parameters ****

lib hansen-roach library
mxx           5 mixtures
msc           6 composition specifications
izm           3 material zones
ge  latticecell  geometry
more          0 0/1 do not read/read optional parameter data
msln          0 fuel solutions


**** problem composition description ****

sc  uo2         standard composition
mx            1 mixture no.
vf        .8400 volume fraction
roth    10.9600 theoretical density
temp     293.0 deg kelvin
          92235   2.35%
          92238  97.65%
end

sc  zr          standard composition
mx            2 mixture no.
vf       1.0000 volume fraction
roth     6.4400 theoretical density
end

sc  h2o         standard composition
mx            3 mixture no.
vf       1.0000 volume fraction
roth      .9982 theoretical density
end

sc  b4c         standard composition
mx            4 mixture no.
vf        .3670 volume fraction
roth     2.5200 theoretical density
end

sc  al          standard composition
mx            4 mixture no.
vf        .6360 volume fraction
roth     2.6989 theoretical density
end

sc  h2o         standard composition
mx            5 mixture no.
vf       1.0000 volume fraction
roth      .9982 theoretical density
end
```

```
**** problem geometry ****

ctp squarepitch  cell type
pitch     1.2751 cm center to center spacing
fuelod     .8230 cm fuel diameter or slab thickness
mfuel         1 mixture no. of fuel
mmod          3 mixture no. of moderator
cladod     .9627 cm clad outer diameter
mclad         2 mixture no. of clad


zone specifications for latticecell geometry

              zone  1 is fuel
              zone  2 is clad
              zone  3 is mod
```

```
sample problem 2  pwr-like fuel bundle

********** data library information **********

   unit                                    volume
  number          data set name            name        unit function
  ------          -------------            ----        -------------

    89     /scale4.2p/datalib/scale.rev05.sclib          standard composition library

    81     /scale4.2p/datalib/scale.rev02.xn16           cross section library

    11     ft11f001                                      short cross section library

                        standard composition library data
                        ---------------------------------

          unit number  :  89

          dataset name :  /scale4.2p/datalib/scale.rev05.sclib

          library title:  scale-4 standard composition library
                          386 standard compositions, 332 nuclides
                          10 elements with variable isotopic distributions.

          creation date:  1/25/94

                        cross section library data
                        --------------------------

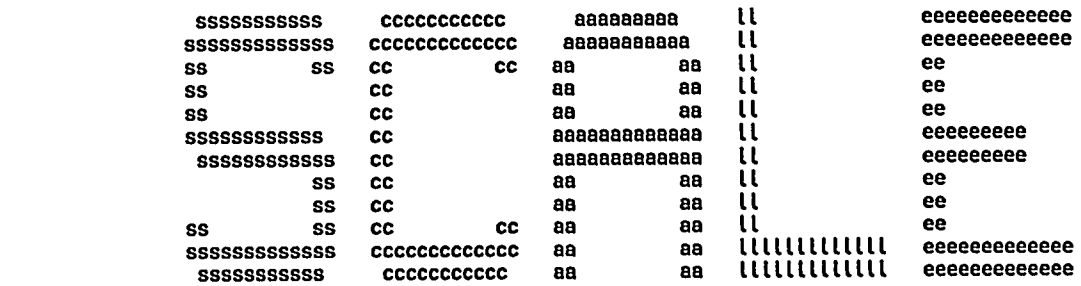
          unit number  :  81

          dataset name :  /scale4.2p/datalib/scale.rev02.xn16

          library title:  scale 4 - 16 neutron group criticality safety library
                            hansen-roach data with knight modifications and some endf/b 4 data
                              compiled for nrc        1/27/89
                                last updated         10/12/89
                                  l.m.petrie         ornl
```

```
........    0 io's were used before reading keno v data    ........
........    0 io's were used reading the keno v parameter data    ........

*************** data reading completed ***************
........    0 io's were used preparing the keno v input data    ........
........    0 io's were used loading the keno v data    ........
........    0 io's were used loading the data    ........
........    0 io's were used checking the keno v geometry data    ........
*****  restart data has been written on unit 95  *****
........    0 io's were used writing the keno v - csas data    ........
........    0 io's were used before reading search data    ........
........    0 io's were used processing csas input data    ........
```



program verification information

code system: scale version: 4.2

program: modify

creation date: 10/25/93

library: /scale4.2p/exe

production code: modify

version: 2.1

jobname: st5

date of execution: 03/14/94

time of execution: 16:34:22

```
*****************************************************************************************************************
***                                                                                                           ***
***                          storage array of pwr-like fuel bundles in poison sheaths                         ***
***                                                                                                           ***
*****************************************************************************************************************
*****************************************************************************************************************
***                              ******          search data          ******                                   ***
***                                                                                                           ***
***                                                                                                           ***
***                              search type                          optimum pitch                            ***
***                                                                                                           ***
***                    pas       number of search passes                 10                                 ***
***                                                                                                           ***
***                    npm       number of search parameters              1                                 ***
***                                                                                                           ***
***                    eps       search convergence tolerance           .0050                               ***
***                    -con      minimum constraint                    -.2450                               ***
***                                                                                                           ***
***                    +con      maximum constraint                     1.2250                              ***
***                                                                                                           ***
***                                                                                                           ***
***                      unit    first   last                                                               ***
***      command         number  region  region  ----------------    search constants    ----------------   ***
***                                                                                                           ***
***                      unit    reg=__  to __   +x or r  -x or +h  +y or -h    -y       +z        -z       ***
***                                                                                                           ***
***  alter/change/modify   1       3       3       1.00      1.00      1.00      1.00      .00       .00      ***
***                                                                                                           ***
*****************************************************************************************************************
*****************************************************************************************************************
```

```
*********************   search pass  1     keff=  7.31988E-01 + or -  6.08683E-03   *********************
                              the parameter was  0.00000E+00
                      *****  modified keno v data has been rewritten on unit 95  *****

*********************   search pass  2     keff=  3.58234E-01 + or -  4.64021E-03   *********************
                              the parameter was -2.45000E-01
                      *****  modified keno v data has been rewritten on unit 95  *****

*********************   search pass  3     keff=  7.44512E-01 + or -  3.79809E-03   *********************
                              the parameter was  1.22500E+00
                      *****  modified keno v data has been rewritten on unit 95  *****

*********************   search pass  4     keff=  8.97264E-01 + or -  4.79952E-03   *********************
                              the parameter was  6.12501E-01
                      *****  modified keno v data has been rewritten on unit 95  *****

*********************   search pass  5     keff=  9.13226E-01 + or -  4.64053E-03   *********************
                              the parameter was  4.12008E-01
```

storage array of pwr-like fuel bundles in poison sheaths

****
****

convergence was achieved on pass 5 the parameter was 4.12008E-01

the equation used in the search was:

k-eff = +7.18481E-01 +1.00598E+00*p -1.54341E+00*p**2 +6.05700E-01*p**3

k-effective= 9.13226E-01 + or - 4.64053E-03 the corresponding geometry follows;

region	media num	bias id	geometry description for those units utilized in this problem
			----- unit 1 -----
1 cylinder	1	1	radius = .41150 +z = 183.00 -z = -183.00 centerline is at x = 0.00000E+00 y = 0.00000E+00
2 cylinder	2	1	radius = .48135 +z = 183.10 -z = -183.10 centerline is at x = 0.00000E+00 y = 0.00000E+00
3 cuboid	3	1	+x = .90023 -x = -.90023 +y = .90023 -y = -.90023 +z = 183.10 -z = -183.10

****
****

storage array of pwr-like fuel bundles in poison sheaths

based on the preceding data, the best estimate of the parameter is 4.39709E-01

the geometry corresponding to this parameter follows:

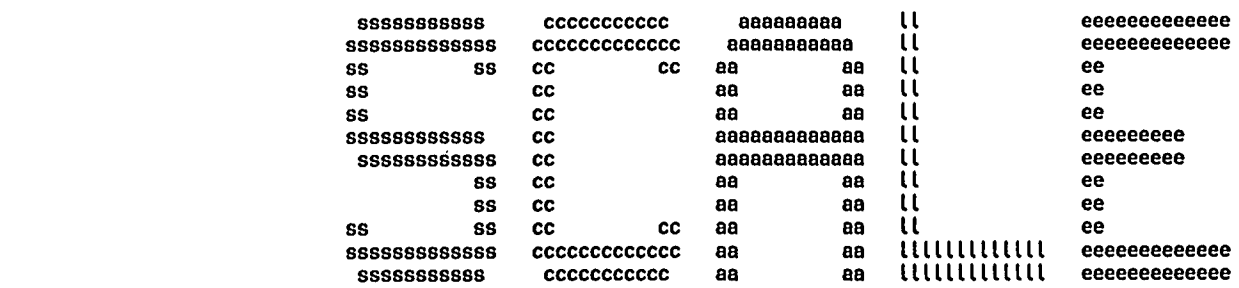
region	media num	bias id	geometry description for those units utilized in this problem
			----- unit 1 -----
1 cylinder	1	1	radius = .41150 +z = 183.00 -z = -183.00 centerline is at x = 0.00000E+00 y = 0.00000E+00
2 cylinder	2	1	radius = .48135 +z = 183.10 -z = -183.10 centerline is at x = 0.00000E+00 y = 0.00000E+00
3 cuboid	3	1	+x = .91789 -x = -.91789 +y = .91789 -y = -.91789 +z = 183.10 -z = -183.10

****
****

***** modified keno v data has been rewritten on unit 95 *****

***** convergence has been achieved in the search package. *****

control module modify is complete.




```
*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                 program verification information                 *****
*****                                                                     *****
*****                 code system:    scale  version:    4.2           *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  csas                                         *****
*****                                                                     *****
*****         creation date:  12/01/93                                    *****
*****                                                                     *****
*****              library:  /scale4.2p/exe                               *****
*****                                                                     *****
*****                                                                     *****
*****       production code:  csas                                        *****
*****                                                                     *****
*****              version:  2.2                                          *****
*****                                                                     *****
*****              jobname:  st5                                          *****
*****                                                                     *****
*****     date of execution:  03/14/94                                    *****
*****                                                                     *****
*****     time of execution:  16:42:11                                    *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

```
sample problem 3  sample fuel cask

**** problem parameters ****

lib hansen-roach library
mxx            6 mixtures
msc            7 composition specifications
izm            3 material zones
ge  latticecell  geometry
more           0 0/1 do not read/read optional parameter data
msln           0 fuel solutions

**** problem composition description ****

sc  uo2          standard composition
mx             1 mixture no.
vf         .8400 volume fraction
roth     10.9600 theoretical density
temp       293.0 deg kelvin
           92235   2.35%
           92238  97.65%
end

sc  zr           standard composition
mx             2 mixture no.
vf        1.0000 volume fraction
roth      6.4400 theoretical density
end

sc  h2o          standard composition
mx             3 mixture no.
vf        1.0000 volume fraction
roth       .9982 theoretical density
end

sc  b4c          standard composition
mx             4 mixture no.
vf         .3670 volume fraction
roth      2.5200 theoretical density
end

sc  al           standard composition
mx             4 mixture no.
vf         .6360 volume fraction
roth      2.6989 theoretical density
end

sc  h2o          standard composition
mx             5 mixture no.
vf        1.0000 volume fraction
roth       .9982 theoretical density
end
```

```
sc  al          standard composition
mx                6 mixture no.
vf        1.0000 volume fraction
roth      2.6989 theoretical density
end

**** problem geometry ****

ctp squarepitch  cell type
pitch     1.2750 cm center to center spacing
fuelod     .8230 cm fuel diameter or slab thickness
mfuel             1 mixture no. of fuel
mmod              3 mixture no. of moderator
cladod     .9627 cm clad outer diameter
mclad             2 mixture no. of clad


zone specifications for latticecell geometry

                  zone  1 is fuel
                  zone  2 is clad
                  zone  3 is mod
```

```
                        sample problem 3  sample fuel cask

                          ********** data library information **********

        unit                                                    volume
        number              data set name                       name        unit function
        ------              -------------                       ----        -------------

          89      /scale4.2p/datalib/scale.rev05.sclib                      standard composition library

          81      /scale4.2p/datalib/scale.rev02.xn16                       cross section library

          11      ft11f001                                                  short cross section library

                                  standard composition library data
                                  ---------------------------------

          unit number  :  89

          dataset name :  /scale4.2p/datalib/scale.rev05.sclib

          library title:  scale-4 standard composition library
                          386 standard compositions, 332 nuclides
                          10 elements with variable isotopic distrbutions.

          creation date:   1/25/94

                                  cross section library data
                                  --------------------------

          unit number  :  81

          dataset name :  /scale4.2p/datalib/scale.rev02.xn16

          library title:  scale 4 - 16 neutron group criticality safety library
                            hansen-roach data with knight modifications and some endf/b 4 data
                              compiled for nrc        1/27/89
                                last updated         10/12/89
                                  l.m.petrie         ornl
```

```
**** xsdrn mesh intervals ****

   4 mesh intervals in zone  1
   4 mesh intervals in zone  2
  14 mesh intervals in zone  3

                    .....    0 io's were used before reading keno v data    .....

                    .....    0 io's were used reading the keno v parameter data    .....

                  ********** data reading completed **********

                    .....    0 io's were used preparing the keno v input data    .....

                    .....    0 io's were used loading the keno v data    .....

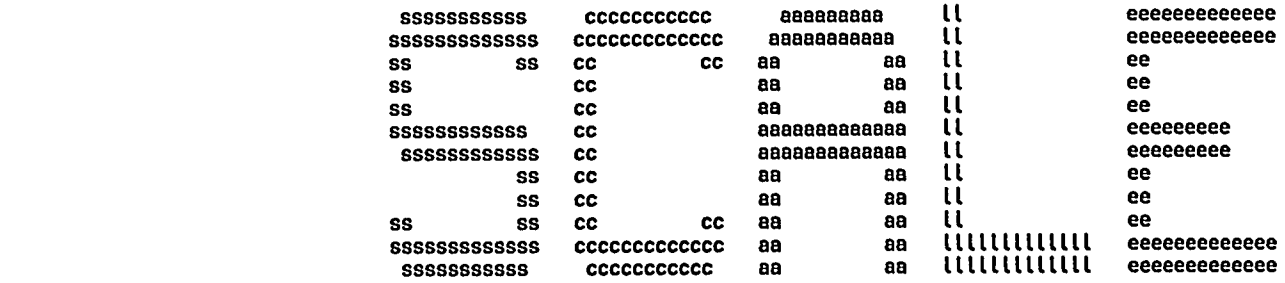
                    .....    0 io's were used loading the data    .....

                    .....    0 io's were used checking the keno v geometry data    .....
                   *****  restart data has been written on unit 95  *****

                    .....    0 io's were used writing the keno v - csas data    .....

                    .....    0 io's were used before reading search data    .....

                    .....    0 io's were used processing csas input data    .....
```




```
*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                  program verification information                *****
*****                                                                     *****
*****                 code system:    scale  version:    4.2           *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  modify                                       *****
*****                                                                     *****
*****         creation date:  10/25/93                                    *****
*****                                                                     *****
*****              library:  /scale4.2p/exe                               *****
*****                                                                     *****
*****                                                                     *****
*****       production code:  modify                                      *****
*****                                                                     *****
*****              version:  2.1                                          *****
*****                                                                     *****
*****              jobname:  st5                                          *****
*****                                                                     *****
*****     date of execution:  03/14/94                                    *****
*****                                                                     *****
*****     time of execution:  16:43:11                                    *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

```
*********************************************************************************************************************
***                                                                                                               ***
***                                        sample square fuel cask                                                ***
***                                                                                                               ***
*********************************************************************************************************************
*********************************************************************************************************************
***                                  ******          search data          ******                                  ***
***                                                                                                               ***
***                                                                                                               ***
***                                  search type                          optimum pitch                           ***
***                                                                                                               ***
***                        pas       number of search passes                 10                                   ***
***                                                                                                               ***
***                        npm       number of search parameters             1                                    ***
***                                                                                                               ***
***                        eps       search convergence tolerance          .0050                                  ***
***                        -con      minimum constraint                   -.0417                                  ***
***                                                                                                               ***
***                        +con      maximum constraint                    .2083                                  ***
***                                                                                                               ***
***                                                                                                               ***
***                          unit    first   last                                                               ***
***       command            number  region  region  ----------------    search constants    ----------------   ***
***                                                                                                               ***
***                          unit    reg=__  to __   +x or r  -x or +h  +y or -h     -y       +z        -z      ***
***                                                                                                               ***
***   alter/change/modify      1       3       3       1.00       1.00       1.00       1.00       .00       .00   ***
***                                                                                                               ***
*********************************************************************************************************************
*********************************************************************************************************************
```

```
**********   search pass  1     keff=  7.11079E-01 + or -  5.77865E-03   **********
                  the parameter was  0.00000E+00
          *****  modified keno v data has been rewritten on unit 95  *****

**********   search pass  2     keff=  7.62379E-01 + or -  4.31515E-03   **********
                  the parameter was -4.16667E-02
          *****  modified keno v data has been rewritten on unit 95  *****

**********   search pass  3     keff=  6.20806E-01 + or -  5.39177E-03   **********
                  the parameter was  2.08333E-01
          *****  modified keno v data has been rewritten on unit 95  *****

**********   search pass  4     keff=  6.43165E-01 + or -  4.71612E-03   **********
                  the parameter was  1.04167E-01
```

****
****

convergence was achieved on pass 2 the parameter was -4.16667E-02

the equation used in the search was:

k-eff = +7.11079E-01 -1.03319E+00*p +4.44000E+00*p**2 -7.49067E+00*p**3

k-effective= 7.62379E-01 + or - 4.31515E-03 the corresponding geometry follows;

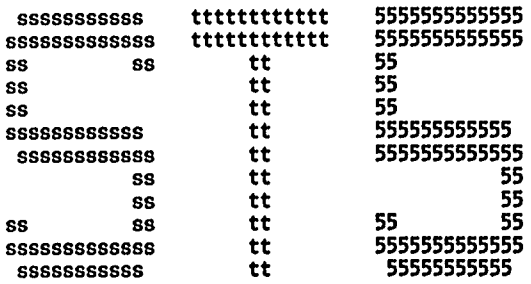
region	media num	bias id	geometry description for those units utilized in this problem					
			----- unit 1 -----					
1 cuboid	500	1	+x = 10.837	-x = -10.837	+y = 10.837	-y = -10.837	+z = 183.00	-z = -183.00
2 cuboid	4	1	+x = 11.500	-x = -11.500	+y = 11.500	-y = -11.500	+z = 183.00	-z = -183.00
3 cuboid	5	1	+x = 11.500	-x = -11.500	+y = 11.500	-y = -11.500	+z = 183.00	-z = -183.00

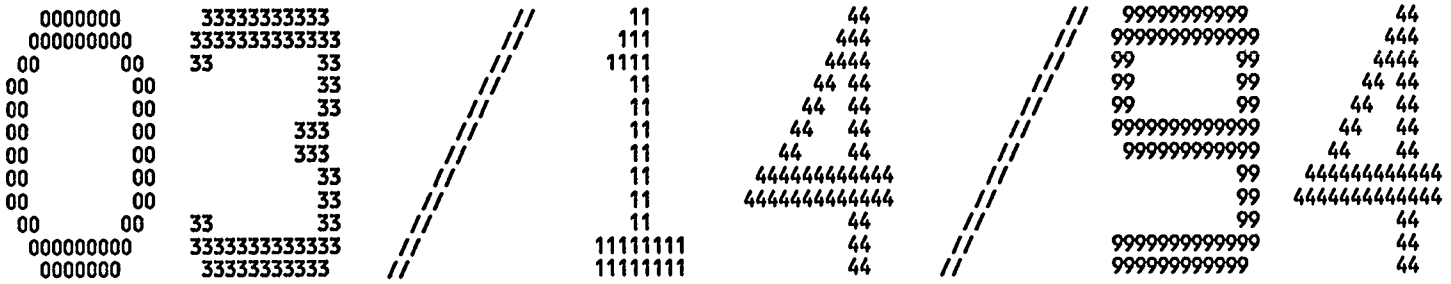
****
****

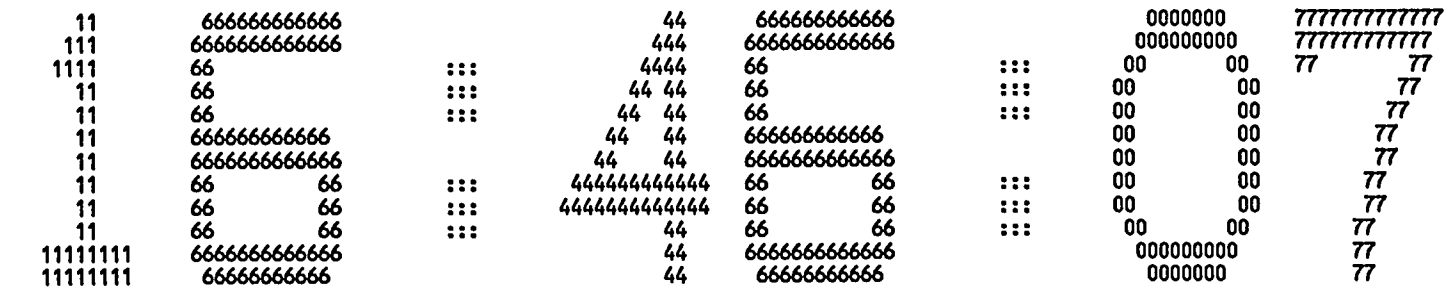
***** modified keno v data has been rewritten on unit 95 *****

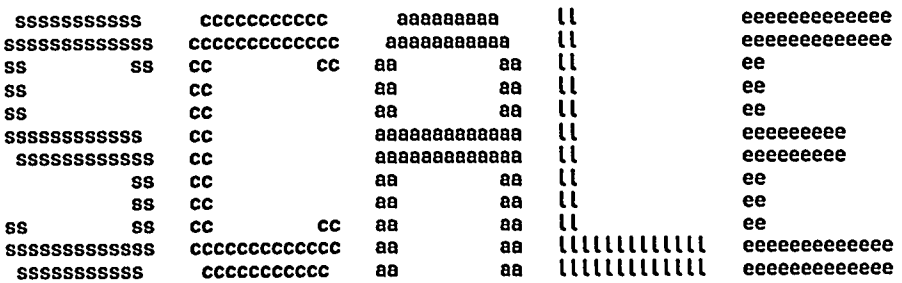
***** convergence has been achieved in the search package. *****

control module modify is complete.









program verification information

code system: scale version: 4.2

program: csas

creation date: 12/01/93

library: /scale4.2p/exe

production code: csas

version: 2.2

jobname: st5

date of execution: 03/14/94

time of execution: 16:46:07

```
sample problem 4  set up 2c8 in csas25


**** problem parameters ****

lib hansen-roach library
mxx            1 mixtures
msc            1 composition specifications
izm            1 material zones
ge  infhommedium geometry
more           0 0/1 do not read/read optional parameter data
msln           0 fuel solutions


**** problem composition description ****

sc  uranium      standard composition
mx             1 mixture no.
vf         .9850 volume fraction
roth     19.0500 theoretical density
temp       293.0 deg kelvin
           92235  93.20%
           92238   5.60%
           92234   1.00%
           92236    .20%
end


**** problem geometry ****


**** infinite homogeneous medium ****
mfuel          1 mixture no. of the infinite homogeneous medium
```

```
                                sample problem 4  set up 2c8 in csas25

                                ********** data library information **********

          unit                                                          volume
          number          data set name                                 name        unit function
          ------          -------------                                 ----        -------------

            89      /scale4.2p/datalib/scale.rev05.sclib                            standard composition library

            81      /scale4.2p/datalib/scale.rev02.xn16                             cross section library

            11      ft11f001                                                        short cross section library

                                        standard composition library data
                                        ---------------------------------

          unit number  :  89

          dataset name :  /scale4.2p/datalib/scale.rev05.sclib

          library title:  scale-4 standard composition library
                          386 standard compositions, 332 nuclides
                          10 elements with variable isotopic distrbutions.

          creation date:   1/25/94

                                        cross section library data
                                        --------------------------

          unit number  :  81

          dataset name :  /scale4.2p/datalib/scale.rev02.xn16

          library title:  scale 4 - 16 neutron group criticality safety library
                            hansen-roach data with knight modifications and some endf/b 4 data
                              compiled for nrc        1/27/89
                                last updated         10/12/89
                                  l.m.petrie         ornl
```

```
........    0 io's were used before reading keno v data    ........

........    0 io's were used reading the keno v parameter data    ........

*************** data reading completed ***************

........    0 io's were used preparing the keno v input data    ........

........    0 io's were used loading the keno v data    ........

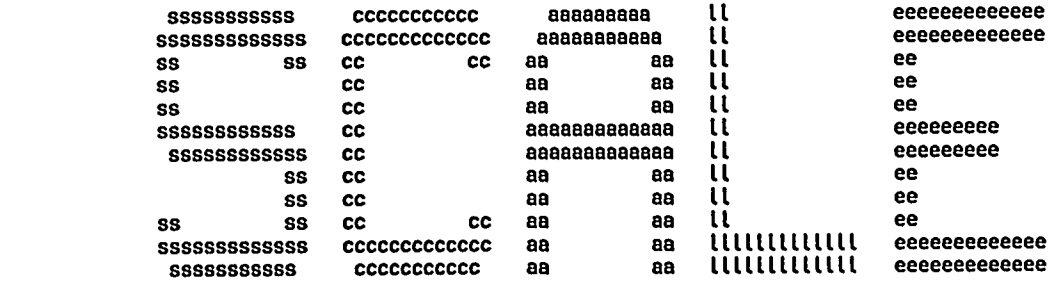
........    0 io's were used loading the data    ........

........    0 io's were used checking the keno v geometry data    ........
*****  restart data has been written on unit 95  *****

........    0 io's were used writing the keno v - csas data    ........

........    0 io's were used before reading search data    ........

........    0 io's were used processing csas input data    ........
```



program verification information

code system: scale version: 4.2

program: modify

creation date: 10/25/93

library: /scale4.2p/exe

production code: modify

version: 2.1

jobname: st5

date of execution: 03/14/94

time of execution: 16:46:26

```
*****************************************************************************************************************
***                          critical pitch search for case 2c8 bare                                          ***
*****************************************************************************************************************
*****************************************************************************************************************
***                              ******          search data          ******                                  ***
***                                                                                                          ***
***                              search type                          critical pitch                          ***
***                                                                                                          ***
***                    pas       number of search passes                 10                               ***
***                                                                                                          ***
***                    npm       number of search parameters              1                               ***
***                                                                                                          ***
***                    eps       search convergence tolerance           .0050                             ***
***                                                                                                          ***
***                    kef       desired k-effective                   1.0000                             ***
***                                                                                                          ***
***                    -con      minimum constraint                    -.2070                             ***
***                                                                                                          ***
***                    +con      maximum constraint                     .0693                             ***
***                                                                                                          ***
***                      unit    first   last                                                              ***
***      command         number  region  region  ----------------   search constants   ----------------     ***
***                                                                                                          ***
***                      unit    reg=__  to __   +x or r  -x or +h  +y or -h    -y       +z       -z       ***
***                                                                                                          ***
***  alter/change/modify   1       2       2       1.00      1.00      1.00      1.00      .00      .00      ***
***                                                                                                          ***
***                                                                                                          ***
***  alter/change/modify   1       2       2        .00       .00       .00       .00     1.00     1.00      ***
*****************************************************************************************************************
*****************************************************************************************************************

     ********************  search pass  1     keff=  9.62581E-01 + or -  4.66186E-03   ********************
                                the parameter was  0.00000E+00
                          *****  modified keno v data has been rewritten on unit 95  *****

     ********************  search pass  2     keff=  9.26968E-01 + or -  4.76267E-03   ********************
                                the parameter was  6.92605E-02
                          *****  modified keno v data has been rewritten on unit 95  *****

     ********************  search pass  3     keff=  1.01030E+00 + or -  4.65530E-03   ********************
                                the parameter was -7.27719E-02
                          *****  modified keno v data has been rewritten on unit 95  *****

     ********************  search pass  4     keff=  1.00968E+00 + or -  4.18861E-03   ********************
                                the parameter was -5.70604E-02
                          *****  modified keno v data has been rewritten on unit 95  *****

     ********************  search pass  5     keff=  9.80129E-01 + or -  5.04216E-03   ********************
                                the parameter was -3.87869E-02
                          *****  modified keno v data has been rewritten on unit 95  *****

     ********************  search pass  6     keff=  9.98210E-01 + or -  4.21917E-03   ********************
                                the parameter was -5.09593E-02
```

critical pitch search for case 2c8 bare

****
****

convergence was achieved on pass 6 the parameter was -5.09593E-02

the equation used in the search was:

k-eff = +9.39989E-01 -9.76969E-01*p +7.86001E+00*p**2 +8.33712E+01*p**3

k-effective= 9.98210E-01 + or - 4.21917E-03 the corresponding geometry follows;

region	media num	bias id	geometry description for those units utilized in this problem
			----- unit 1 -----
1 cylinder	1	1	radius = 5.7480 +z = 5.3825 -z = -5.3825 centerline is at x = 0.00000E+00 y = 0.00000E+00
2 cuboid	0	1	+x = 6.8786 -x = -6.8786 +y = 6.8786 -y = -6.8786 +z = 6.5318 -z = -6.5318

****
****

critical pitch search for case 2c8 bare

based on the preceding data, the best estimate of the parameter is -5.17118E-02

the geometry corresponding to this parameter follows:

region	media num	bias id	geometry description for those units utilized in this problem
			----- unit 1 -----
1 cylinder	1	1	radius = 5.7480 +z = 5.3825 -z = -5.3825 centerline is at x = 0.00000E+00 y = 0.00000E+00
2 cuboid	0	1	+x = 6.8732 -x = -6.8732 +y = 6.8732 -y = -6.8732 +z = 6.5266 -z = -6.5266

****
****

***** modified keno v data has been rewritten on unit 95 *****

***** convergence has been achieved in the search package. *****

control module modify is complete.

ABSTRACT

The SAS1 control module was developed to provide an easy-to-use tool for a one-dimensional, discrete-ordinates shielding analysis. Automated preparation of a working cross-section library is performed using the BONAMI and NITAWL-II functional modules of SCALE. Cell-weighting of cross sections is optionally allowed by a call to XSDRNPM. The one-dimensional radiation transport calculation is also done using XSDRNPM. The XSDOSE functional module then uses the surface angular flux from XSDRNPM to generate dose rates at points on, or some distance from, the shield surface.

Simplified, free-form input is used in SAS1. Default values are provided for all nonphysical calculational parameters (e.g., angular quadrature, number of iterations, etc.) except the spatial mesh. Radiation sources can be optionally read from an ORIGEN-S output file. In addition, the angular boundary flux from a preliminary XSDRNPM criticality calculation can be optionally used as the input source to the final XSDRNPM shielding calculation.

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ACKNOWLEDGMENTS

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S1.1 INTRODUCTION

Shielding Analysis Sequence No. 1 (SAS1) is a SCALE control module developed for problem-dependent cross-section preparation and subsequent one-dimensional (1-D) shielding calculations. The control module has two analytic sequences—SAS1 and SAS1X. Input for the module is designed to be simple and direct. The SCALE free-form reading routines (see Sect. M3) are used for data input.

The SAS1 module basically consists of three major steps: (1) preparation of the cross sections and mixing table used for the shielding calculation, (2) execution of a 1-D radiation transport analysis, and (3) calculation of dose rates outside the defined shield. The first step is accomplished using the Material Information Processor, which is described in Sect. M7. This processor uses the standard input data for the cross-section library, material compositions, and problem geometry (see Sect. M7.4) to generate input data automatically for calls to the BONAMI and NITAWL-II modules of SCALE. BONAMI performs resonance self-shielding calculations for materials having Bondarenko data (see Sects. F1, M7.2.5.1, and M7.A), while NITAWL-II applies the Nordheim resonance self-shielding correction to materials having resonance parameters (see Sects. F2, M7.2.5.2, M7.2.5.3, and M7.A). The radiation transport analysis of the second step is performed via a call to the XSDRNPM module of SCALE (see Sect. F3). This module performs the 1-D fixed source calculation that provides the neutron and/or gamma fluxes used to determine the dose rates. It also calculates the dose rates inside the system. The last step of the SAS1 sequence is a call to the XSDOSE module of SCALE (see Sect. F4) that calculates the dose rate for selected points outside the system (or at the surface) using XSDRNPM fluxes and standard flux-to-dose conversion factors available in SCALE.

The SAS1X sequence follows the steps of the SAS1 sequence except that an additional call is made to the XSDRNPM module to prepare cell-weighted cross sections or perform a simple criticality analysis to obtain a boundary source for the final XSDRNPM shielding analysis. The SAS1X sequence can prepare cell-weighted cross sections for one problem region where a homogeneous representation of a heterogeneous configuration is needed. The boundary source option was added to allow an easy means to evaluate the dose from a postulated criticality accident as a function of shield design or detector location.

S1.2 METHODS AND TECHNIQUES

The SAS1 module was designed to enable general 1-D shielding analyses to be performed without requiring the user to be experienced in the use of such functional modules as NITAWL-II, BONAMI, XSDRNPM, or XSDOSE. The modeling approximations and validity, along with the solution techniques associated with each of these functional modules, is described in detail in other sections of the SCALE manual, viz. Sects. M7 and F1-F4. Likewise, the Material Information Processor (which uses engineering-type input data for problem mixtures, geometry, and boundary conditions to prepare much of the functional module input automatically) is described in detail in Sect. M7. This section highlights various methods, techniques, or features incorporated into SAS1 for ease of use and/or flexibility.

S1.2.1 SOURCE SPECIFICATION

The SAS1 control module allows source spectra to be input from (1) cards, (2) an ORIGEN-S binary output file (see Sect. F7), and (3) an XSDRNPM boundary flux distribution calculated within SAS1X. The last option was added to allow multiple shielding analyses to be performed using the leakage spectrum from an XSDRNPM MULTIREGION criticality calculation as a boundary source. This option is discussed in more detail in Sect. S1.2.4. The second option was added to allow easy input of the neutron and gamma source spectra calculated by ORIGEN-S for spent fuel assemblies and/or other radiation sources. Neutron, gamma, or coupled neutron-gamma libraries and sources may be used. (Note: The ORIGEN-S source spectra must have the same energy group structure as the cross-section library used in SAS1.) Depending on the cross-section library type (neutron only, gamma only, or coupled) used in the calculation, SAS1 will employ the appropriate portion of the coupled source located on the ORIGEN-S output file. Source spectra from cards or the ORIGEN-S output file can be specified for more than one zone. For applications involving spent nuclear fuel, the SAS2(H) module (see Sect. S2) within SCALE could be used to simulate the fuel depletion and generate the fuel source spectra. Saving the output from unit 71 for a SAS2(H) case provides the ORIGEN-S output file containing the source spectra (see Sect. S2.5.6).

The shielding module of the SAS1 sequence—XSDRNPM—requires the source spectra normalized on a per unit volume basis. For spectra from ORIGEN-S output files, the SAS1 module assumes a source spectra normalized on a per assembly basis [standard from a SAS2(H) case] and uses the following formula to modify the source spectra to a per unit volume basis:

$$s_i = \frac{S_i \cdot NASS}{ZVOL} ,$$

where

s_i = source strength for energy group i per unit volume
S_i = source strength for energy group i per assembly from ORIGEN-S output file
NASS = SAS1 input parameter (integer) indicating the number of assemblies in the source zone
ZVOL = SAS1 input parameter indicating the volume of the actual source zone.

If an assembly fraction is required (as may be for consolidated fuel), the ZVOL parameter can be adjusted since NASS must be an integer.

For stand-alone ORIGEN-S cases, the units for the source spectra on the ORIGEN-S output file depend on the BASIS card provided in data block 6 of the ORIGEN-S input. The "basis" or units for the source spectra on the file can be obtained from the printout for the corresponding ORIGEN-S case. Knowing the units for the source, the SAS1 user can convert the source units to the per unit volume basis by using appropriate input values for the ZVOL and NASS parameters. SAS1 always uses the above formula to convert the ORIGEN-S file source to the properly normalized source for use in SAS1.

Source spectra input from card records are renormalized to the input source strength per unit volume. For flexibility, variables to specify the total unit volume neutron source strength (XNN) and total unit volume photon source strength (XNG) are provided in SAS1.

Boundary source spectra input from the XSDRNPM-S criticality calculation in SAS1X require no normalization.

S1.2.2 MESH INTERVAL SIZE SPECIFICATION

For each zone entered in the SAS1 input, the user is required to input the number of equal-size mesh intervals desired for that zone. This method of specifying the mesh was selected because it is easy to input while still providing the user with control of the mesh size from zone to zone. The completely automatic mesh generator developed for the SAS2 control module (see Sect. S2.2.9) is adequate for the specific class of problems for which it was designed, but unsatisfactory mesh intervals can be generated when it is applied to other classes of problems. Because SAS1 was developed for solving general 1-D shielding problems, the currently available automatic mesh generator was not used. Therefore, the SAS1 user must exercise some judgment in specifying the number of zone mesh intervals, or unsatisfactory results could be obtained.

Ideally, the mesh spacing in a material should be no more than the shortest mean free path obtained by comparing neutron and gamma cross sections for *all* energy groups. This procedure has the potential to generate a very fine, but perhaps costly and unneeded, mesh spacing. For example, in heavy metal shields where the mean free path for low-energy gammas is very short, these criteria can be loosened. Trial and error, or a lot of *a priori* experience, is necessary to obtain a sufficiently adequate and efficient mesh size for a problem. The final criterion by which to judge the input mesh is the flux profile. A smoothly varying flux profile is desired. However, some general suggestions can be provided for the novice user seeking a point of reference from which to start a calculation:

1. In a gamma radiation field, the mesh size for a heavy-metal shield should range from about 0.3 (uranium) to 0.7 cm (iron). If no gammas are present, the mesh size can be increased to about 1.0 cm.

2. In a neutron radiation field, typical neutron moderators should have a mesh size of 0.8 to 1.0 cm. For some materials such as carbon, the mesh size can be increased to about 2.0 cm.

3. A typical mesh spacing for light elements is 1.0 cm.

4. For gases and voids, the mesh spacing can be rather large, 3 to 5 cm.

5. Radical changes in the mesh size from one zone to the next can be detrimental, particularly because greater flux gradients typically occur at material interfaces. If necessary, the SAS1 user can provide extra zones with intermediate mesh spacings on either side of a material interface to provide for better transition from one material mesh size to another. (Note: Radical mesh size changes within the same material can also cause large undesirable flux changes between the mesh intervals.)

The previous suggestions provide a minimum of guidance to the inexperienced user, but all users are duly cautioned that only after the calculation is complete can the results be analyzed and the mesh judged adequate. The appropriate check is the groupwise scalar fluxes (in XSDRNPM output). These should not undergo significant changes (>50%) from one interval to the next. Again, exceptions occur because the low-energy fluxes may be allowed to change radically from interval to interval without affecting the validity of the final doses. Thus, when there is uncertainty in the user's mind, the safest and best approach is to repeat the calculation with a finer mesh until successive calculations show little or no change in the desired dose results.

S1.2.3 COMBINED CRITICALITY AND SHIELDING CALCULATIONS

After the original SAS1 module was developed and tested, an enhancement was added that allows the user to take the leakage spectrum from an XSDRNPM criticality calculation and input it as a boundary source to subsequent shielding calculations. This option can be valuable in assessing the effectiveness of criticality accident alarms at various locations when shielded by different materials. The modifications were made using existing input variables such that there is no impact on the input for previous SAS1 and SAS1X calculations.

The SAS1X procedure executes BONAMI, NITAWL-II, and XSDRNPM to process cross sections for subsequent shielding calculations by XSDRNPM. Although the first XSDRNPM calculation called by SAS1X was originally intended by producing cell-weighted cross sections, the analysis can also be used to provide the value and the leakage spectrum for the 1-D geometry input with the MULTIREGION treatment (see Sect. M7.2.4.3). When properly specified, the SAS1X sequence reads the angular flux file written by the first XSDRNPM criticality calculation and prepares a boundary source for input to subsequent XSDRNPM shielding calculations. This boundary source is input to the boundary of the first zone of the shielding problem. This first zone must be designated as a void region, and its boundary dimension must be identical to the outer boundary of the XSDRNPM criticality calculation.

Error checking for consistent input is performed to ensure that the input for this SAS1X option is accurate. The following checks are performed:

1. The geometry option input to the Material Information Processor must be MULTIREGION.

2. The zone designated for the boundary flux input must be a void region and must be the first zone of the shielding analysis.

3. The boundary dimension of the zone designated for the boundary flux input must be identical to the outer boundary dimension of the XSDRNPM criticality calculation.

4. The number of intervals in the zone designated for the boundary flux input must equal one.

5. The angular quadrature (ISN) for the XSDRNPMS criticality and shielding calculations must be identical.

No mixture that is used in the XSDRNPM criticality calculations may be used in the XSDRNPM shielding calculation.

In order to obtain a calculation of activities from XSDRNPM with SAS1X, the user must input a trace amount of the ACTIVITIES dummy nuclide from the Standard Composition Library in one of the mixtures in the XSDRNPM shielding calculation. This is not necessary when using the SAS1 sequence because the sequence automatically places the ACTIVITIES dummy nuclide on the cross-section library. However, in the SAS1X sequence the XSDRNPM criticality calculation generates a second

cross-section library with the cell-weighted cross sections that are used in the XSDRNPM shielding calculation. This library does not contain the ACTIVITIES nuclide; thus it must be input by the user.

The dose results from SAS1X are given in rem/hour normalized to a fission source rate of 1 fission neutron born/second. In order to normalize the dose to total fissions, the following calculation should be performed:

$$\text{Dose (rem)} = \text{total fission} * \text{dose rate}\left(\frac{\text{rem/h}}{\text{neutrons/s}}\right) * \frac{1 \text{ neutron/s}}{\text{fission rate (fissions/s)}} * \frac{1 \text{ h}}{3600 \text{ s}}$$

The dose rate is taken from the XSDOSE output, and the fission rate is taken from the XSDRNPM criticality case output. Dose rates from the optional XSDRNPM calculation of activities can be interpreted in the same manner.

In order to normalize the dose rate to power, the following calculation should be performed:

$$\text{Dose rate (rem/h)} = \text{dose rate}\left(\frac{\text{rem/h}}{\text{neutrons/s}}\right) * \text{power (watts)} * \frac{1 \text{ neutron/s}}{\text{fission rate(fissons/s)}} * \frac{1}{\text{energy per fission}\left(\frac{\text{watt-s}}{\text{fission}}\right)}$$

where energy per fission is typically on the order of 3×10^{-11} watt-s/fission. Caution should be exercised in using the equations presented above if dose factors other than the default ANSI standard are used. The units of measure for other dose factors may differ, requiring modifications to the above equations.

S1.2.4 SPECIAL FEATURES AND PARAMETER DEFAULT VALUES

The SAS1 control module has been developed to enable several different shielding calculations to be run using the same cross-section working library. This is done by separating data for the cross-section processing and data for the shielding analysis by a Problem Control Card. If the Problem Control Card in the input data is left blank, additional shielding problems following the current problem will be solved using the same cross-section set and mixing table. If this card contains LAST, the program terminates on completion of the current problem. Generation of the cross-section working library can also be skipped (i.e., calls to BONAMI, NITAWL-II, XSDRNPM for cell-weighting are bypassed) by saving the working library from a previous SAS1 case (output by NITAWL-II to the file in unit 4) and using the PARM=RESTART option on the module specification card (see Sect. S1.4). For the restart case, the working library is read from the file in unit 4, and the Material Information Processor portion of the data (see Sect. S1.4) must be the same as that used in preparation of the working library (to ensure a valid mixing table is generated). Generation of a working library without execution of the shielding analysis can also be done by using the PARM=HALT option on the module specification card. These features for using the same working library with multiple shielding calculations are very beneficial for design analyses when only the geometry or source specification differs between problems. To use the PARM=HALT and PARM=RESTART options with the SAS1X sequence, the working library output by XSDRNPM to the file in unit 3 must also be saved. If the XSDRNPM boundary flux from the criticality calculation is to be used as a source in the shielding calculation, the file in unit 94 (containing the angular boundary fluxes) must also be saved.

Another attractive feature of the SAS1 module is the optional COLLAPSE parameter. This keyword parameter is available as an option in the MORE DATA section of data for the Material Information Processor. Engaging the COLLAPSE parameter causes the thermal neutron groups available

on the cross-section set to be collapsed to one group. The collapse is done using a typical thermal reactor flux spectrum (Maxwellian to 1/E to fission). The sources read from an ORIGEN-S file are also collapsed to remove multiple thermal neutron groups. *However, sources input from cards are assumed to be collapsed by the user prior to input.* In shielding problems where the neutron thermal group structure is not needed, the COLLAPSE option can significantly enhance the calculational efficiency with little or no impact on the final dose rates. In particular, this option is aimed at the 27-group neutron and 27n-18-γ group libraries available in SCALE that contain 13 thermal neutron groups. As shown in the sample problems (Sect. S1.5), the COLLAPSE option can prove very beneficial in reducing cpu time without affecting results.

Default values are provided in SAS1 for parameters commonly used in XSDRNPM (for shielding analysis) and XSDOSE. Parameters for which default values are provided, but that can be easily modified, are shown in Table S1.4.7.* The default values were selected for a variety of reasons. An angular quadrature order (ISN) of 16 was chosen for use in XSDRNPM because it generally provides enough scattering angles for the typical 1-D shielding problem. An angular quadrature of 8 is often adequate, but ISN = 16 is a more prudent choice for thick shields. The outer iteration limit (ICM) of 4 was selected based on experience with evaluating doses from spent fuel shipping casks using the SCALE 27n-18γ group library. Cases run without the COLLAPSE option typically took more than four outer iterations to converge (because of the large amount of thermal upscatter), but the dose results were only slightly affected.

Default dose factor identifiers (IDs) and detector locations for use by XSDOSE are also provided in SAS1. The default dose factors are the ANSI standard neutron and gamma flux-to-dose-rate factors.[1] The default detector locations are at 0, 1, 2, and 4 m from the outer shield surface. In addition to the dose rates available from the XSDOSE output of SAS1, the dose rates internal to the shield are always provided in the activity tables at the end of the XSDRNPM output. Activity No. 1 is the neutron dose (rem/h) based on the ANSI neutron dose conversion factors, while Activity No. 2 is the gamma dose (rem/h) based on the ANSI gamma dose conversion factors. A calculation of activities for the same dose factor identifiers may also be obtained from XSDRNPM by inputing a trace amount of the ACTIVITIES dummy nuclide from the Standard Composition Library in one of the mixtures in the shielding analysis. If optional dose factors are specified in the input, the activities provided by XSDRNPM will use those specified.

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*Note that the optional parameter data in the Material Information Processor input (see Table S1.4.5) does not affect the XSDRNPM-S case run for the shielding analysis.

S1.3 PROGRAM FLOW

The general flow of the SAS1 control module is given in this section along with a brief description of the subroutines. An abbreviated flowchart for the SAS1 sequence is shown in Fig. S1.3.1. In the figure, the SCALE driver is represented as the large rectangular block at the left, functional modules are represented by hexagons, major program segments are contained in rectangularized ovals, and subroutines are denoted by boxes. The SCALE driver (described in Sect. M1) initiates the correct sequence based on the module name read from the first card (module specification card) in the user input data file. Subroutine SAS1 or subroutine SAS1X is then accessed by the driver. Data are transferred from the SAS1 module to the functional modules and between functional modules by sequential data files.

As noted in previous sections, the functional modules accessed in SAS1 are described in detail in Sects. F1-F4 of the SCALE Manual. Likewise, the Material Information Processor is described in Sect. M7. In fact, all documentation pertaining to the Material Information Library is valid here. Thus, only the initiating subroutine C4DATA is described in the following subroutine descriptions. All subroutines in the Shielding Data Processor program segment are briefly described.

SAS1 - This subroutine initiates an analytic sequence to perform cross-section processing without cell-weighting, solve one or more 1-D radiation transport problems by discrete ordinates calculations, and generate the radiation doses at points in, or outside of, the problem boundary. It sets information in common to communicate with the SCALE driver. It sets the sequence indicator and loads it in common. MAIN is called to activate the data reading and checking procedure, and to provide information to the SCALE driver so that the desired functional modules will be executed in the proper order.

SAS1X - This subroutine is identical to subroutine SAS1 except the sequence initiated performs an eigenvalue calculation using the XSDRNPM module. Cell-weighted cross sections or the leakage spectrum from this XSDRNPM analysis are used in the subsequent shielding calculation.

MAIN - This routine is called from subroutines SAS1 or SAS1X and opens the appropriate input/output units based on the sequence to be run. Subroutine IONUMS is called to define the input/output units used by the free-form data routines. On the first call to MAIN, data preparation is initiated, and module execution flags are set for processing the cross-section data. Flags are set to signal the SCALE driver to execute BONAMI and NITAWL-II. If called from SAS1X, execution of XSDRNPM is also flagged. MAIN uses the library subroutine ALOCAT to call C4DATA and initiate the Material Information Processor (see Sect. M7.3 for more details). These program segments are accessed to read and check the control module input data and prepare input data for the functional modules. After completion of cross-section processing, the driver returns control to MAIN (via the SAS1 or SAS1X subroutines). Flags are set to direct the SCALE driver to execute XSDRNPM and XSDOSE for the shielding and dose analysis. DATIN is called via ALOCAT to initiate the program segment entitled Shielding Data Processor. This program segment reads data input to the control module and prepares the input data for execution of the functional modules. If the program control card is set to LAST, a flag is set to terminate the control module following execution of XSDOSE. If there are other cases to follow, the program control card is blank, and the SCALE driver is instructed to return to MAIN following

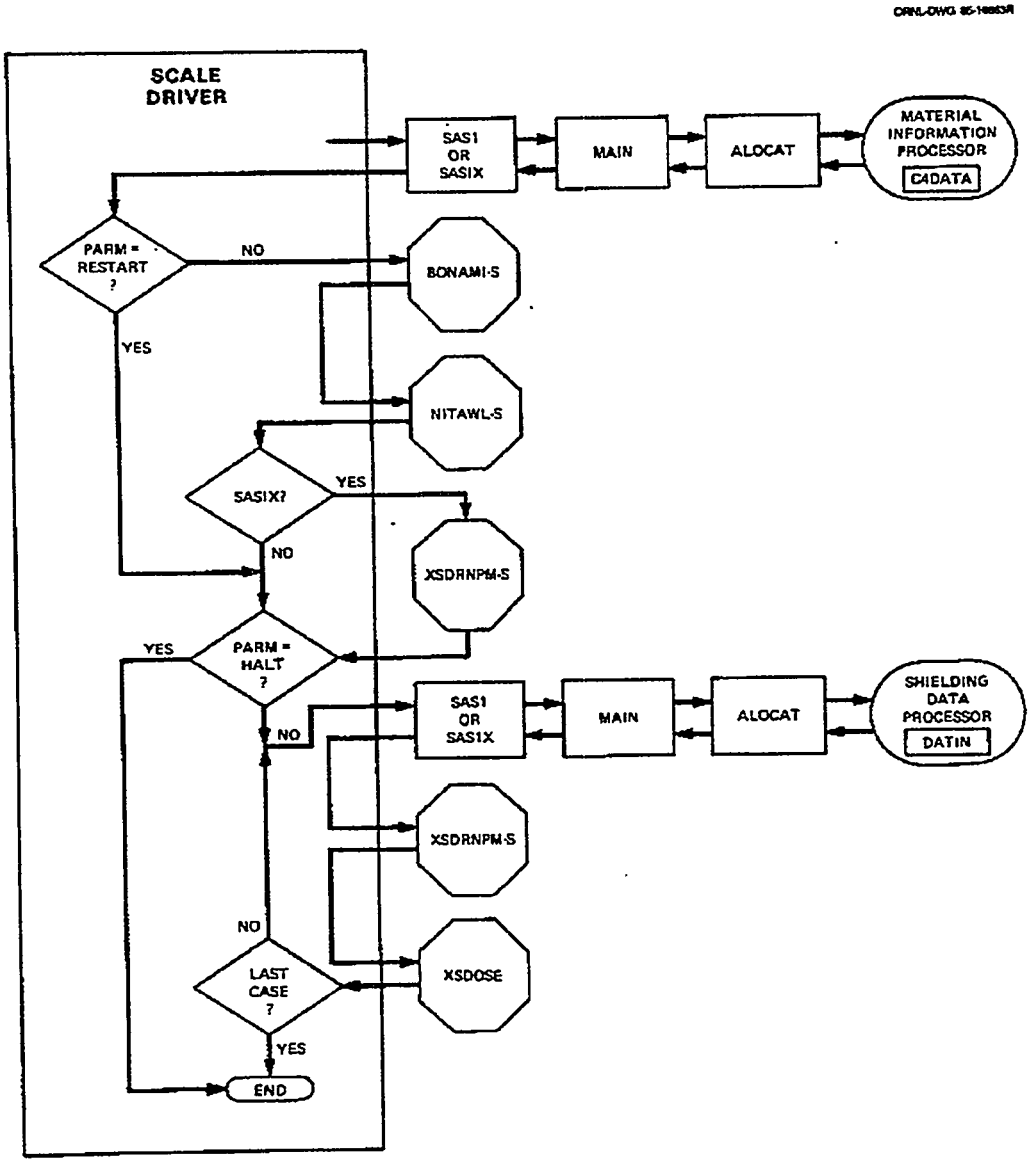


Figure S1.3.1 General SAS1 flow diagram

the execution of XSDOSE in order to repeat the shielding analysis portion of the sequence with another set of data.

ALOCAT- This routine is part of the SCALE subroutine library. It is used to dynamically allocate an array and pass it, along with its dimension, to another subroutine supplied as an argument. It is used in SAS1 to call C4DATA and DATIN.

C4DATA - This is the subroutine through which the Material Information Processor is activated. It opens the units that will be used to pass data to the functional modules (96 for BONAMI, 97 for NITAWL-II, and 98 for XSDRNPM). Throughout the subroutine, pointers are defined for various types of data, and the STOP subroutine library is called to write a message if the data arrays require more storage than is available. All other subroutines called by C4DATA carry out operations to prepare and check data that will be used by the functional modules activated by the sequence. A description of the other subroutines in the Material Information Processor is provided in Sect. M7.3. A list of warning and error messages issued by the Material Information Processor is provided in Sect. M7.7.

DATIN - This subroutine is called from MAIN via ALOCAT to initiate the program segment designated the Shielding Data Processor. It calls all the subroutines used for data input and data processing needed to prepare the XSDRNPM and XSDOSE input data files.

FREE-FORM READING ROUTINES - Subroutines SCANON, SCANOF, IREAD, FREAD, and AREAD are a part of the SCALE subroutine library and are called at various places throughout the program to control the reading of free-form data. SCANON and SCANOF turn on and off the scan-ahead feature that checks to see if the next item in the input is an END. IREAD, FREAD, and AREAD read input as integer, floating-point decimal, or alphanumeric data, respectively. See Sects. M2 and M3 for more detailed descriptions of these library routines.

RDICE - This subroutine is called twice from DATIN. On the first call the ICE binary input file (written by the Material Information Processor) is read to obtain the dimensions of the mixing table. The second call reads the mixing table data from the ICE input file.

SETA - This subroutine is called by DATIN to read the problem title, coordinate system specification, and the left boundary condition needed for slab and disc geometries. Library routines SCANON, SCANOF, and AREAD are called.

RDZON - This subroutine reads the zone description data and transfers it to a scratch data set. It counts the number of various types of entries for use in dimensioning the appropriate data storage arrays. Library routines SCANON, SCANOF, AREAD, IREAD, and FREAD are called.

BFLUX - This subroutine reads the XSDRNPM angular flux file to obtain the boundary flux from the XSDRNPM criticality analysis input to the shielding analysis.

ZONDAT - This subroutine reads the scratch data set written by RDZON and loads the zone data into the appropriate arrays.

SOURCE - This subroutine is called from DATIN to read the input source spectra from an ORIGEN-S binary output data set and/or from input cards. Library routine FREAD is called.

SETB - This subroutine is called from DATIN to read optional parameter values that override the default values. Library routines AREAD, FREAD, and IREAD are called.

DOSD1 - This subroutine reads the dimensions needed by XSDOSE and sets the array sizes for the rest of the XSDOSE data arrays. Library routine FREAD is called.

DOSD2 - This subroutine is called by DATIN to read the remainder of the data used by XSDOSE. It sets the default values of dose factor IDs and detector locations when the default values are used. Library routines FREAD, SCANON, and SCANOF are called.

CORMIX - This subroutine modifies the mixing table to make homogenized mixtures of source zone material with other input mixtures as required by the module data input. It is called from DATIN.

SNORM - This subroutine normalizes the input source spectra to the correct values for each source zone. Normalization of both ORIGEN-S and card input source spectra are done. SNORM is called by DATIN.

XSDRNA - This subroutine is called by DATIN to prepare the input data required by the functional module XSDRNPM. The data are written, in binary, on the appropriate units for use in the XSDRNPM execution by the SCALE driver.

XSDOSA - This subroutine is called by DATIN to prepare the input data required by the functional module XSDOSE. The data are written, in binary, on the appropriate unit for use in the subsequent XSDOSE execution by the SCALE driver.

Besides the subroutines described above, the SAS1 module makes use of several of the subroutines described in the SCALE subroutine library (Sect. M2).

S1.4 INPUT DATA DESCRIPTION

The input to SAS1 consists of an Analytical Sequence Specification Card, the Material Information Processor data, a problem control card, and the shielding problem data. An outline of the SAS1 input is provided in Tables S1.4.1-S1.4.6. The data for each segment are entered using the SCALE free-form reading routines described in detail in Sect. M3. A review of the free-form input features is provided below, followed by the input requirements for each segment of data.

The word "END" is a special data item. An "END" may have a name or label associated with it. The name or label associated with an "END" is separated from the "END" by a single blank and is a maximum of 12 characters long. *At least 2 blanks MUST follow every labeled and unlabeled "END." It is the user's responsibility to ensure compliance with this restriction. Failure to observe this restriction can result in the use of incorrect or incomplete data without the benefit of warning or error messages.*

S1.4.1 ANALYTICAL SPECIFICATION CARD

The analytical sequence specification =SAS1 or =SAS1X (# can also be used in place of =) should begin in column 1. The SAS1X sequence prepares cell-weighted cross sections (by XSDRNPM) for use as a homogenized mixture in the subsequent XSDRNPM shielding calculations. Input data for the sequence can be checked, or portions of the sequence execution can be skipped, by entering various keyword options beginning in column 11.

PARM=CHECK PARM=CHK	This option causes the input data to be read and checked without execution of any functional modules. Appropriate error messages are printed.
PARM=SIZE=nnnnnn	The region size for a problem can be specified by the user by entering PARM=SIZE=nnnnnn starting after column 10 of the analytical sequence specification. The region size, nnnnnn, is specified in words.
PARM=HALT	This option causes the sequence to halt after generation of the cross-section library. The Shielding Problem Data input is read and checked even though the shielding modules are not executed.
PARM=RESTART	This option allows a mixing table to be generated with the input material information data but allows the cross-section preparation modules to be skipped and, instead, uses an existing working library (consistent with the material information data) read on unit 4 and the boundary flux file on unit 94 (if XSDRNPM boundary source is input).

The PARM=HALT and PARM=RESTART options can be cost-effective when many shielding analyses are to be performed with a single cross-section library over a period of time.

To run SAS1 and utilize more than one of the PARM options, use commas between each option and parentheses or single quotes at the beginning and end:

```
=SAS1    PARM=(CHECK,SIZE=120000)
=SAS1    PARM=(SIZE=120000,CHECK)
=SAS1    PARM='CHECK,SIZE=120000'
=SAS1    PARM='SIZE=120000,CHECK'
```

Table S1.4.1 Outline of data for SAS1 module

Data position	Type of data	Data entry	Comments
1	Sequence specification	=SAS1 or =SAS1X	Begin in column 1. PARM=CHK beginning in column 11 checks the input for errors, while PARM=HALT and PARM=RESTART, respectively, stop and restart the sequence after completion of the Material Information Processor
2	Title	Enter a title	80 characters (prints 72 in XSDRNPM)
3	Cross-section library name	**27N-18COUPLE** **22N-18COUPLE** **18GROUPGAMMA** **27BURNUPLIB**	These are the commonly used cross-section libraries available in SCALE for shielding analyses. See Sect. M4
4	Type of calculation	**INFHOMMEDIUM** **LATTICECELL** **MULTIREGION**	These are the available options. See the explanation in Sect. M7.4.3. Note the LATTICECELL specification is normally applicable only for the SAS1X sequence where cell-weighted cross sections are desired
5	Standard composition specification data	Enter the appropriate data	Terminate this data block with **END COMP**. See Table S1.4.2. Section C4.4.4 provides a detailed explanation
6	Cell geometry specification	Enter the appropriate data (Omit for **INFHOMMEDIUM**)	Omit for **INFHOMMEDIUM**. See Table S1.4.3 for **LATTICECELL**. See Table S1.4.4 for **MULTIREGION**. Detailed explanations are provided in Sects. M7.4.6 and M7.4.7
7	Optional parameter data	Enter the desired data	Precede this data block by **MORE DATA** if more parameter data are to be entered. Otherwise, omit these data entirely. See Table S1.4.5 for parameter description. See Sect. M7.4.8 for more information
8	Terminate information processor data	**END**	Must begin in column 1. Except for **END COMP**, this is the only END keyword in the Material Information Processor data that should start in column one
9	Problem control card	Blank or **LAST**	Keyword LAST (begin column one) indicates the subsequent shielding problem data is the last to be entered. A blank record indicates another problem control card/shielding problem data combination is expected
10	Shielding problem data	Enter appropriate data	See Table S1.4.6
11	Terminate analytic sequence	END	Must begin in column 1

Table S1.4.2 Material Information Processor data: standard composition specification[a]

Entry number	Variable name	Type of data	Entry requirement	Comments
1	SC	Standard composition component name	Always	Enter once for each standard composition. Enter the alphanumeric description from Table M8.2.1. Additional allowed names include those beginning with ARBM for arbitrary materials, and SOLN for solutions
A1	ROTH	Theoretical density of material (g/cc)	ARBM	Enter once for each standard composition component that is an arbitrary material
A2	NEL	Number of elements in the material	ARBM	Enter once for each standard composition component that is an arbitrary material
A3	IVIS	Multiple isotope indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 for a material that does not contain multiple isotope elements. Enter 1 if the material contains a multiple isotope element. An arbitrary material cannot have more than one multiple isotope element. If necessary, several arbitrary materials may be used in a single mixture
A4	ICP	Compound indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 1 for a compound and 0 for alloys, mixtures, etc.
A5	IRS	Resonance indicator	ARBM	Enter once for each standard composition component that is an arbitrary material. Enter 0 if all the nuclides in the material are nonresonance nuclides; enter 1 if one or more have resonance data. See Sect. M8.2, Table M8.2.1
A6	NCZA	ID number (from far right column of Table M8.2.1)	ARBM	Repeat the sequences A6 and A7 for each element in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1. (Premixed standard compositions cannot be used in an arbitrary material definition.)
A7	ATPM	Number of atoms of this element per molecule of arbitrary material	ARBM and ICP=1	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry 2. Do not enter a value unless ICP=1
		or	or	or
		Weight percent of this element in this arbitrary material	ARBM and ICP=O	Repeat the sequence A6 and A7 for each element in the arbitrary material before entering entry number 2. Do not enter a value unless ICP=0
2	MX	Mixture ID number	Always	Enter once for each standard composition component

Table S1.4.2 (continued)

Entry number	Variable name	Type of data	Entry requirement	Comments
S1	FD	Fuel density (grams of U or Pu per liter of solution)	SOLN	Enter once for a solution
S2	AML	Acid molarity of the solution	SOLN	Enter once for a solution. AML=0 if there is no acid in the solution
01	SPGR or ROTH	Specific gravity of the solution or Density of the basic standard composition	Optional	If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR or If the density of a basic standard composition (ROTH) is to be entered, use DEN=ROTH
3	VF	Density multiplier	See comment column	Enter the density multiplier (density fraction, volume fraction, or a combination). Default value is 1. This item can be omitted if entries 4, 5, 6a, and 6b are also omitted. VF=0 is not allowed for SOLN or ARBM
4	ADEN	Number density (atoms/b-cm) for the nuclide	VF=O	Enter only if VF=0.0
5	TEMP	Temperature, in degrees K	See comment column	Default value is 293 K. This entry can be omitted if entries 6a and 6b are also omitted
6a	IZA	Isotope's ZA number	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
6b	WTP	Weight percent of the isotope	VF≠0	Enter for each isotope in the standard composition component. Omit if VF=0.0. Entries 6a and 6b are entered in pairs until each isotope in the component is defined
7[b]	END	Terminate a standard composition	Always	Enter once for each standard composition component. This terminates the data for a standard composition component. Enter END to terminate the component. Repeat entries 1 through 7 until all the mixtures have been defined. At least two blanks must separate entry 7 from the next entry
	END COMP	Terminate the data block	Terminus	Enter once for a problem. Enter the words END COMP when all the standard composition components have been described. At least two blanks must follow the END COMP

[a]See Sect. M7.4.4 for detailed description of each input variable.

[b]NOTE: Entry 7 should not begin in column 1 unless a name is associated with it. At least two blanks should separate the last entry 7 from the END COMP.

Table S1.4.3 Material Information Processor data: unit cell specification for LATTICECELL problems[a]

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CTP	Type of lattice	Always		Describes the type of lattice or array configuration
				SQUAREPITCH	Use for cylindrical rods in a square pitch
				ASQUAREPITCH	Use for annular cylindrical rods in a square pitch
				ASQP	Use for annular cylindrical rods in a square pitch
				TRIANGPITCH	Use for cylindrical rods in a triangular pitch
				ATRIANGPITCH	Use for annular cylindrical rods in a triangular pitch
				ATRP	Use for annular cylindrical rods in a triangular pitch
				SPHSQUAREP	Use for spherical pellets in a cubic lattice
				ASPHSQUAREP	Use for annular spherical pellets in a cubic lattice
				ASSP	Use for annular spherical pellets in a cubic lattice
				SPHTRIANGP	Use for spherical pellets in a bicentered or face-centered hexagonal close-packed lattice
				ASPHTRIAGP	Use for spherical pellets in a bicentered or face-centered hexagonal close-packed lattice
				ASTP	Use for spherical pellets in a bicentered or face-centered hexagonal close-packed lattice
				SYMMSLABCELL	Use for a symmetric array of slabs
				ASYMSLABCELL	Use for a periodic but asymmetric array of slabs
2	PITCH	Array pitch (cm)	Always	Appropriate dimension	The center-to-center spacing (cm) between fuel lumps. For asymmetric slab cell, enter the distance from the center of one moderator to the center of the other moderator (cm)
3	FUELOD	Outside dimension of fuel (cm)	Always	Appropriate dimension	Outside diameter of fuel (cm), or the thickness of the fuel in a slab
4	MFUEL	Fuel mixture number	Always	Mixture number	Mixture number representing the fuel
5	MMOD	Moderator mixture number	Always	Mixture number	Mixture number representing the moderator
6	MMOD2	2nd moderator mixture number	Annular cell	Mixture number	Mixture number representing the second moderator
7	TKMOD2	2nd moderator thickness	ASYMSLABCELL	Thickness	Thickness of the second moderator (cm) for ASYMSLABCELL
		or	or	or	or
		2nd moderator diameter (cm)	annular cell	Diameter	Diameter of inner moderator (cm) for other annular cells
8	CLADOD	Outside diameter of clad (cm)	If clad	Clad OD	OMIT IF NO CLAD. For a slab, CLADOD is the sum of thickness of the fuel, gap, and clad
9	MCLAD	Clad mixture number	If clad	Mixture number	OMIT IF NO CLAD. Mixture number representing the clad
10	CLADID	Inside diameter of clad (cm)	If gap	Clad ID	OMIT IF NO GAP between the fuel and clad
11	MGAP	Gap mixture number	If gap	Mixture number	OMIT IF NO GAP between the fuel and clad. A mixture number of zero is often used
12	END	Terminate LATTICELL data	Always	END	Terminate the LATTICECELL input data by entering the word END. Do not start in column 1. At least two blanks must follow entry 12

[a]See Sect. M7.4.6 for detailed description of each input variable.

Table S1.4.4 Material Information Processor data: geometry specification for MULTIREGION problems[a]

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	CS	Type of geometry	Always		Describes the type of geometry. The options are listed below
				SLAB	Use for slab geometry
				CYLINDRICAL	Use for cylindrical geometry
				SPHERICAL	Use for spherical geometry
				BUCKLEDSLAB	Use for slab geometry with a buckling correction for the two transverse directions
				BUCKLEDCYL	Use for cylindrical geometry with a buckling correction in the axial direction
					Default is VACUUM. Describes the right/outside boundary condition
2	BR	Right boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	VACUUM	This provides a nonreturn condition at the boundary. Do not use for cylindrical or spherical
				REFLECTED	Do not use for cylindrical or spherical
				PERIODIC	
				WHITE	This provides isotopic return at the boundary
					Default is REFLECTED. Describes the left boundary condition
3	BL	Left boundary condition	Required for BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	VACUUM	This provides a nonreturn condition at the boundary
				REFLECTED	Recommended for cylindrical or spherical
				PERIODIC	Do not use for cylindrical or spherical
				WHITE	This provides isotropic return at the boundary
4	ORGN	Location of left boundary on the x-axis (cm)	BUCKLEDSLAB & BUCKLEDCYL Optional for other geometries	Appropriate dimension	Default is 0.0. Should not be changed for cylindrical or spherical geometry. A value must be entered if subsequent data are to be entered
5	DY	Buckling height (cm)	BUCKLEDSLAB & BUCKLEDCYL	Appropriate dimension	OMIT FOR SLAB, CYLINDRICAL, and SPHERICAL. This corresponds to one of the transverse dimensions of an actual 3-D slab assembly or to the length of a finite cylinder
6	DZ	Buckling depth (cm)	BUCKLEDSLAB	Appropriate dimension	OMIT UNLESS BUCKLEDSLAB WAS SPECIFIED. This is the buckling depth corresponding to the second transverse
7	END	End geometry parameters	Always	END	Enter the word END. Do not start in column 1. At least two blanks must separate entry 7 from the first entry 8
8	MXZ	Mixture number in the zone	Always	Mixture number	Repeat entry numbers 8-10 until all zones are defined. Enter the mixture number for this zone
9	RZ	Outside radius of the zone (cm)	Always	Appropriate dimension	Repeat entry numbers 8-10 until all zones are defined. Enter the outside dimension of the zone (cm)
10	XMOD	External moderator index	Optional		Repeat entry numbers 8-10 until all zones are defined
					Entry 10 is optional and can be omitted. If it is omitted, repeat entries 8 and 9 until all zones are defined
				NOEXTERMOD	No moderating materials in the adjacent zones
				ONEEXTERMOD	A moderating material is present in one adjacent zone
				TWOEXTERMOD	Moderating materials are present in two adjacent zones
	END ZONE	Terminate zone data		END ZONE	Enter when all zones have been defined by repeating entries 8 through 10 for each zone. At least two blanks must follow this entry

[a]See Sect. M7.4.7 for detailed information on each input variable.

Table S1.4.5 Material Information Processor data: optional parameter data[a]

Entry number	Keyword name	Type of data	Module using data	Comments
		Summary of available optional parameter data (see Sect. M7.4.8)		
1	MORE DATA	Input flag	XSDRNPM	This signals that optional parameter data are to be entered
2	ISN=	Order of angular quadrature	XSDRNPM	The default value is 8. This allows using another value
3	SZF=	Spatial mesh size factor	XSDRNPM	The default value is 1.0 SZF<1.0 gives a finer mesh SZF>1.0 gives a coarser mesh
4	IIM=	Maximum number of inner iterations	XSDRNPM	The default value is 20. This allows using another value
5	ICM=	Maximum number of outer iterations	XSDRNPM	The default value is 25. This allows using another value
6	EPS=	Overall convergence criteria	XSDRNPM	
7	PTC=	Point convergence criteria	XSDRNPM	The default value is 0.0001. This allows using another value
8	BKL= factor	Buckling	XSDRNPM	The default value is 1.420892. Use ONLY for a MULTIREGION problem that specifies BUCKLEDSLAB or BUCKLEDCYL
9	IUS	Upscattering scaling factor	XSDRNPM	The default value is zero. IUS=0 does not utilize upscatter scaling. IUS=1 uses upscatter scaling to accelerate the solution and/or speed convergence
10	RES=	Resonance data	BONAMI NITAWL	Enter the mixture number, geometry type (SLAB, CYLINDER, SPHERE) and the thickness of the slab or radius of the sphere or cylinder, in cm
11	DAN(mm)=	Dancoff factor for the specified mixture	BONAMI NITAWL	Enter the mixture number mm to which the Dancoff factor applies inside the parentheses; enter the Dancoff factor after the equal sign Repeat items 10 and 11 for all resonance mixtures used in the problem that are not treated in the LATTICECELL or MULTIREGION description

Table S1.4.5 (continued)

Entry number	Keyword name	Type of data	Module using data	Comments
12	BAL=	Key to print balance tables	XSDRN	The default is FINE. BAL=NONE causes the balance table print to be suppressed. BAL=ALL prints all balance tables. BAL=FINE prints only the fine-group balance tables
13	DY=	First transverse dimension	XSDRN	The first transverse dimension in centimeters used in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a slab or a cylinder)
14	DZ=	Second transverse dimension		The second transverse dimension in centimeters used for a buckling correction (i.e., the width of a slab)
15	COF=	Diffusion coefficient option for transverse leakage corrections	XSDRNPM	The default is 0. See Sect. F3.5, 3$ array, variable IPN
16	FRD=	Unit from which fluxes will be read	XSDRNPM	Enter the unit number from which the flux guess for XSDRN will be read
17		Unit on which fluxes will be written	XSDRNPM	Enter the unit number where the binary fluxes from XSDRN will be written
18	DAB=	Number of direct access data blocks	MIP	The default is 200. Number of blocks allocated for direct access unit 8
19	COLL	Key to activate collapse of thermal groups	MIP	Enter COLL to collapse all thermal groups into one group for the shielding sequences
20	END	Terminus		Terminate the optional parameter data

[a]See Sect. M7.4.8 for detailed information on each variable.
[b]MIP is the Material Information Processor.

Table S1.4.6 Input for shielding problem data*a*

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
1	TITLE	Title	Always	Enter a title	80 characters
2	CS	Type of geometry	Always	SPHERICAL CYLINDRICAL SLAB DISC	For spherical geometry For cylindrical geometry For slab geometry For slab geometry with only disc-shaped portion of surface used for dose evaluation; dose from top of a cylinder
3	BL	Left boundary condition	SLAB or DISC	VACUUM REFLECTED	No return condition at boundary Mirror reflection at boundary
4	MXZ	Mixture number in zone	Always	Valid mixture number for zone	Repeat items 4-15 for each zone Enter 0 for void, 500 for cell-weighted mixture
5	RZ	Outer zone dimension	Always	Appropriate outside dimension of zone (cm)	Repeat items 4-15 for each zone
6	IMZ	Mesh intervals for zone	Always	Number of equal mesh intervals	Repeat items 4-15 for each zone. Enter 1 for the first zone if a boundary source is used (see Sect. S1.2.3)
7	ISZ	Source identifier for zone	Always	0, no source; N, source from ORIGEN-S file or from XSDRNPM criticality case; -N, source from cards	Repeat items 4-15 for each zone
8	MIXC	Mixture number to mix with MXZ	ISZ≠0	Valid mixture number or 0 for void	Repeat items 4-15 for each zone
9	VFC	Volume fraction of MIXC	ISZ≠0	Volume fraction or 0 if not used	Repeat items 4-15 for each zone If nonzero, zone will be composed of mixture MIXC and mixture MXZ so that $\rho_{ZONE} = (VFC)/(\rho_{MIXC}) + (1 - VFC)(\rho_{MXZ})$
10	NSOU	Unit number with ORIGEN-S output file	ISZ>0	=0 XSDRNPM boundary source >0 unit number with ORIGEN-S file	Repeat items 4-15 for each zone
11	NPOS	Source position number on ORIGEN-S file	ISZ>0 & NSOU>0	Source position number	Repeat items 4-15 for each zone Position number obtained from ORIGEN-S printout
12	ZVOL	Values to convert source to per cm³ basis	ISZ>0 & NSOU>0	Zone volume (cm³) conversion parameter	For spectra in per assembly units Enter inverse of value for conversion to per cm³ of zone (see Sect. S1.2.1). Repeat items 4-15 for each zone
13	NASS	Number of fuel assemblies in a zone	ISZ>0 & NSOU>0	Integer number of assemblies in zone	For spectra in per assembly units (see Sect S1.2.1) Set to 1 if not used Repeat items 4-15 for each zone
14	XNN	Neutron normalization factor	ISZ<0	Total source strength per cm³	Repeat items 4-15 for each zone
15	XNG	Gamma normalization factor	ISZ<0	Total source strength per cm³	Repeat items 4-15 for each zone

Table S1.4.6 (continued)

Entry number	Variable name	Type of data	Entry requirement	Data entry	Comments
END ZONE	Keyword to terminate zone	Completion of zone input data	END ZONE	Enter once for a problem after all data for zones have been entered.	
16	SOU	Source spectra	Any ISZ<0	One entry per group	Repeat spectrum entries for each source
17		Optional parameter data	Optional	ISN=integer	Enter to change order of angular quadrature (16)
				IIM=integer	Enter to change inner iteration limit (20)
				ICM=integer	Enter to change outer iteration limit (4)
				ID1=-1/0/1	Enter to change flux edit option (-1)
				SCT=integer	Enter to change order of Legendre expansion used (3)
				PRT=-2/-1/O/N	Enter to change cross-section print option (-2)
				PBT=-1/0/1	Enter to change balance table print (0)
				EPS=floating point number	Enter to change overall convergence (1E-4)
				PTC=floating point number	Enter to change flux convergence (1E-4)
				DY=floating point number	Buckling height of cylinder or slab (0)
				DZ=floating point number	Buckling width of slab (0)
				IFS=0/1	Enter 1 to eliminate fission source (0)
				NDETEC=integer	Enter to change default detector locations
				NFACTR=integer	Enter to change default dose factor IDs
18	READ XSDOSE	Keyword	Items 19, 20, 21, or 22 to be entered	READ XSDOSE	Input to allow entry of data for XSDOSE—items 21, 19–22
19	DIMEN1	Shield dimensions in cm	If SLAB, DISC, or CYLINDRICAL geometries	Height for SLAB Disc radius for DISC Height for CYLINDRICAL	Omit if SPHERICAL geometry
20	DIMEN2	Shield dimensions in cm	SLAB geometry	Width of SLAB	Omit if DISC, CYLINDRICAL, or SPHERICAL geometries
21	DOSE	Dose factor IDs	NFACTR>0	NFACTR entries	See Table S1.4.8 NFACTR=0 provides ANSI IDs
22		Detector coordinates in cm	NDETEC>0	NDETEC detector	NDETEC=0 gives 0, 1, 2, 4 m from surface at centerline
				R for SPHERICAL	
				R,Z for CYLINDRICAL	Z from cylinder bottom
				R,Z for DISC	Z from surface
				Y,Y,Z for SLAB	X from surface of Y,Z slab

[a]See Sect. S1.4.4 for detailed description of each input variable. Note dashed lines indicate blocking of input data into records whose input should begin on a new card.

S1.4.2 MATERIAL INFORMATION PROCESSOR DATA

These data are needed to generate the mixing table and cross sections used in the shielding analysis. The input for this portion of the data is described in detail in Sects. M7.4.3-M7.4.8. An outline of the data entry requirements is provided in Table S1.4.1. Tables S1.4.2-S1.4.5 provide a summary of the input format for the standard composition data, cell geometry specifications, and optional parameter data. These data must be terminated with an END beginning in column 1.

S1.4.3 PROBLEM CONTROL CARD

This card allows the user to control the number of subsequent shielding analyses performed with the cross-section working library. If this card contains **LAST** (starting in column one), the job will terminate at the end of the calculation for the Shielding Problem Data following this card. If this card is left blank, another Problem Control Card/Shielding Problem Data combination is expected, and the same working library and mixing table will be utilized.

S1.4.4 SHIELDING PROBLEM DATA

The Shielding Problem Data are used to describe the shielding geometry, radiation sources, detector, and dose information used by the problem. This input segment must be terminated with an **END** beginning in column 1. Other ENDs used in this input segment must not begin in column 1. If a blank Problem Control Card precedes this set of Shielding Problem Data, then another combination of Problem Control Card and Shielding Problem Data is expected by the control module. Input for the Shielding Problem Data is outlined in Table S1.4.6. The following detailed explanation denotes variable names with capital letters and input keywords or variable names by boldface capital letters.

1. TITLE An 80-character title of the shielding problem (only 72 characters will be printed by XSDRNPM).

2. CS Type of geometry. The available input keywords are listed below.

   SPHERICAL The shielding problem uses spherical geometry.

   CYLINDRICAL The shielding problem uses cylindrical geometry.

   SLAB The shielding problem uses slab geometry.

   DISC XSDRNPM solves the radiation transport problem in slab geometry, and XSDOSE calculates the dose rates from a disc-shaped portion of the outer slab surface. This is the option to use in evaluating the dose out the top of a cylinder.

3. BL Left boundary condition. This parameter is required only when **SLAB** or **DISC** geometries are specified. A reflected left boundary condition is automatically used by SPHERICAL and CYLINDRICAL coordinate systems because the left boundary corresponds to the centerline. The right boundary condition is set to vacuum for all geometry options. The available input keywords are listed below.

REFLECTED All particles crossing the left boundary of the system are specularly reflected (i.e., mirror image reflection).

VACUUM All particles crossing the left boundary of the system leave the system.

Items 4 through 15 of the Shielding Problem Data comprise the zone input data. Items 4 through 7 are required for each zone, while items 8 through 15 are used only for source zones. If a zone has no source, only items 4 through 7 are entered. If a boundary source or a source from an ORIGEN-S output file is to be used in a zone, items 4 through 9 and 14 through 15 are entered. The zone data must be terminated with an **END ZONE** keyword.

4. MXZ Mixture number of material in this zone. This must be a mixture number defined in the Material Information Processor data. To use cell-weighted cross sections generated by the SAS1X sequence, enter 500. *Mixtures used to create the cell-weighted mixture 500 should not be used as a zone mixture.* Enter 0 for a void (SAS1 will instruct XSDRNPM to put the first nonzero mixture in the zone and give it a density factor of 0.0). A 0 is required in the first zone if a combined criticality/shielding case is desired (see Sect. S1.2.3).

5. RZ Outer radius of this zone for spheres or cylinders, or distance from left boundary for slabs and discs, in centimeters.

6. IMZ Number of space mesh intervals used by XSDRNPM in this zone (see Sects. S1.2.2 and S1.2.3). Enter 1 for the first zone if a boundary source is used (see Sect. S1.2.3).

7. ISZ Source identification number for this zone.
Enter 0 for zones with no source.
Enter a **positive** source identification number for a source spectrum input from an ORIGEN-S output file or from the XSDRNPM criticality analysis.
Enter a **negative** source identification number for a source spectrum input from cards.

If this zone has no source (ISZ=0), this ends the data for the zone.

8. MIXC Mixture number of material to be mixed homogeneously with the source zone material such that $\rho_{ZONE} = VFC \times \rho_{MIXC} + (1 - VFC)\rho_{MXZ}$. Enter 0 to designate a void or if the first zone of a combined criticality/shielding case (see Sect. S1.2.3).

9. VFC Volume fraction of mixture MIXC to be blended with mixture MXZ in the source zone. The volume fraction of mixture MIXC in this zone will be VFC, while the volume fraction of mixture MXZ actually used in this zone will then be (1.0 -VFC). Enter 0 if not used.

If the source spectrum is entered from cards, skip to item 14.

10. NSOU Unit number for data set with ORIGEN-S output file containing the source spectrum. Enter 0 if a boundary source is used and terminate the data for this zone.

11. NPOS Position number of source spectrum on the ORIGEN-S output file. The position number and the associated burnup and decay times are given in the ORIGEN-S printout. See Sect. F7 for information needed to generate and save an ORIGEN-S output file. The output file is saved in a SAS2 case by saving output to unit 71 (see Sect. S2.5.6).

12. ZVOL Parameter used for converting ORIGEN-S output file spectra to per-zone-unit volume (cm^3). *Division* of the spectra by this parameter value should Convert it to a per-cm^3 basis. For file spectra with per assembly units, ZVOL should be the zone volume in cm^3. See Sect. S1.2.1 for a discussion.

13. NASS For file spectra with per assembly units [from SAS2(H) cases and many ORIGEN-S cases], NASS is the number of assemblies in the zone. See Sect. S1.2.1 for a discussion. Set to 1 if not needed. *Entering 0 will eliminate source entirely.*

Items 12 and 13 are used to convert the ORIGEN-S source spectra (S_i) to a per-cm^3 basis (s_i) by the formula

$$s_i = \frac{S_i \cdot NASS}{ZVOL}$$

Knowing the units on S_i (from ORIGEN-S or SAS2 printout), ZVOL and NASS can be input accordingly. If the source spectra is from ORIGEN-S, this ends the data for the zone.

14. XNN Normalization factor for neutron source from cards. Enter 0 if not used.

15. XNG Normalization factor for gamma source from cards. Enter 0 if not used.

XNN and XNG are typically the total neutron and gamma source strength per unit volume (per cm^3) in the zone. For a coupled neutron/photon problem, if only one of these factors is nonzero, *both* sources will be normalized such that the spectrum corresponding to the nonzero value gives the correct total source. For example, if XNG=0 and XNN is nonzero, the final neutron source total will be correct, and the gamma source, if any, will be altered by the same factor as the neutron source. For photon-only problems, XNN should be zero, while for neutron-only problems, XNG should be zero.

END ZONE is used to terminate the zone data. Enter these keywords (do not start in column 1) after input of data for the last zone.

16. SOU Source spectrum from cards *in order from highest to lowest energy group*. Repeat for each source spectra from cards. Each spectrum must have one entry for each group. If more than one source is entered, they must be in order of the zone number the source is used in. If the same source is used in more than one zone, the spectrum must be repeated for each additional zone. If the COLLAPSE feature is used, SOU should already be collapsed to reduce the thermal neutron groups to one.

17. Optional Parameters

Some of the commonly used parameters for XSDRNPM shielding calculations and XSDOSE are assigned default values that are useful for many problems. If a value different from the default is desired, it may be entered by inputing the parameter name followed immediately (no space) by an equal sign and the desired value. For example, ICM=10 changes the outer iteration limit to 10. One or more of the parameters can be entered in any order. Default values are used for parameters not entered. Each entry should be separated from the previous by a blank. Table S1.4.7 provides a description of the optional parameters and their default values.

18. READ XSDOSE
Keyword allowing entry of shield and detector data used by XSDOSE. Must be entered to allow entry of items 19-21.

19. DIMEN1
Dimension (cm) describing the extent and/or location of the outer shield surface. For **SLAB**, enter the slab height.
For **DISC**, enter the disc radius.
For **CYLINDRICAL** geometry option, enter the height.
Omit for the **SPHERICAL** geometry option.

20. DIMEN2
Secondary dimension (cm) describing the extent and/or location of the outer shield surface of slab. Enter slab width. Omit for other geometries.

21. DOSE Dose factor IDs (NFACTR entries). The available dose factor IDs in SCALE are provided in Table S1.4.8. If NFACTR=0 (the default value), the ANSI dose factor IDs are used and these entries can be omitted.

22. Detector Coordinates (cm)
Omit if NDETEC=0 (the default value), and the detectors will be located by default at the surface, and at 100, 200, and 400 cm from the surface along the centerline. If NDETEC > 0, then NDETEC sets of coordinate entries are required. The input coordinates depend on the geometry option selected:

R	Sphere radius for **SPHERICAL** geometry option.
R,Z	Cylinder radius and height from bottom for **CYLINDRICAL** geometry option.
R,Z	Disc radius and height from surface for **DISC** geometry option.
X,Y,Z	Slab, x distance from the surface of a y by z section for **SLAB** geometry option.

23. **END** Terminate Shielding Problem Data. Always entered starting in column 1. This h.keyword also terminates the analytic sequence if **LAST** is entered in the preceding Problem Control Card.

Table S1.4.7 Optional parameter input for the shielding problem data

Name	Default	Meaning, comments
ISN=	16	Order of angular quadrature
IIM=	20	Inner iteration maximum
ICM=	4	Outer iteration maximum. After ICM outer iterations, the problem will be forced into the termination phase and the program will continue as if full convergence was attained. A message to this effect is printed
ID1=	-1	Flux edit option: -1 no flux print, 0 scalar flux print, 1 scalar flux and angular flux print
SCT=	3	Order of Legendre expansion to be used
PRT=	-2	Cross-section print option: -2 no cross-section print, -1 print 1-D cross sections, O/N print P^L arrays through order N
PBT=	0	Balance table print option: -1 no balance table print, 0 fine group balance table print, 1 fine and broad group balance table prints
EPS=	1.E-4	Overall problem convergence. This is used by XSDRNPM after each outer iteration to determine if the problem has converged. A value less than 0.0001 tightens the convergence criteria; a larger value loosens the convergence criteria. See Sect. M7.2.5.8 for additional information
PCT=	1.E-4	Scalar flux convergence. This is the point flux convergence criteria used by XSDRNPM to determine if convergence has been achieved after an inner iteration. A smaller value tightens convergence; a larger value loosens it
DY=	0	First transverse dimension (cm) used by XSDRNPM in a buckling correction to calculate leakage normal to the principal calculation direction (i.e., the height of a cylinder or slab)
DZ=	0	Second transverse dimension (cm) used by XSDRNPM for buckling correction (i.e., the width of a slab)
IFS=	0	A value of 1 will cause the fission source to be eliminated
NDETEC=	0	Number of detectors for XSDOSE dose rate calculation. The default value of NDETEC will automatically provide detectors located on the centerline at the surface and at 100, 200, and 400 cm from the surface
NFACTR=	0	Number of dose factor IDs for dose rate calculation. The NFACTR default provides dose factor IDs for the ANSI standard neutron and gamma dose factors

Table S1.4.8 Special dose factor ID numbers available in SCALE

ID No.	Response function	Availability[a]
9001	Hurst dose factors (mrad/h)/(neutrons/cm^2/s)	1,2,5
9002	Snyder-Neufeld dose factors (mrad/h)/(neutrons/cm^2/s)	1,2,5
9026	Snyder-Neufeld conversion from flux to biological dose (mrem/h)/(neutrons/cm^2/s)	1,2,5
9027	Henderson conversion from neutron flux to absorbed dose rate in tissue (rad/h)/(neutrons/cm^2/s)	1,2,5
9028	Straker-Morrison conversion factors (mrem/h)/(neutrons/cm^2/s)	1
9029	ANSI standard neutron flux-to-dose-rate factors (rem/h)/(neutrons/cm^2/s)	1,2,3,5,6
9501	Straker-Morrison conversion factors (mR/h)/(photons/cm^2/s)	1,4
9502	Henderson conversion factors (rad/h)/(photons/cm^2/s)	1,2,4
9503	Claiborne-Trubey conversion factors (rad/h)/(photons/cm^2/s)	1,2,4
9504	ANSI standard gamma-ray flux-to-dose-rate factors (rem/h)/(photons/cm^2/s)	1,2,4

[a]Reference numbers of cross-section libraries:
1. 22N-18COUPLE
2. 27N-18COUPLE
3. 27BURNUPLIB
4. 18GROUPGAMMA
5. 123GROUPGMTH
6. 27GROUPNDF4

S1.5 SAMPLE PROBLEMS

S1.5.1 GENERAL DISCUSSION

The SAS1 control module provides automated analytic sequences that use the XSDRNPM and XSDOSE codes to calculate the neutron and gamma fluxes and dose rates on the surface of a spent fuel shipping cask or other shielded body and at other points beyond the outer surface of the body. XSDRNPM is used to model one-dimensional (1-D) radiation transport through the shield, while XSDOSE is used to model radiation transport from the exterior surface, through an external void, to the point or points of interest. Preliminary cross-section processing is performed automatically as the SAS1 control module first invokes the BONAMI and NITAWL-II resonance self-shielding codes. In the SAS1X sequence, a preliminary XSDRNPM calculation is performed to prepare cell-weighted cross sections for one region (typically the source region) where a homogeneous representation of a heterogeneous configuration is desired. For example, the resulting mixture 500 from a SAS1X LATTICECELL calculation can be used to represent the homogenized fuel assemblies in one or more zones of the final XSDRNPM shielding calculation of the sequence. On the other hand, if the cell weighting of the cross-section data is not deemed of great importance (as is frequently the case in shielding calculations), the user may specify the actual volume fraction for each material in the homogenized representation of the fuel (or other radioactive material) and invoke the basic SAS1 sequence.

Although the SAS1 control module is designed to solve a variety of 1-D shielding problems, the feature of the module will be mainly illustrated via analysis of the spent fuel shipping cask shown in Fig. S1.5.1. The cases that are illustrated are summarized in Tables S1.5.1 and S1.5.2. The heavily annotated input data for each case is included to illustrate how such a cask may be described under accident and nonaccident conditions using a variety of modeling approximations and input options.* The modeling approximations and input options illustrated included calculations (1) with and without the neutron shield, (2) with and without the axial shock absorber, (3) using the latticecell, multiregion, and infinite homogeneous media cross-section processing options, (4) collapsing down to 1 thermal group or retaining as many as 13, (5) using or not using the buckling approximation in the 1-D shielding analysis, (6) entering the source spectrum directly or reading an ORIGEN-S source file, (7) using lower order angular quadratures, (8) allowing more outer iterations, (9) including more detector locations than those shown in Fig. S1.5.1, and (10) using alternate sets of flux-to-dose conversion factors. The radial and axial analyses for the shipping casks are discussed in Sects. S1.5.2 and S1.5.3. The final sample problem discussed in Sect. S1.5.4 demonstrates the use of the SAS1X sequence for a combined criticality and shielding problem as described in Sect. S1.2.3.

Note that all problem results shown in Sects. S1.5.2-S1.5.4 represent those obtained during testing of the module on the IBM-3090 at ORNL. These results will not exactly match those distributed with the code package. The input for the SAS1 cases tested at ORNL were prepared to ensure an exact match between the source input directly and the source provided by the ORIGEN-S file. Users wishing to compare results between cases run at their installation will need to ensure their sources also match (i.e., the ORIGEN-S source used by ORNL to test will not exactly duplicate that generated at any specific installation).

---

*Lines of input data containing an apostrophe (') in column 1 will be ignored by the SAS1 input processor and treated as an embedded comment. This feature is very helpful in documenting user input.

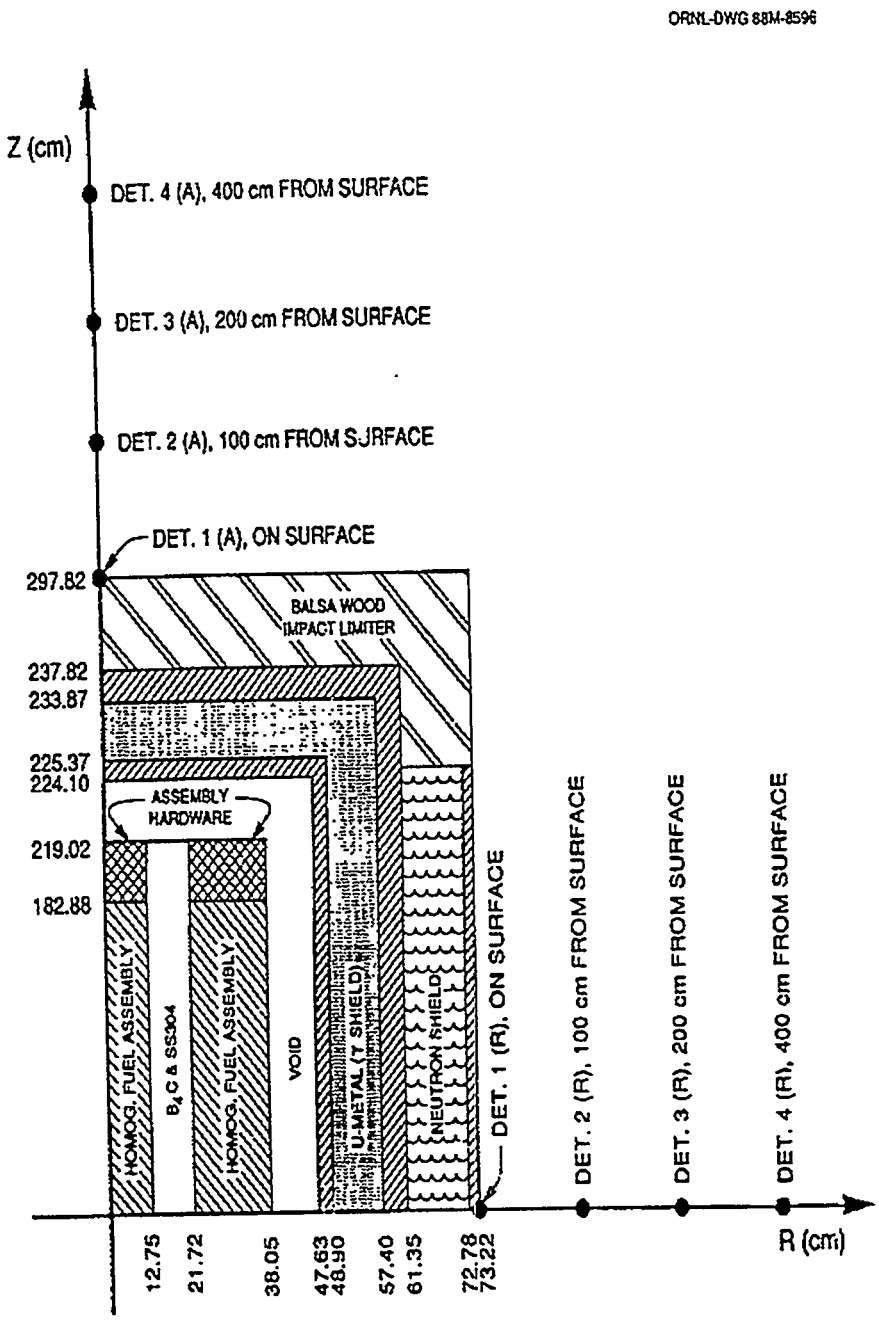


Figure S1.5.1 Seven assembly, depleted uranium metal, spent fuel shipping casks described by SAS1 sample problems

Table S1.5.1 Effect of using various options in the solution of the radial SAS1 sample problem under different conditions[a]

Fuel model used in cross-section calculation	Collapse option used	Neutron shield present	ORIGEN source file used	ISN=default (16) ICM=default (4)	ISN=default (16) ICM=10	ISN=9 ICM=default (4)
LATTICECELL (SAS1X)	No	Yes	No	9.35/23.71 [1,245][b]	—	—
LATTICECELL (SAS1X)	No	Yes	Yes	9.35/23.71 [2,245]	—	—
LATTICECELL (SAS1X)	Yes	Yes	No	9.72/23.89 [3,96][b]	—	—
LATTICECELL (SAS1X)	Yes	Yes	Yes	9.72/23.92 [4,96]	—	—
INFHOMMEDIUM (SAS1)	No	Yes	Yes	9.32/23.788 [5,242][c]	9.55/24.02 [6,440]	—
INFHOMMEDIUM (SAS1)	No	No	Yes	269.9/29.28 [7,238]	273.3/29.29 [8,370]	—
INFHOMMEDIUM (SAS1)	Yes	Yes	Yes	9.70/24.00 [9,94]	—	9.61/24.20 [10,33][d,e]
INFHOMMEDIUM (SAS1)	Yes	No	Yes	269.9/29.28 [13,90]	—	269.6/29.63 [14,32]

[a]The tabulated results (Dn/Dg) show the calculated neutron and gamma dose rates in mrem/h on the surface of the cask under the various conditions. The data in brackets [id, t] show the case id number corresponding to the sample input and the XSDRNPM running time (s) for the shielding problem on an IBM-3090.

[b]Dose rates obtained using the collapsed 15n-library vs the 27n-library may differ more if one had a thermal-neutron-absorbing/gamma-producing material like boron in the neutron shield near the outer portion of the cask. Such situations may be evaluated on a case-by-case basis.

[c]Input for case [5] also illustrates use of additional detector sites (NDETEC=6) and an additional set of flux-to-dose conversion factors.

[d]Case [11] was identical to case [10] except that an axial buckling of 595.64 cm was used in the XSDRNPM shielding calculation. In this case, Dn = 8.99 mrem/h, Dg = 23.40 mrem/h, and the required cpu time was 33 s.

[e]Case [12] was identical to case [10] except that the outer fuel region and the adjacent void were smeared together in the XSDRNPM shielding calculation. In this case, DN 9.92 mrem/h, Dg = 24.05 mrem/h, and the required cpu time was 32 s.

Table S1.5.2 Effect of using various options in the solution of the axial SAS1 sample problem under different conditions

Geometric model for the NITAWL cross-section calculation	Geometric model for the XSDRNPM shielding calculation[b]	Collapse neutron cross sections	With axial shock absorber on the end	Without axial shock absorber on the end
MULTIREGION INFINITE SLAB	BUCKLED SLAB	Yes	15.28/12.40 [15,40][c] 15.27/12.38 [16,39][c]	143.2/19.13 [17,29]
MULTIREGION INFINITE SLAB	INFINITE SLAB	Yes	132.0/31.74 [18,41]	912.7/24.45 [19,31]
INFHOMMEDIUM	BUCKLED SLAB	No	15.30/12.34 [20,115]	143.2/19.13 [21.85]
INFHOMMEDIUM	BUCKLED SLAB	Yes	15.27/12.38 [22,39]	143.2/19.13 [23,29]
INFHOMMEDIUM	BUCKLED SLAB	Yes	132.0/31.74 [24,41]	912.7/24.45 [25,31]

[a]The tabulated results (Dn/Dg) show the calculated neutron and gamma dose rates in mrem/h on the end of the cask under the various conditions. The data in brackets [id, t] show the case ID number corresponding to the sample input, and the XSDRNPM running time (s) for the shielding problem on an IBM-3090.

[b]In all cases the finite radius of a circular disk corresponding to the end of the cask was used in the XSDOSE portion of the shielding calculation. For values at points on the surface (reported above), this will make no difference, but for those points farther away from the end of the cask, the actual size will affect the calculated dose rate and is correctly accounted for by XSDOSE in all cases.

[c]Cases [15] and [16] are identical except that case [15] illustrates how to input the 27n-18γ source spectra for the spent fuel directly after the zone input data, while case [16] shows how to use the same data directly from an ORIGEN-S binary source file.

S1.5.2 DISCUSSION OF THE RADIAL PROBLEMS

Cases 1 through 14 of Table S1.5.1 illustrate different approaches to the 1-D radial problem for the cask shown in Fig. S1.5.1.

Dose results using the ANSI-standard flux-to-dose conversion factors[1] are summarized in Table S1.5.1 with the respective case number and computation time. Comparisons of these results show the effect of using the various options and modeling approximations—both in terms of the calculated neutron and gamma dose rates on the surface of the cask and the corresponding running time for the 1-D XSDRNPM shielding calculation. Listings of the annotated input data for cases 1 through 14 may be found in the following tables:

Table S1.5.3	Cases 1-2
Table S1.5.4	Cases 3-4
Table S1.5.5	Cases 5-8
Table S1.5.6	Cases 9-14

Table S1.5.3 Annotated Input for Case 1 and 2

```
#SAS1X
CASES 1 & 2 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=NO
27N-18COUPLE  LATTICECELL
'
' DESCRIPTION OF MATERIALS IN A PWR FUEL PIN:
' [SEE MIX 8, BELOW, FOR ADDITIONAL COMMENTS]
UO2  1  0.90172   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  2  1  560  END
'
' MIX 3 IS USED BETWEEN THE INNER AND OUTER ROW OF ASSEMBLIES IN THE CASK:
SS304   3  2.1712E-2  END
B4C     3  7.7066E-2  END
'
' MIX 4 IS THE STRUCTURAL STEEL USED IN THE CASK BODY
' MIX 5 IS THE U-METAL GAMMA SHIELD
' MIX 6 IS THE NEUTRON SHIELD  (DEFINED HERE;  USED IN SOME CASES, BUT NOT ALL)
' MIX 7 IS THE INTERNAL BASKET MATERIAL (SS304) BETWEEN ASSEMBLIES
' MIX 8 CORRESPONDS TO NITROGEN AT 2 ATM PRESSURE, 560 DEG-K (0.00122 G/CC).
'
'    NOTE: USERS ARE GENERALLY FREE TO USE MIXTURE NUMBER 0 TO REPRESENT A VOID
'    IN ANY GEOMETRIC ZONE. THE SINGLE EXCEPTION IS THAT IT CANNOT BE USED AS
'    THE "MODERATOR" WHEN PERFORMING A LATTICE CELL CALCULATION FOR A DRY CASK.
'    IN THIS CASE, THE USER MUST ACTUALLY ENTER THE STANDARD COMPOSITION
'    SPECIFICATIONS FOR SOME OTHER MATERIAL THAT, FOR ALL PRACTICAL PURPOSES,
'    IS THE SAME AS A VOID. HERE MIX 8 HAS BEEN USED FOR THAT PURPOSE.
'
SS304         4  END
U(.27)METAL   5  END
H2O           6  0.944  END
SS304         7  0.11879  560  END
N             8  0.00122  560  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
' DESCRIPTION OF LATTICE IN A WESTINGHOUSE 17*17 PWR FUEL ASSEMBLY:
SQUAREPITCH  1.2598  0.8357  1  8  0.94996  2  END
'
END

CASE 1 -- LATTICECELL X-SECT PROC, COLLAPSE=NO, SOURCE SPEC ENTERED BELOW
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' THE -1 INDICATES THAT SOURCE SPECTRUM 1 IS ENTERED BELOW (AFTER ZONE DATA)
' XNN=6.91E+02 N/S/CC IN HOMOGENIZED SPENT FUEL;  XNG=2.59E+10 PHOTONS/S/CC
500  12.75  20 -1     7  0.17994     6.91E+02   2.59E+10
3    21.72   8  0
'
' ZONE 3 (LIKE ZONE 1) CONSISTS OF 17.994 VOL% SS304 (MIX 7), PLUS
' 82.006 VOL% (= 100.0-17.994) HOMOGENIZED FUEL CELLS (MIX 500)
500  38.05  30 -1     7  0.17994     6.91E+02   2.59E+10
0    47.63   5  0
4    48.90   2  0
5    57.40  30  0
4    61.35   6  0
6    72.78  16  0
4    73.22   1  0
' NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
```

Table S1.5.3 (continued)

```
'
' 27N-18G SOURCE SPECTRUM 1 IS NOW ENTERED:
1.27E+01  1.45E+02  1.62E+02  9.06E+01  1.22E+02  1.33E+02  2.60E+01
20Z
3.92E-01  1.84E+00  9.41E+00  2.34E+01  4.45E+04  3.58E+05  1.20E+07
4.83E+06  2.74E+08  1.08E+09  1.39E+09  9.90E+09  3.10E+09  2.83E+08
4.18E+08  1.52E+09  1.75E+09  6.19E+09
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
LAST
CASE 2 -- LATTICECELL X-SECT PROC, COLLAPSE=NO, SOURCE SPEC FROM ORIGEN-S FILE
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
500  12.75  20 +1     7  0.17994     60  2  1.8679E+5  1
3    21.72   8  0
'
' ZONE 3 (LIKE ZONE 1) CONSISTS OF 17.994 VOL% SS304 (MIX 7), PLUS
' 82.006 VOL% (= 100.0-17.994) HOMOGENIZED FUEL CELLS (MIX 500)
500  38.05  30 +1     7  0.17994     60  2  1.1215E+6  6
0    47.63   5  0
4    48.90   2  0
5    57.40  30  0
4    61.35   6  0
6    72.78  16  0
4    73.22   1  0
' NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
```

Table S1.5.4 Annotated input for cases 3 and 4

```
#SAS1X
CASES 3 & 4 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=YES
27N-18COUPLE  LATTICECELL
'
' DESCRIPTION OF MATERIALS IN A PWR FUEL PIN:
UO2  1  0.90172   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  2  1  560  END
'
' MIX 3 IS USED BETWEEN THE INNER AND OUTER ROW OF ASSEMBLIES IN THE CASK:
SS304   3  2.1712E-2  END
B4C     3  7.7066E-2  END
'
' MIX 4 IS THE STRUCTURAL STEEL USED IN THE CASK BODY
' MIX 5 IS THE U-METAL GAMMA SHIELD
' MIX 6 IS THE NEUTRON SHIELD  (DEFINED HERE;  USED IN SOME CASES, BUT NOT ALL)
' MIX 7 IS THE INTERNAL BASKET MATERIAL (SS304) BETWEEN ASSEMBLIES
' MIX 8 CORRESPONDS TO NITROGEN AT 2 ATM PRESSURE, 560 DEG-K (0.00122 G/CC).
'
'    NOTE: USERS ARE GENERALLY FREE TO USE MIXTURE NUMBER 0 TO REPRESENT A VOID
'    IN ANY GEOMETRIC ZONE. THE SINGLE EXCEPTION IS THAT IT CANNOT BE USED AS
'    THE "MODERATOR" WHEN PERFORMING A LATTICE CELL CALCULATION FOR A DRY CASK.
'    IN THIS CASE, THE USER MUST ACTUALLY ENTER THE STANDARD COMPOSITION
'    SPECIFICATIONS FOR SOME OTHER MATERIAL THAT, FOR ALL PRACTICAL PURPOSES,
'    IS THE SAME AS A VOID. HERE MIX 8 HAS BEEN USED FOR THAT PURPOSE.
'
SS304        4  END
U(.27)METAL  5  END
H2O          6  0.944  END
SS304        7  0.11879  560  END
N            8  0.00122  560  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
' DESCRIPTION OF LATTICE IN A WESTINGHOUSE 17*17 PWR FUEL ASSEMBLY:
SQUAREPITCH  1.2598  0.8357  1  8  0.94996  2  END
'
' TO COLLAPSE THE 27 NEUTRON GROUPS DOWN TO 15 GROUPS ENTER:
MORE DATA  COLLAPSE  END
'
END

CASE 3 -- LATTICECELL X-SECT PROC, COLLAPSE=YES, SOURCE SPEC ENTERED BELOW
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' THE -1 INDICATES THAT SOURCE SPECTRUM 1 IS ENTERED BELOW (AFTER ZONE DATA)
' XNN=6.91E+02 N/S/CC IN HOMOGENIZED SPENT FUEL;  XNG=2.59E+10 PHOTONS/S/CC
500  12.75  20 -1     7  0.17994     6.91E+02   2.59E+10
3    21.72   8  0
'
' ZONE 3 (LIKE ZONE 1) CONSISTS OF 17.994 VOL% SS304 (MIX 7), PLUS
' 82.006 VOL% (= 100.0-17.994) HOMOGENIZED FUEL CELLS (MIX 500)
500  38.05  30 -1     7  0.17994     6.91E+02   2.59E+10
0    47.63   5  0
4    48.90   2  0
5    57.40  30  0
4    61.35   6  0
6    72.78  16  0
4    73.22   1  0
' NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
```

Table S1.5.4 (continued)

```
' COLLAPSED 15N-18G SOURCE SPECTRUM 1 IS NOW ENTERED:
1.27E+01  1.45E+02  1.62E+02  9.06E+01  1.22E+02  1.33E+02  2.60E+01
8Z
3.92E-01  1.84E+00  9.41E+00  2.34E+01  4.45E+04  3.58E+05  1.20E+07
4.83E+06  2.74E+08  1.08E+09  1.39E+09  9.90E+09  3.10E+09  2.83E+08
4.18E+08  1.52E+09  1.75E+09  6.19E+09
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
LAST
CASE 4 - LATTICECELL X-SECT PROC, COLLAPSE=YES, SOURCE SPEC FROM ORIGEN-S FILE
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
500  12.75  20 +1     7  0.17994     60  2  1.8679E+5  1
3    21.72   8  0
'
' ZONE 3 (LIKE ZONE 1) CONSISTS OF 17.994 VOL% SS304 (MIX 7), PLUS
' 82.006 VOL% (= 100.0-17.994) HOMOGENIZED FUEL CELLS (MIX 500)
500  38.05  30 +1     7  0.17994     60  2  1.1215E+6  6
0    47.63   5  0
4    48.90   2  0
5    57.40  30  0
4    61.35   6  0
6    72.78  16  0
4    73.22   1  0
' NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
```

Table S1.5.5 Annotated input for cases 5-8

```
#SAS1
CASES 5-8 (PREP) -- INFHOMMEDIA USED FOR X-SECT PROCESSING, COLLAPSE=NO
27N-18COUPLE  INFHOMMEDIA
'
' THE UO2 AND ZIRCALLOY VOLUME FRACTIONS PRESERVE THE AMOUNT OF FUEL ASSOCIATED
' WITH THE 264 FUEL PINS IN THE SPACE OCCUPIED BY A WESTINGHOUSE 17*17 ASSEMBLY
' (IN A 17*17 ASSEMBLY, ONLY 264 OF THE 289 AVAILABLE PIN POSITIONS ARE USED.)
' HERE, THE HOMOGENIZED FUEL (MIX 1) NOW CONTAINS SOME SS304 REPRESENTING THE
' INTERNAL BASKET MATERIAL BETWEEN ASSEMBLIES. (IN THE LATTICECELL X-SECT
' MODEL, THIS WAS CALLED MIX 7 AND WAS LATER BLENDED WITH MIX 500 IN THE
' ZONE INPUT DATA FOR THE CASK SHIELDING CALCS -- SEE CASES 1, 2, 3 OR 4.)
UO2  1  0.25553   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  1  0.08282  560  END
SS304   1  2.1375E-2   560  END
'
' MIX 2 IS USED BETWEEN THE INNER AND OUTER ROW OF ASSEMBLIES IN THE CASK:
SS304   2  2.1712E-2  END
B4C     2  7.7066E-2  END
'
' MIX 3 IS A DUMMY MATERIAL NOT USED IN THESE EXAMPLES
' MIX 4 IS THE STRUCTURAL STEEL USED IN THE CASK BODY
' MIX 5 IS THE U-METAL GAMMA SHIELD
' MIX 6 IS THE NEUTRON SHIELD  (DEFINED HERE;  USED IN SOME CASES, BUT NOT ALL)
HE           3  END
SS304        4  END
U(.27)METAL  5  END
H2O          6  0.944  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
END

CASE 5 -- INFHOMMEDIA X-SECTS; COLLAPSE=N; N-SHIELD PRESENT; ISN=16,ICM=4
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
' FOR THE FOLLOWING SHIELDING CALCULATION.  THIS IS ALSO TRUE FOR ANY
' ADDITIONAL SHIELDING CALCULATIONS THAT FOLLOW THIS CASE.
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' NOTES REGARDING THE DATA FOR ZONE 1:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
'  THE  0  0.0  INDICATES THAT ZONE 1 IS NOT TO BE DILUTED WITH MIX 0 (VOID)
'  ORIGEN SOURCE:  ON UNIT 60, 2-ND DECAY TIME IN FILE, ZVOL=1.8679E+5,
'  NUMBER OF FUEL ASSEMBLIES IN THIS FIRST ZONE = 1
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
'  NUMBER OF FUEL ASSEMBLIES IN THIRD ZONE = 6
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
'  INNER STEEL SHELL:
4  48.90   2  0
'  U-METAL GAMMA SHIELD:
5  57.40  30  0
'  OUTER STEEL SHELL:
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
'    [FOR THE ACCIDENT SCENARIO WHERE THE N-SHIELD IS ASSUMED
'    TO BE LOST, SIMPLY CHANGE THE "6" TO A "0" ON NEXT CARD]
6  72.78  16  0
'  OUTSIDE STEEL BARREL:
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
```

Table S1.5.5 (continued)

```
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' NOTE: THE FOLLOWING LIST OF OPTIONAL CONTROL PARAMETERS FOR THE SHIELDING
' PORTION OF THE CALCULATION DOESN'T START WITH "MORE DATA" AND DOESN'T END
' WITH "END" --  IF USED, THEY'RE JUST ENTERED BY THEMSELVES.
' THE FOLLOWING LIST IS INCLUDED FOR ILLUSTRATIVE PURPOSES ONLY.
' GENERALLY ONE DOES NOT NEED ANY OF THE OPTIONAL CONTROL PARAMETERS,
' AND THE FOLLOWING CARD MAY SIMPLY BE DELETED.  THE CODE WILL SUPPLY
' THE NECESSARY DEFAULT VALUES SHOWN IN THE MANUAL.
ISN=16  ICM=4  NDETEC=5  NFACTR=4
'
READ XSDOSE
'
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
'
' BECAUSE WE HAD SET  NFACTR=4  (ABOVE), WE MUST NOW ENTER THE CORRESPONDING
' ID NUMBERS FOR THE FOUR FLUX-TO-DOSE CONVERSION FACTORS OF INTEREST.  HAD
' THE "NFACTR=" PARAMETER NOT APPEARED ABOVE, THIS DATA WOULD NOT HAVE BEEN
' REQUIRED, AND THE CODE WOULD HAVE AUTOMATICALLY USED THE ANSI-STANDARD
' FLUX-TO-DOSE CONVERSION FACTORS (9029 FOR NEUTRONS AND 9504 FOR GAMMAS).
' NO HARM IS DONE IF SOME OF THE ID'S ENTERED ARE NOT AVAILABLE IN THE
' PARTICULAR X-SECT LIBRARY BEING USED (LIKE THE STRAKER-MORRISON FACTORS,
' 9028 AND 9503, IN THE "27N-18COUPLE" LIBRARY).  IN SUCH CASES, THE CODE
' WILL SIMPLE IGNORE THOSE ID'S.
9029  9504
9028  9503
'
' BECAUSE WE HAD SET  NDETEC=5  (ABOVE), WE MUST NOW ENTER THE CORRESPONDING
' LOCATION FOR EACH OF THE FIVE DETECTORS.  NOTE THAT THESE WILL OVERRIDE AND
' REPLACE THE 4 DETECTOR LOCATIONS THAT SAS1 WOULD NORMALLY USE BY DEFAULT
' HAD THE "NDETEC=" PARAMETER NOT APPEARED ABOVE.  FOR CYL GEOMETRY ENTER:
' R(1)  H(1)
' R(2)  H(2)
' ETC...WHERE H IS THE HEIGHT OF THE DETECTOR ABOVE THE BASE OF THE CASK.
'       NOTE: H=0.0 ALWAYS CORRESPONDS TO THE BASE OF THE CASK, AND
'       HERE, H=595.64 WOULD CORRESPOND TO THE TOP OF THE CASK
 73.22  297.82
173.22  297.82
273.22  297.82
473.22  297.82
473.22  595.64
'
END

CASE 6 - INFHOMMEDIA X-SECTS; COLLAPSE=N; N-SHIELD PRESENT; ISN=DEFAULT,ICM=10
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
6  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
```

Table S1.5.5 (continued)

```
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
ICM=10
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END

CASE 7 - INFHOMMEDIA X-SECTS; COLLAPSE=N; NO N-SHIELD USED; ISN,ICM=DEFAULTS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (NOW VOID):
'    FOR THE ACCIDENT SCENARIO HERE, THE N-SHIELD IS ASSUMED
'    TO BE LOST, SO MIXTURE 0 WAS USED IN PLACE OF MIXTURE 6.
0  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
LAST
CASE 8 - INFHOMMEDIA X-SECTS; COLLAPSE=N; NO N-SHIELD USED; ISN=DEFUALT,ICM=10
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (NOW VOID):
'    FOR THE ACCIDENT SCENARIO HERE, THE N-SHIELD IS ASSUMED
'    TO BE LOST, SO MIXTURE 0 WAS USED IN PLACE OF MIXTURE 6.
0  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
```

Table S1.5.5 (continued)

```
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
ICM=10
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
```

Table S1.5.6 Annotated input for cases 9-14

```
#SAS1
CASES 9-14 (PREP) -- INFHOMMEDIA USED FOR X-SECT PROCESSING, COLLAPSE=YES
27N-18COUPLE  INFHOMMEDIA
'
' THE UO2 AND ZIRCALLOY VOLUME FRACTIONS PRESERVE THE AMOUNT OF FUEL ASSOCIATED
' WITH THE 264 FUEL PINS IN THE SPACE OCCUPIED BY A WESTINGHOUSE 17*17 ASSEMBLY
' (IN A 17*17 ASSEMBLY, ONLY 264 OF THE 289 AVAILABLE PIN POSITIONS ARE USED.)
' HERE, THE HOMOGENIZED FUEL (MIX 1) NOW CONTAINS SOME SS304 REPRESENTING THE
' INTERNAL BASKET MATERIAL BETWEEN ASSEMBLIES. (IN THE LATTICECELL X-SECT
' MODEL, THIS WAS CALLED MIX 7 AND WAS LATER BLENDED WITH MIX 500 IN THE
' ZONE INPUT DATA FOR THE CASK SHIELDING CALCS -- SEE CASES 1, 2, 3 OR 4.)
UO2  1  0.25553   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  1  0.08282  560  END
SS304   1  2.1375E-2   560  END
'
' MIX 2 IS USED BETWEEN THE INNER AND OUTER ROW OF ASSEMBLIES IN THE CASK:
SS304   2  2.1712E-2  END
B4C     2  7.7066E-2  END
'
' MIX 3 IS A DUMMY MATERIAL NOT USED IN THESE EXAMPLES
' MIX 4 IS THE STRUCTURAL STEEL USED IN THE CASK BODY
' MIX 5 IS THE U-METAL GAMMA SHIELD
' MIX 6 IS THE NEUTRON SHIELD  (DEFINED HERE;  USED IN SOME CASES, BUT NOT ALL)
HE           3  END
SS304        4  END
U(.27)METAL  5  END
H2O          6  0.944  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
' TO COLLAPSE THE 27 NEUTRON GROUPS DOWN TO 15 GROUPS ENTER:
MORE DATA  COLLAPSE  END
'
END

CASE 9 -- INFHOMMEDIA X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; ISN,ICM=DEFAULTS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
' FOR THE FOLLOWING SHIELDING CALCULATION.  THIS IS ALSO TRUE FOR ANY
' ADDITIONAL SHIELDING CALCULATIONS THAT FOLLOW THIS CASE.
'
CYLINDRICAL
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' NOTES REGARDING THE DATA FOR ZONE 1:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
'  THE  0  0.0  INDICATES THAT ZONE 1 IS NOT TO BE DILUTED WITH MIX 0 (VOID)
'  ORIGEN SOURCE:  ON UNIT 60, 2-ND DECAY TIME IN FILE, ZVOL=1.8679E+5,
'  NUMBER OF FUEL ASSEMBLIES IN THIS FIRST ZONE = 1
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
'  NUMBER OF FUEL ASSEMBLIES IN THIRD ZONE = 6
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
'  INNER STEEL SHELL:
4  48.90   2  0
'  U-METAL GAMMA SHIELD:
5  57.40  30  0
'  OUTER STEEL SHELL:
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
'    [FOR THE ACCIDENT SCENARIO WHERE THE N-SHIELD IS ASSUMED
'    TO BE LOST, SIMPLY CHANGE THE "6" TO A "0" ON NEXT CARD]
6  72.78  16  0
'  OUTSIDE STEEL BARREL:
```

Table S1.5.6 (continued)

```
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS WOULD GO NEXT (IF USED)
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END

CASE 10 - INFHOMMEDIA X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; ISN=8,ICM=DEFAULT
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
6  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
' IN THIS CASE, A LOW-ORDER S8 ANGULAR QUADRATURE IS BEING USED FOR CHEAP
' SCOPING CALCULATIONS.  A HIGHER-ORDER S16 (DEFAULT), S24, OR S32 SET
' SHOULD NORMALLY BE USED IN THE FINAL ANALYSIS.
ISN=8
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END

CASE 11 - SAME AS CASE 10, WITH AXIAL BUCKLING OF 595.64 CM USED IN XSDRN CALC
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
6  72.78  16  0
```

Table S1.5.6 (continued)

```
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
' IN THIS CASE, A LOW-ORDER S8 ANGULAR QUADRATURE IS BEING USED FOR CHEAP
' SCOPING CALCULATIONS, AND AN AXIAL BUCKLING OF 595.64 CM IS BEING USED IN
' THE XSDRNPM CALCULATION. (AS NOTED IN SECTION F4.1.2.1 OF THE SCALE MANUAL,
' HOWEVER, THE USE OF AN AXIAL BUCKLING CORRECTION IN 1-D RADIAL SHIELDING
' CALCULATIONS SHOULD GENERALLY BE AVOIDED.  A HIGHER-ORDER S16 [DEFAULT],
' S24, OR S32 QUADRATURE SET SHOULD ALSO BE USED IN THE FINAL ANALYSIS.)
ISN=8  DY=595.64
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END

CASE 12 - SAME AS CASE 10, WITH OUTER FUEL ZONE SMEARED WITH ADJACENT VOID
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
'  IN CASE 10, THE OUTER FUEL ZONE EXTENDED FROM R=21.72 CM TO R=38.05 CM,
'  WITH AN ADJACENT  VOID REGION  EXTENDING FROM R=38.05 CM TO R=47.63 CM.
'  IN THIS CASE [12], THE TWO ZONES HAVE BEEN MODELED AS ONE COMBINED ZONE.
'  THIS COMBINED ZONE CONTAINS 45.68 VOL% VOID (MIX 0), PLUS 54.32 VOL%
'  (=100.00-45.68)  FUEL  MIX 1.  NOTE THAT THE VOLUME (ZVOL) OF THE
'  COMBINED FUEL REGION IS NOW 2.0647E+6 CC RATHER THAN 1.1215E+6 CC
'  [2.0647E+6 = PI*(47.63**2 - 21.72**2)*(144*2.54)].  WHEN USING SOURCE
'  TERMS & SPECTRA FROM AN ORIGEN FILE (N/S/ASSY & PHOTONS/S/ASSY), THIS
'  VOLUME (ZVOL) MUST BE ENTERED SO THAT SAS1 PROPERLY NORMALIZES THE
'  SOURCE PER UNIT VOLUME, WHICH IS THEN USED IN THE XSDRNPM CALCULATION.
'  AS IN THE PREVIOUS CASE, THIS ZONE CONTAINS 6 PWR FUEL ASSEMBLIES.
1  47.63  30 +1      0  0.4568   60  2  2.0647E+6  6
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (WATER):
6  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
' IN THIS CASE, A LOW-ORDER S8 ANGULAR QUADRATURE IS BEING USED FOR CHEAP
' SCOPING CALCULATIONS.  A HIGHER-ORDER S16 (DEFAULT), S24, OR S32 SET
' SHOULD NORMALLY BE USED IN THE FINAL ANALYSIS.
ISN=8
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
```

Table S1.5.6 (continued)

```
CASE 13 - INFHOMMEDIA X-SECTS; COLLAPSE=Y; NO N-SHIELD USED; ISN,ICM=DEFAULTS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (NOW VOID):
'    FOR THE ACCIDENT SCENARIO HERE, THE N-SHIELD IS ASSUMED
'    TO BE LOST, SO MIXTURE 0 WAS USED IN PLACE OF MIXTURE 6.
0  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
LAST
CASE 14 - INFHOMMEDIA X-SECTS; COLLAPSE=Y; NO N-SHIELD USED; ISN=8,ICM=DEFAULT
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD
' TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE ABOVE TITLE CARD.
'
CYLINDRICAL
'  DESCRIPTION OF EACH ZONE FOLLOWS:
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE
1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
2  21.72   8  0
1  38.05  30 +1      0  0.0      60  2  1.1215E+6  6
0  47.63   5  0
4  48.90   2  0
5  57.40  30  0
4  61.35   6  0
'  NEUTRON SHIELD (NOW VOID):
'    FOR THE ACCIDENT SCENARIO HERE, THE N-SHIELD IS ASSUMED
'    TO BE LOST, SO MIXTURE 0 WAS USED IN PLACE OF MIXTURE 6.
0  72.78  16  0
4  73.22   1  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE 1 AND CASE 3.
'
' OPTIONAL CONTROL PARAMETERS GO NEXT (IF USED):
' IN THIS CASE, A LOW-ORDER S8 ANGULAR QUADRATURE IS BEING USED FOR CHEAP
' SCOPING CALCULATIONS.  A HIGHER-ORDER S16 (DEFAULT), S24, OR S32 SET
' SHOULD NORMALLY BE USED IN THE FINAL ANALYSIS.
ISN=8
'
READ XSDOSE
' ENTER FULL HEIGHT OF CASK TO BE USED BY XSDOSE CALC (=2*297.82):
595.64
END
```

Cases 1 through 4 of Table S1.5.1 show how the user may invoke the SAS1X control module to perform a preliminary XSDRNPM latticecell calculation for a Westinghouse 17 x 17 fuel assembly to obtain cell-weighted cross-section data that may later be referred to as "mixture 500" in the specification of one or more zones in the 1-D shielding problem. While all four cases utilize the SCALE 27n-18γ cross-section library (see Sect. M4.2.7 for more information), cases 1 and 2 retain all 27 neutron groups in the final 1-D shielding calculation, while cases 3 and 4 collapse the 13 neutron energy groups below 3.05 eV down to one thermal energy group prior to performing the 1-D shielding calculation. Because of these differences, cases 1 and 2 were both run as separate steps in one SAS1X calculation, while cases 3 and 4 were both run as separate steps in another SAS1X calculation (cf. Table S1.5.1). Note that in cases 1 and 2, the running time for each XSDRNPM shielding calculation was approximately 4 min on an IBM-3090, while cases 3 and 4 using the collapsed neutron data required only 1.6 min for each XSDRNPM case. It should also be noted that the calculated neutron and gamma dose rates on the surface of the cask are not significantly different in this case, although they may differ more if one had a strong thermal-neutron-absorbing/gamma-producing material like boron in the neutron shield near the outer portion of the cask.

Cases 1 and 3 illustrate how the user may describe the neutron/gamma source spectra directly in the SAS1 or SAS1X input file for the general case when one retains all 27 neutron groups and for the collapsed case where the 13 thermal groups have been collapsed to one thermal sink group, leaving a total of 15 neutron groups and 18 gamma groups. Cases 2 and 4 solve exactly the same problem but illustrate how the neutron/gamma source spectra may be read from an ORIGEN-S source file on logical unit 60. Note that the same ORIGEN-S source file may be used regardless of whether or not the COLLAPSE option has been invoked. If the COLLAPSE option is used, the SAS1 or SAS1X control modules will collapse the source spectra as well as the cross-section data. (To avoid listing the 27n-18γ or 15n-18γ spectral data, an excessive number of times for the various sample input cases, most of the cases shown here assume that these data are being read from an ORIGEN-S source file. Primarily for completeness, the exact same data have been given explicitly in cases 1 and 3.) In all four cases the neutron shield was assumed to be present.

Although mixture 500 may indeed be typical of the homogenized spent fuel in the innermost radial zone of the 1-D shielding calculation, it does not include any of the stainless steel in the basket between assemblies (mixture 7). In cases 1 through 4, the zone input data for zone 3 are used to indicate that (azimuthally) the material in this zone is 82% spent fuel and 18% stainless steel from the basket.

Cases 5 through 14 assume that the user has simply entered the appropriate volume fraction of UO_2, zircalloy, and stainless steel necessary to describe the spent fuel and the internal basket structure as a single homogenized material that will be treated as an infinite homogeneous media in the resonance self-shielding calculation. Because a preliminary XSDRNPM latticecell calculation will not be performed, the SAS1 sequence should be used in lieu of the SAS1X sequence. Cases 5 through 8 use all 27 neutron groups, while cases 9 through 14 use an assumed Maxwellian neutron spectrum to collapse the 13 thermal neutron groups down to one thermal sink group prior to the 1-D shielding calculation. While the two sets of results are generally in good agreement, a 3% difference in the external neutron dose rate is seen in those analyses where the neutron shield is present (cf. Table S1.5.1, case 5 vs case 9). Cases 6 and 8 show the effect of using additional outer iterations (ICM=10) to better converge the flux spectrum. While four outer iterations are generally adequate to converge the internal fission source in a heavily poisoned cask with one thermal sink group, unpoisoned casks (or analyses performed with more thermal energy neutron groups) may require additional iterations. Better convergence of the thermal neutron flux in the outermost portion of the neutron shield may also have a slight impact on the external dose rate (cf. Table S1.5.1, case 6 vs case 5). However, the penalty for increasing the number of outer iterations is approximately 50 to 100% for the cases shown.

Cases 10 and 14 (15n-18γ, with and without the neutron shield) are similar to cases 9 and 13, respectively, except that a lower order S_8 quadrature was used for illustrative purposes. While an S_{16} or higher quadrature is recommended for final analysis, a lower order S_8 quadrature may be used for

debugging purposes and/or for large series of scoping calculations where the need for accuracy is not paramount. As shown in Table S1.5.1, the S_{16} shielding calculations each required approximately 1.6 min of cpu time on an IBM-3090, while the S_8 calculations required only 0.55 min each and gave surface dose rates that were less than 1% different from S_{16} results. For problems involving thicker shields or for problems having only gamma source terms, the sensitivity to the quadrature will generally be somewhat greater. Also, while the dose rates at the surface of the cask may be relatively insensitive to the order of the quadrature, the calculated dose rates at more distant points outside the cask will always be more sensitive to the order of the quadrature.

The input data for case 11 are listed below (cf. Table S1.5.6) to illustrate how an axial buckling correction may be used in the XSDRNPM 1-D radial analysis. In this case an axial buckling of 595.64 cm was used to approximate the axial leakage from the cask. As noted in the footnote to Table S1.5.1, the calculated dose rate on the outside of the cask is just marginally lower than the normal (more conservative) case where a buckling correction is not used. This insensitivity is characteristic of the 1-D radial calculation due to the length of the cask relative to its radius. It should also be realized that the $DB^2\phi$ correction is treated as an absorption term in the transport equation solved by XSDRNPM and that it, therefore, represents an "isotropic" correction; whereas, in reality, some of the angular fluxes would be affected greatly by the finite dimensions of the cask, while the most outward-directed angular fluxes important in shielding calculations would be affected to a much smaller degree. For that reason the use of an axial buckling correction should generally be avoided when performing 1-D calculations in the radial direction. For 1-D calculations in the axial direction, however, failure to use a realistic buckling correction may cause the calculated dose rates to be unrealistically high (cf. cases 16 and 18 in Sect. S1.5.3).

Lastly, the input for case 12 is listed below (cf. Table S1.5.6) to illustrate still another way in which the interior of the cask could be modeled. Here, the outer fuel region and the adjacent void were smeared together in the XSDRNPM shielding calculation. This more conservative model tends to dilute the fuel in the outer region so that it provides less spatial self-shielding than what one might actually have when modeled as shown in Fig. S1.5.1. The calculated results show a 3% increase in the external neutron dose rate and a negligible change in the gamma dose rate. Nevertheless, this is the type of modeling sensitivity that users should investigate when analyzing any new shielding configuration. More extensive notes have also been provided, as commented in the input data listing, to show how the source terms for the smeared zone (zone 3) should be modified to correctly account for the volumetric dilution of the spent fuel.

S1.5.3 DISCUSSION OF THE 1-D AXIAL PROBLEMS

Cases 15 through 25 (cf. Table S1.5.2) illustrate different approaches to the 1-D axial problem with and without the axial shock absorber on the end of the cask. The effect of collapsing the cross-section data using different geometric models and the effect of using a buckling correction in the 1-D shielding analysis were all examined. In addition, the annotated input listed in Tables S1.5.7 through S1.5.9 is used to illustrate (1) how the fuel should be smeared over the entire inner volume of the cask and how the zone description data may be used to accomplish that task, (2) how the source terms on the zone description card(s) should be renormalized to accurately represent the neutron and gamma sources in the fuel (cf. cases 15 and 16), and (3) how one might account for the activation sources in the hardware at the top of the fuel assemblies (cf. case 15). Alternate ways of entering these data are also illustrated in Tables S1.5.7 through S1.5.9.

Cases 15 through 19 used a multiregion infinite slab model in the Nordheim resonance self-shielding calculation for the cross-section data, while cases 20 through 25 performed the resonance self-shielding calculation for each material as if one had an infinite homogeneous region of the given material. In the multiregion case, the resonance energy neutrons in each material have a finite free-flight escape

Table S1.5.7 Annotated input for cases 15-19

```
#SAS1
CASES 15-19 (PREP) -- MULTIREGION SLAB USED FOR X-SECT PROCESSING, COLLAPSE=YES
27N-18COUPLE  MULTIREGION
'
' THE UO2 AND ZIRCALLOY VOLUME FRACTIONS PRESERVE THE AMOUNT OF FUEL ASSOCIATED
' WITH THE 264 FUEL PINS IN THE SPACE OCCUPIED BY A WESTINGHOUSE 17*17 ASSEMBLY
' (IN A 17*17 ASSEMBLY, ONLY 264 OF THE 289 AVAILABLE PIN POSITIONS ARE USED.)
' HERE, THE HOMOGENIZED FUEL (MIX 1) ALSO CONTAINS SOME SS304 REPRESENTING THE
' INTERNAL BASKET MATERIAL BETWEEN ASSEMBLIES.  NOTE THAT THIS DESCRIPTION OF
' MIX 1 IS THE SAME AS THAT USED FOR THE MATERIAL IN ZONES 1 & 3 OF THE 1-D
' RADIAL CALCULATIONS (SEE CASES [5] THROUGH [14]). FOR THE AXIAL CALCULATIONS,
' HOWEVER, THE FUEL SHOULD BE SMEARED OVER THE ENTIRE INNER VOLUME OF THE CASK
' CAVITY (I.E., OVER WHAT WERE ZONES 1-4 IN THE RADIAL MODEL). THIS ADDITIONAL
' DILUTION IS ACCOMPLISHED BELOW, BY USING THE MIXING OPTION IN THE ZONE
' DESCRIPTION DATA FOR THE AXIAL SHIELDING CALCULATION.
UO2  1  0.25553   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  1  0.08282  560  END
SS304   1  2.1375E-2   560  END
'
' MIX 2 IS AN HOMOGENIZED MODEL OF THE HARDWARE ON THE END OF THE ASSEMBLY:
SS304      2  4.8714E-2  END
ZIRCALLOY  2  1.2838E-2  END
'
' MIX 3 IS THE STAINLESS STEEL USED IN THE CASK LID
' MIX 4 IS THE U-METAL GAMMA SHIELD EMBEDDED WITHIN THE LID
' MIX 5 IS THE EXTERNAL SHOCK ABSORBER (BALSA WOOD) ON THE END OF THE CASK;
'  WHILE MIX 5 IS DEFINED HERE, IT IS ONLY USED IN SOME OF THE CASK MODELS.
SS304        3  END
U(.27)METAL  4  END
BALSA        5  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
' GEOMETRY SPECIFICATION CARD FOR X-SECT PROCESSING CALC
' (NOTE: NO GEOM SPEC CARD IS REQUIRED FOR INFHOMMEDIA)
SLAB  END
'
' MULTIREGION ZONE DESCRIPTION USED IN THE CROSS SECTION
' RESONANCE SELF-SHIELDING CALCULATION PERFORMED BY NITAWL:
1   182.88  NOEXTERMOD
2   219.02  NOEXTERMOD
0   224.10  NOEXTERMOD
3   225.37  NOEXTERMOD
4   233.87  NOEXTERMOD
3   237.82  NOEXTERMOD
5   297.82  NOEXTERMOD
'
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' TO COLLAPSE THE 27 NEUTRON GROUPS DOWN TO 15 GROUPS ENTER:
MORE DATA  COLLAPSE  END
'
END

CASE 15 -- MULTIREGION X-SECTS; COLLAPSE=Y; BUCKLED SLAB MODEL; WITH SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
' FOR THE FOLLOWING SHIELDING CALCULATION.  THIS IS ALSO TRUE FOR ANY
' ADDITIONAL SHIELDING CALCULATIONS THAT FOLLOW THIS CASE.
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' NOTES REGARDING THE DATA FOR ZONES 1 & 2:
' ----------------------------------------
```

Table S1.5.7 (continued)

```
'  TOGETHER, ZONES 1 & 2 REPRESENT THE TOP HALF OF THE FUEL ASSEMBLY.
'  TWO ZONES WERE USED HERE SO THAT A COARSE MESH OF ABOUT 2.74 CM
'  [=137.16/50] COULD BE USED IN THE LOWER REGION WHILE A FINER MESH OF
'  ABOUT 0.91 CM [=(182.88-137.16)/50] COULD BE USED NEAR THE TOP OF THE
'  ASSEMBLY WHERE THE FUEL ITSELF PROVIDES LESS SPATIAL SELF-SHIELDING.
'
'  THE -1 INDICATES THAT SOURCE SPECTRUM 1 IS ENTERED BELOW (AFTER ZONE DATA).
'  IN THE RADIAL SHIELDING CALCULATIONS (CF. CASES [1] THROUGH [14]) THE
'  HOMOGENIZED FUEL REPRESENTED BY MIX 1 ABOVE WAS LOCATED IN RADIAL ZONES 1
'  (EXTENDING FROM R=0.0 CM TO R=12.75 CM) AND 3 (EXTENDING FROM R=21.72 CM TO
'  R=38.05 CM), WITH A VOID REGION [ZONE 4] EXTENDING FROM R=38.05 CM TO THE
'  INNER WALL OF THE CASK AT R=47.63 CM.  THE ACTUAL VOLUME FRACTION OF THIS
'  HOMOGENIZED FUEL MIXTURE INSIDE THE CASK IS THEREFORE GIVEN BY
'  VFMIX1=(FVOL/ZVOL)=0.50189, WHERE
'
'  FVOL=  1.30834E+6 CC = PI*(12.75**2 + 38.05**2 - 21.72**2)*(2*182.88)
'  ZVOL = 2.60680E+6 CC = PI*(47.63**2)*(2*182.88)
'
'  IN THE AXIAL CALC, THE SOURCE DENSITY IN THIS LARGER HOMOGENIZED REGION
'  CORRESPONDING TO THE CASK CAVITY MUST BE REDUCED BY A SIMILAR AMOUNT. THUS,
'  XNN(CASE15)=0.50189*XNN(CASE1)  AND  XNG(CASE15)=0.50189*XNG(CASE1), IE:
'  XNN(CASE15)=3.468E+2 NEUT/S/CC  AND  XNG(CASE15)=1.300E+10 PHOTONS/S/CC.
'
'  SINCE THE BORATED STEEL BETWEEN THE INNER AND OUTER ROW OF ASSEMBLIES DOES
'  NOT PROVIDE ANY SHIELDING IN THE AXIAL DIRECTION, THE MATERIAL IN RADIAL
'  ZONE 2 (LIKE RADIAL ZONE 4) SHOULD BE TREATED AS A VOID.  THE EFFECTIVE
'  VOLUME FRACTION OF THE VOID SPACE INSIDE THE CASK CAVITY (I.E. THE SPACE
'  NOT OCCUPIED BY MIX 1) IS THEN GIVEN BY  VFVOID = 1.0-VFMIX1 = 0.49811.
'  THE "0  0.49811" THEREFORE INDICATES THAT AXIAL ZONES 1 & 2 CONTAIN
'  49.81 VOL% VOID (MIX 0), PLUS 50.19 VOL% (=100-49.81) FUEL MIX 1.
' ------------------------------------
1  137.16  50  -1       0  0.49811       3.468E+2  1.300E+10
1  182.88  50  -1       0  0.49811       3.468E+2  1.300E+10
'
'
' HARDWARE ON THE END OF THE ASSEMBLY (ZONE 3):
' ----------------------------------------
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'
'  XNN = 0.0 N/S/CC IN THIS ZONE  &  XNG = 1.2984E+7 PHOTONS/S/CC IN THIS ZONE.
'
'  THE GAMMA SOURCE IN THIS ZONE REPRESENTS ALL THE ACTIVATION SOURCES IN THE
'  STEEL COMPONENTS AT THE END OF THE CASK.  FOR MANY 1-D AXIAL CALCULATIONS,
'  THE DOSE RATE DUE TO THIS ACTIVATION IS NOT NEGLIGIBLE.  ACTUAL ACTIVATION
'  SOURCE STRENGTHS (& SPECTRA) "PER MTIHM" OR "PER ASSEMBLY" OR "PER KG OF
'  HARDWARE" MAY BE OBTAINED FROM AN ORIGEN-S ANALYSIS.  THE TOTAL VOLUMETRIC
'  SOURCE TERMS (XNN & XNG) WILL THEN HAVE TO BE NORMALIZED BY THE USER TO
'  ACCOUNT FOR THE AMOUNT OF ACTIVATED HARDWARE IN THIS PORTION OF THE 1-D
'  AXIAL MODEL OF THE PARTICULAR SHIPPING CASK.
' ------------------------------------
2  219.02  40  -2       0  0.0           0.0  1.2984E+7
'
'
'  VOID BETWEEN TOP OF ASSEMBLY AND INNER LID OF CASK (OCCUPIED
'  BY SMALL LOCKING DEVICES NOT INCLUDED IN THIS MODEL):
0  224.10   5  0
'
'  INNER PORTION OF CASK LID (SS304):
3  225.37   2  0
'
'  U-METAL GAMMA SHIELD IN CASK LID:
4  233.87  30  0
'
'  OUTER PORTION OF CASK LID (SS304):
3  237.82   6  0
'
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5  297.82  60  0
'
```

Table S1.5.7 (continued)

```
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
'
' SOURCE SPECTRUM 1 IS BEING ENTERED DIRECTLY AND GOES NEXT.
' NOTE: WHILE THE COLLAPSED 15N-18G SPECTRUM ENTERED HERE IS IDENTICAL
' TO THAT USED IN CASE [3], THE ACTUAL SPECTRAL SOURCE DENSITIES FOR
' THIS AXIAL PROBLEM WILL BE RENORMALIZED USING THE VALUES OF XNN AND
' XNG GIVEN ABOVE (SEE INPUT DATA FOR ZONES 1 & 2).
1.27E+01  1.45E+02  1.62E+02  9.06E+01  1.22E+02  1.33E+02  2.60E+01
8Z
3.92E-01  1.84E+00  9.41E+00  2.34E+01  4.45E+04  3.58E+05  1.20E+07
4.83E+06  2.74E+08  1.08E+09  1.39E+09  9.90E+09  3.10E+09  2.83E+08
4.18E+08  1.52E+09  1.75E+09  6.19E+09
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT.
' THIS 15N-18G SPECTRUM REPRESENTS THE ACTIVATION SOURCE IN
' THE HARDWARE NEAR THE END OF THE FUEL ASSEMBLY. BECAUSE OF
' THAT, THE SOURCE IS NON-ZERO IN ONLY TWO GAMMA ENERGY GROUPS.
' SUCH ACTIVATION DATA MAY BE OBTAINED FROM AN ORIGEN-S ANALYSIS.
' THE ACTUAL SPECTRAL SOURCE DENSITIES FOR THIS AXIAL PROBLEM
' WILL BE RENORMALIZED USING THE VALUES OF XNN AND XNG GIVEN
' ABOVE (SEE INPUT DATA FOR ZONE 3).
15Z  8Z  0.1574  0.8426  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' UNLIKE THE 1-D RADIAL CALCULATIONS WHERE THE BUCKLING CORRECTION
' GENERALLY MADE VERY LITTLE DIFFERENCE IN THE EXTERNAL DOSE RATE,
' THE 1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION
' IF THE CALCULATED DOSE RATES AT THE SURFACE ARE TO BE ANYWHERE
' CLOSE TO REALISTIC.  EVEN WITH A REALISTIC BUCKLING CORRECTION, ONE
' CAN GENERALLY ONLY GET WITHIN 10-50% OF THE CORRECT DOSE RATE USING
' A 1-D AXIAL MODEL.  WITHOUT A BUCKLING CORRECTION THE SAS1 RESULTS
' AT THE SURFACE MAY BE OFF BY AN ORDER OF MAGNITUDE.  SEE TABLE 7.4
' OF ORNL/CSD/TM-246 FOR MORE DETAILED COMPARISONS AGAINST 3-D MORSE
' MONTE CARLO RESULTS.
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END

CASE 16 -- SAME AS CASE 15, BUT WITH SOURCE SPECTRUM FROM ORIGEN SOURCE FILE
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' NOTES REGARDING THE DATA FOR ZONES 1 & 2:
' ----------------------------------------
'  TOGETHER, ZONES 1 & 2 REPRESENT THE TOP HALF OF THE FUEL ASSEMBLY.
'  TWO ZONES WERE USED HERE SO THAT A COARSE MESH OF ABOUT 2.74 CM
'  [=137.16/50] COULD BE USED IN THE LOWER REGION WHILE A FINER MESH OF
'  ABOUT 0.91 CM [=(182.88-137.16)/50] COULD BE USED NEAR THE TOP OF THE
'  ASSEMBLY WHERE THE FUEL ITSELF PROVIDES LESS SPATIAL SELF-SHIELDING.
'
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  ORIGEN SOURCE:  ON UNIT 60, 2-ND DECAY TIME IN FILE, ZVOL=2.60680E+6,
'  NO. OF FUEL ASSEMBLIES IN THESE FIRST TWO AXIAL ZONES (I.E. IN CASK)=7
'
'  IN THE RADIAL SHIELDING CALCULATIONS (CF. CASES [5] THROUGH [14]) THE
'  HOMOGENIZED FUEL REPRESENTED BY MIX 1 ABOVE WAS LOCATED IN RADIAL ZONES 1
'  (EXTENDING FROM R=0.0 CM TO R=12.75 CM) AND 3 (EXTENDING FROM R=21.72 CM TO
'  R=38.05 CM), WITH A VOID REGION [ZONE 4] EXTENDING FROM R=38.05 CM TO THE
'  INNER WALL OF THE CASK AT R=47.63 CM.  THE ACTUAL VOLUME FRACTION OF THIS
```

Table S1.5.7 (continued)

```
'  HOMOGENIZED FUEL MIXTURE INSIDE THE CASK IS THEREFORE GIVEN BY
'  VFMIX1=FVOL/ZVOL, WHERE
'
'  FVOL=  1.30834E+6 CC = PI*(12.75**2 + 38.05**2 - 21.72**2)*(2*182.88)
'  ZVOL = 2.60680E+6 CC = PI*(47.63**2)*(2*182.88)
'
'  THIS YIELDS VFMIX1=0.50189.  SINCE THE BORATED STEEL BETWEEN THE INNER AND
'  OUTER ROW OF ASSEMBLIES DOES NOT PROVIDE ANY SHIELDING IN THE AXIAL
'  DIRECTION, THE MATERIAL IN RADIAL ZONE 2 (LIKE RADIAL ZONE 4) SHOULD BE
'  TREATED AS A VOID.  THE EFFECTIVE VOLUME FRACTION OF THE VOID SPACE INSIDE
'  THE CASK CAVITY (I.E. THE SPACE NOT OCCUPIED BY MIX 1) IS THEN GIVEN BY
'  VFVOID = 1.0-VFMIX1 = 0.49811.  THE "0  0.49811" THEREFORE INDICATES THAT
'  AXIAL ZONES 1 & 2 CONTAIN 49.81 VOL% VOID (MIX 0), PLUS 50.19 VOL%
'  (=100-49.81) FUEL MIX 1.  WHEN USING SOURCE TERMS & SPECTRA FROM AN ORIGEN
'  FILE (N/S/ASSY & PHOT/S/ASSY), THE SMEARED SOURCE VOL (ZVOL=2.60680E+6 CC)
'  MUST BE ENTERED SO THAT SAS1 PROPERLY NORMALIZES THE SOURCE PER UNIT VOLUME,
'  WHICH IS THEN USED IN THE XSDRNPM SHIELDING CALCULATION.  THE 7 INDICATES
'  THAT THIS SMEARED SOURCE VOLUME CONTAINS 7 FUEL ASSEMBLIES.
' ----------------------------------
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'
'
' HARDWARE ON THE END OF THE ASSEMBLY (ZONE 3):
' -------------------------------------------
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'
'  IN THIS CASE, XNN & XNG WOULD NORMALLY EQUAL THE NUMBER OF NEUTRONS/S/CC
'  IN THIS ZONE AND THE NUMBER OF PHOTONS/S/CC IN THIS ZONE.  WHEN BOTH ARE
'  SPECIFIED AS ZERO (AS SHOWN HERE), IT INDICATES THAT THE SOURCE SPECTRUM
'  ENTERED BELOW (AFTER THE ZONE DATA) HAS ALREADY BEEN NORMALIZED BY THE USER
'  TO THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS PARTICULAR
'  ZONE, AND THAT THIS SPECTRUM IS NOT TO BE RENORMALIZED BY THE CODE.
'
'  THE SPECTRUM REFERRED TO IN THIS CASE REPRESENTS THE ACTIVATION SOURCE IN
'  THE STEEL COMPONENTS AT THE END OF THE CASK.  FOR MANY 1-D AXIAL CALCULA-
'  TIONS, THE DOSE RATE DUE TO THIS ACTIVATION SOURCE IS NOT NEGLIGIBLE.
' ----------------------------------
2  219.02  40  -2       0  0.0           0.0  0.0
'
'  DATA FOR REMAINING ZONES:
0  224.10   5  0
3  225.37   2  0
4  233.87  30  0
3  237.82   6  0
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5  297.82  60  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15]. (NOTE THAT XNN & XNG
' ON THE ZONE 1 DESCRIPTION CARD FOR CASE [15] HAVE BEEN ADJUSTED
' FOR THE SMEARED FUEL VOLUME IN ZONE 1 OF THE 1-D AXIAL MODEL.)
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT.
' THIS 15N-18G SPECTRUM REPRESENTS THE ACTIVATION SOURCE IN
' THE HARDWARE NEAR THE END OF THE FUEL ASSEMBLY. BECAUSE OF
' THAT, THE SOURCE IS NON-ZERO IN ONLY TWO GAMMA ENERGY GROUPS.
' SUCH ACTIVATION DATA MAY BE OBTAINED FROM AN ORIGEN-S ANALYSIS.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' (1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION)
DY=146.44  DZ=146.44
'
READ XSDOSE
```

Table S1.5.7 (continued)

```
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END

CASE 17 -- MULTIREGION X-SECTS; COLLAPSE=Y; BUCKLED SLAB; WITHOUT SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  IF THE EXTERNAL AXIAL SHOCK ABSORBER WERE PRESENT IT WOULD BE NEXT.
'  IN THIS "ACCIDENT" SCENARIO, IT IS ASSUMED TO BE LOST OR DESTROYED.
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' (1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION)
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END

CASE 18 -- MULTIREGION X-SECTS; COLLAPSE=Y; INFINITE SLAB MODEL; WITH SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5  297.82  60  0
 END ZONE
'
```

Table S1.5.7 (continued)

```
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION
' WOULD GO HERE IF USED. [SINCE THE TRANSVERSE DIMENSIONS (DY & DZ) ARE
' NOT SPECIFIED HERE, XSDRNPM WILL USE AN "INFINITE" SLAB MODEL WITH NO
' BUCKLING CORRECTION.  FOR 1-D AXIAL MODELS, THIS WILL YIELD CONSERVA-
' TIVE (BUT UNREALISTICALLY HIGH) DOSE RATES AT THE CASK SURFACE.]
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END
LAST
CASE 19 -- MULTIREGION X-SECTS; COLLAPSE=Y; INFINITE SLAB; WITHOUT SHOCK ABS
'
' NOTE THAT A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD TO BE PLACED
' BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD FOR THIS FINAL CASE
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  IF THE EXTERNAL AXIAL SHOCK ABSORBER WERE PRESENT IT WOULD BE NEXT.
'  IN THIS "ACCIDENT" SCENARIO, IT IS ASSUMED TO BE LOST OR DESTROYED.
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION
' WOULD GO HERE IF USED. [SINCE THE TRANSVERSE DIMENSIONS (DY & DZ) ARE
' NOT SPECIFIED HERE, XSDRNPM WILL USE AN "INFINITE" SLAB MODEL WITH NO
' BUCKLING CORRECTION.  FOR 1-D AXIAL MODELS, THIS WILL YIELD CONSERVA-
' TIVE (BUT UNREALISTICALLY HIGH) DOSE RATES AT THE CASK SURFACE.]
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END
```

Table S1.5.8 Annotated input for cases 20 and 21

```
#SAS1
CASES 20-21 (PREP) -- INFHOMMEDIA USED FOR X-SECT PROCESSING, COLLAPSE=NO
27N-18COUPLE  INFHOMMEDIA
'
' THE UO2 AND ZIRCALLOY VOLUME FRACTIONS PRESERVE THE AMOUNT OF FUEL ASSOCIATED
' WITH THE 264 FUEL PINS IN THE SPACE OCCUPIED BY A WESTINGHOUSE 17*17 ASSEMBLY
' (IN A 17*17 ASSEMBLY, ONLY 264 OF THE 289 AVAILABLE PIN POSITIONS ARE USED.)
' HERE, THE HOMOGENIZED FUEL (MIX 1) ALSO CONTAINS SOME SS304 REPRESENTING THE
' INTERNAL BASKET MATERIAL BETWEEN ASSEMBLIES.  NOTE THAT THIS DESCRIPTION OF
' MIX 1 IS THE SAME AS THAT USED FOR THE MATERIAL IN ZONES 1 & 3 OF THE 1-D
' RADIAL CALCULATIONS (SEE CASES [5] THROUGH [14]). FOR THE AXIAL CALCULATIONS,
' HOWEVER, THE FUEL SHOULD BE SMEARED OVER THE ENTIRE INNER VOLUME OF THE CASK
' CAVITY (I.E., OVER WHAT WERE ZONES 1-4 IN THE RADIAL MODEL). THIS ADDITIONAL
' DILUTION IS ACCOMPLISHED BELOW, BY USING THE MIXING OPTION IN THE ZONE
' DESCRIPTION DATA FOR THE AXIAL SHIELDING CALCULATION.
UO2  1  0.25553   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  1  0.08282  560  END
SS304   1  2.1375E-2   560  END
'
' MIX 2 IS AN HOMOGENIZED MODEL OF THE HARDWARE ON THE END OF THE ASSEMBLY:
SS304      2  4.8714E-2  END
ZIRCALLOY  2  1.2838E-2  END
'
' MIX 3 IS THE STAINLESS STEEL USED IN THE CASK LID
' MIX 4 IS THE U-METAL GAMMA SHIELD EMBEDDED WITHIN THE LID
' MIX 5 IS THE EXTERNAL SHOCK ABSORBER (BALSA WOOD) ON THE END OF THE CASK;
'  WHILE MIX 5 IS DEFINED HERE, IT IS ONLY USED IN SOME OF THE CASK MODELS.
SS304         3  END
U(.27)METAL   4  END
BALSA         5  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
END

CASE 20 -- INFHOMMEDIA X-SECTS; COLLAPSE=N; BUCKLED SLAB MODEL; WITH SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  TOGETHER, ZONES 1 & 2 REPRESENT THE FUEL ASSEMBLY (Z < 182.88 CM).
'  TWO ZONES WERE USED SO THAT THE SPATIAL MESH SIZE COULD BE VARIED.
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  THE "0  0.49811" INDICATES THAT AXIAL ZONES 1 & 2 CONTAIN 49.81 VOL% VOID
'  (MIX 0), PLUS 50.19 VOL% (=100-49.81) FUEL MIX 1.  SEE CASE [16] FOR
'  ADDITIONAL COMMENTS ON THIS AND THE SOURCE NORMALIZATION FACTOR (ZVOL).
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED TO
'  THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS REGION.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5  297.82  60  0
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE.  NOTE THAT SINCE THE COLLAPSE=Y OPTION WAS NOT
```

Table S1.5.8 (continued)

```
' USED, THE SPECTRUM WOULD HAVE TO BE INPUT USING THE 27N-18G FORMAT
' SHOWN IN CASE [1] -- NOT THE 15N-18G FORMAT SHOWN IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
' SINCE THE COLLAPSE=Y OPTION WAS NOT USED, THIS SPECTRUM MUST BE INPUT
' USING A 27N-18G FORMAT (NOT THE 15N-18G FORMAT SHOWN FOR CASES 16-20).
27Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' (1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION)
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC: .
73.22
END
LAST
CASE 21 -- INFHOMMEDIA X-SECTS; COLLAPSE=N; BUCKLED SLAB; WITHOUT SHOCK ABS
'
' NOTE THAT A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD TO BE PLACED
' BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD FOR THIS FINAL CASE
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  TOGETHER, ZONES 1 & 2 REPRESENT THE FUEL ASSEMBLY (Z < 182.88 CM).
'  TWO ZONES WERE USED SO THAT THE SPATIAL MESH SIZE COULD BE VARIED.
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  THE "0  0.49811" INDICATES THAT AXIAL ZONES 1 & 2 CONTAIN 49.81 VOL% VOID
'  (MIX 0), PLUS 50.19 VOL% (=100-49.81) FUEL MIX 1.  SEE CASE [16] FOR
'  ADDITIONAL COMMENTS ON THIS AND THE SOURCE NORMALIZATION FACTOR (ZVOL).
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED TO
'  THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS REGION.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  IF THE EXTERNAL AXIAL SHOCK ABSORBER WERE PRESENT IT WOULD BE NEXT.
'  IN THIS "ACCIDENT" SCENARIO, IT IS ASSUMED TO BE LOST OR DESTROYED.
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE.  NOTE THAT SINCE THE COLLAPSE=Y OPTION WAS NOT
' USED, THE SPECTRUM WOULD HAVE TO BE INPUT USING THE 27N-18G FORMAT
' SHOWN IN CASE [1] -- NOT THE 15N-18G FORMAT SHOWN IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
' SINCE THE COLLAPSE=Y OPTION WAS NOT USED, THIS SPECTRUM MUST BE INPUT
' USING A 27N-18G FORMAT (NOT THE 15N-18G FORMAT SHOWN FOR CASES 16-20).
27Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' (1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION)
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END
```

Table S1.5.9 Annotated input for cases 22-25

```
#SAS1
CASES 22-25 (PREP) -- INFHOMMEDIA USED FOR X-SECT PROCESSING, COLLAPSE=YES
27N-18COUPLE  INFHOMMEDIA
'
' THE UO2 AND ZIRCALLOY VOLUME FRACTIONS PRESERVE THE AMOUNT OF FUEL ASSOCIATED
' WITH THE 264 FUEL PINS IN THE SPACE OCCUPIED BY A WESTINGHOUSE 17*17 ASSEMBLY
' (IN A 17*17 ASSEMBLY, ONLY 264 OF THE 289 AVAILABLE PIN POSITIONS ARE USED.)
' HERE, THE HOMOGENIZED FUEL (MIX 1) ALSO CONTAINS SOME SS304 REPRESENTING THE
' INTERNAL BASKET MATERIAL BETWEEN ASSEMBLIES.  NOTE THAT THIS DESCRIPTION OF
' MIX 1 IS THE SAME AS THAT USED FOR THE MATERIAL IN ZONES 1 & 3 OF THE 1-D
' RADIAL CALCULATIONS (SEE CASES [5] THROUGH [14]). FOR THE AXIAL CALCULATIONS,
' HOWEVER, THE FUEL SHOULD BE SMEARED OVER THE ENTIRE INNER VOLUME OF THE CASK
' CAVITY (I.E., OVER WHAT WERE ZONES 1-4 IN THE RADIAL MODEL). THIS ADDITIONAL
' DILUTION IS ACCOMPLISHED BELOW, BY USING THE MIXING OPTION IN THE ZONE
' DESCRIPTION DATA FOR THE AXIAL SHIELDING CALCULATION.
UO2  1  0.25553   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
ZIRCALLOY  1  0.08282  560  END
SS304   1  2.1375E-2   560  END
'
' MIX 2 IS AN HOMOGENIZED MODEL OF THE HARDWARE ON THE END OF THE ASSEMBLY:
SS304      2  4.8714E-2  END
ZIRCALLOY  2  1.2838E-2  END
'
' MIX 3 IS THE STAINLESS STEEL USED IN THE CASK LID
' MIX 4 IS THE U-METAL GAMMA SHIELD EMBEDDED WITHIN THE LID
' MIX 5 IS THE EXTERNAL SHOCK ABSORBER (BALSA WOOD) ON THE END OF THE CASK;
'  WHILE MIX 5 IS DEFINED HERE, IT IS ONLY USED IN SOME OF THE CASK MODELS.
SS304        3  END
U(.27)METAL  4  END
BALSA        5  END
'
' THE KEYWORDS "END COMP" SHOULD BEGIN IN COLUMN 1:
END COMP
'
' TO COLLAPSE THE 27 NEUTRON GROUPS DOWN TO 15 GROUPS ENTER:
MORE DATA  COLLAPSE  END
'
END

CASE 22 -- INFHOMMEDIA X-SECTS; COLLAPSE=Y; BUCKLED SLAB MODEL; WITH SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
' FOR THE FOLLOWING SHIELDING CALCULATION.  THIS IS ALSO TRUE FOR ANY
' ADDITIONAL SHIELDING CALCULATIONS THAT FOLLOW THIS CASE.
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
'
' NOTES REGARDING THE DATA FOR ZONES 1 & 2:
' ----------------------------------------
'  TOGETHER, ZONES 1 & 2 REPRESENT THE TOP HALF OF THE FUEL ASSEMBLY.
'  TWO ZONES WERE USED HERE SO THAT A COARSE MESH OF ABOUT 2.74 CM
'  [=137.16/50] COULD BE USED IN THE LOWER REGION WHILE A FINER MESH OF
'  ABOUT 0.91 CM [=(182.88-137.16)/50] COULD BE USED NEAR THE TOP OF THE
'  ASSEMBLY WHERE THE FUEL ITSELF PROVIDES LESS SPATIAL SELF-SHIELDING.
'
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  ORIGEN SOURCE:  ON UNIT 60, 2-ND DECAY TIME IN FILE, ZVOL=2.60680E+6,
'  NO. OF FUEL ASSEMBLIES IN THESE FIRST TWO AXIAL ZONES (I.E. IN CASK)=7
'
'  IN THE RADIAL SHIELDING CALCULATIONS (CF. CASES [5] THROUGH [14]) THE
'  HOMOGENIZED FUEL REPRESENTED BY MIX 1 ABOVE WAS LOCATED IN RADIAL ZONES 1
'  (EXTENDING FROM R=0.0 CM TO R=12.75 CM) AND 3 (EXTENDING FROM R=21.72 CM TO
'  R=38.05 CM), WITH A VOID REGION [ZONE 4] EXTENDING FROM R=38.05 CM TO THE
'  INyER WALL OF THE CASK AT R=47.63 CM.  THE ACTUAL VOLUME FRACTION OF THIS
'  HOMOGENIZED FUEL MIXTURE INSIDE THE CASK IS THEREFORE GIVEN BY
```

Table S1.5.9 (continued)

```
'  VFMIX1=FVOL/ZVOL, WHERE
'
'  FVOL=  1.30834E+6 CC = PI*(12.75**2 + 38.05**2 - 21.72**2)*(2*182.88)
'  ZVOL = 2.60680E+6 CC = PI*(47.63**2)*(2*182.88)
'
'  THIS YIELDS VFMIX1=0.50189.  SINCE THE BORATED STEEL BETWEEN THE INNER AND
'  OUTER ROW OF ASSEMBLIES DOES NOT PROVIDE ANY SHIELDING IN THE AXIAL
'  DIRECTION, THE MATERIAL IN RADIAL ZONE 2 (LIKE RADIAL ZONE 4) SHOULD BE
'  TREATED AS A VOID.  THE EFFECTIVE VOLUME FRACTION OF THE VOID SPACE INSIDE
'  THE CASK CAVITY (I.E. THE SPACE NOT OCCUPIED BY MIX 1) IS THEN GIVEN BY
'  VFVOID = 1.0-VFMIX1 = 0.49811.  THE "0  0.49811" THEREFORE INDICATES THAT
'  AXIAL ZONES 1 & 2 CONTAIN 49.81 VOL% VOID (MIX 0), PLUS 50.19 VOL%
'  (=100-49.81) FUEL MIX 1. WHEN USING SOURCE TERMS & SPECTRA FROM AN ORIGEN
'  FILE (N/S/ASSY & PHOT/S/ASSY), THE SMEARED SOURCE VOL (ZVOL=2.60680E+6 CC)
'  MUST BE ENTERED SO THAT SAS1 PROPERLY NORMALIZES THE SOURCE PER UNIT VOLUME,
'  WHICH IS THEN USED IN THE XSDRNPM SHIELDING CALCULATION.  THE 7 INDICATES
'  THAT THIS SMEARED SOURCE VOLUME CONTAINS 7 FUEL ASSEMBLIES.
' ----------------------------------
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'
'
' HARDWARE ON THE END OF THE ASSEMBLY (ZONE 3):
' ------------------------------------------
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'
'  IN THIS CASE, XNN & XNG WOULD NORMALLY EQUAL THE NUMBER OF NEUTRONS/S/CC
'  IN THIS ZONE AND THE NUMBER OF PHOTONS/S/CC IN THIS ZONE.  WHEN BOTH ARE
'  SPECIFIED AS ZERO (AS SHOWN HERE), IT INDICATES THAT THE SOURCE SPECTRUM
'  ENTERED BELOW (AFTER THE ZONE DATA) HAS ALREADY BEEN NORMALIZED BY THE USER
'  TO THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS PARTICULAR
'  ZONE, AND THAT THIS SPECTRUM IS NOT TO BE RENORMALIZED BY THE CODE.
'
'  THE SPECTRUM REFERRED TO IN THIS CASE REPRESENTS THE ACTIVATION SOURCE IN
'  THE STEEL COMPONENTS AT THE END OF THE CASK.  FOR MANY 1-D AXIAL CALCULA-
'  TIONS, THE DOSE RATE DUE TO THIS ACTIVATION SOURCE IS NOT NEGLIGIBLE.
'
'  ACTUAL ACTIVATION SOURCE STRENGTHS (& SPECTRA) "PER MTIHM" OR "PER ASSEMBLY"
'  OR "PER KG OF HARDWARE" MAY BE OBTAINED FROM AN ORIGEN-S ANALYSIS.  THE
'  TOTAL VOLUMETRIC SOURCE TERMS (OR SPECTRA) WILL THEN HAVE TO BE NORMALIZED
'  BY THE USER TO ACCOUNT FOR THE AMOUNT OF ACTIVATED HARDWARE IN THIS PORTION
'  OF THE 1-D AXIAL MODEL OF THE PARTICULAR SHIPPING CASK.
' ----------------------------------
2  219.02  40  -2       0  0.0           0.0  0.0
'
'
'  VOID BETWEEN TOP OF ASSEMBLY AND INNER LID OF CASK (OCCUPIED
'  BY SMALL LOCKING DEVICES NOT INCLUDED IN THIS MODEL):
0  224.10   5  0
'
'  INNER PORTION OF CASK LID (SS304):
3  225.37   2  0
'
'  U-METAL GAMMA SHIELD IN CASK LID:
4  233.87  30  0
'
'  OUTER PORTION OF CASK LID (SS304):
3  237.82   6  0
'
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5 297.82  60  0
'
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
```

Table S1.5.9 (continued)

```
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15]. (NOTE THAT XNN & XNG
' ON THE ZONE 1 DESCRIPTION CARD FOR CASE [15] HAVE BEEN ADJUSTED
' FOR THE SMEARED FUEL VOLUME IN ZONE 1 OF THE 1-D AXIAL MODEL.)
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT.
' THIS 15N-18G SPECTRUM REPRESENTS THE ACTIVATION SOURCE IN
' THE HARDWARE NEAR THE END OF THE FUEL ASSEMBLY. BECAUSE OF
' THAT, THE SOURCE IS NON-ZERO IN ONLY TWO GAMMA ENERGY GROUPS.
' SUCH ACTIVATION DATA MAY BE OBTAINED FROM AN ORIGEN-S ANALYSIS.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' UNLIKE THE 1-D RADIAL CALCULATIONS WHERE THE BUCKLING CORRECTION
' GENERALLY MADE VERY LITTLE DIFFERENCE IN THE EXTERNAL DOSE RATE,
' THE 1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION
' IF THE CALCULATED DOSE RATES AT THE SURFACE ARE TO BE ANYWHERE
' CLOSE TO REALISTIC.  EVEN WITH A REALISTIC BUCKLING CORRECTION, ONE
' CAN GENERALLY ONLY GET WITHIN 10-50% OF THE CORRECT DOSE RATE USING
' A 1-D AXIAL MODEL.  WITHOUT A BUCKLING CORRECTION THE SAS1 RESULTS
' AT THE SURFACE MAY BE OFF BY AN ORDER OF MAGNITUDE.  SEE TABLE 7.4
' OF ORNL/CSD/TM-246 FOR MORE DETAILED COMPARISONS AGAINST 3-D MORSE
' MONTE CARLO RESULTS.
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END

CASE 23 -- INFHOMMEDIA X-SECTS; COLLAPSE=Y; BUCKLED SLAB; WITHOUT SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  TOGETHER, ZONES 1 & 2 REPRESENT THE FUEL ASSEMBLY (Z < 182.88 CM).
'  TWO ZONES WERE USED SO THAT THE SPATIAL MESH SIZE COULD BE VARIED.
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  FOR ADDITIONAL COMMENTS ABOUT DATA ON NEXT TWO CARDS, SEE CASE [22].
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED TO
'  THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS REGION.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  IF THE EXTERNAL AXIAL SHOCK ABSORBER WERE PRESENT IT WOULD BE NEXT.
'  IN THIS "ACCIDENT" SCENARIO, IT IS ASSUMED TO BE LOST OR DESTROYED.
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
```

Table S1.5.9 (continued)

```
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION:
' IN THIS CASE, DY & DZ ARE BOTH SET TO THE DIAMETER OF THE CASK.
' (1-D AXIAL CALCULATIONS GENERALLY REQUIRE A BUCKLING CORRECTION)
DY=146.44  DZ=146.44
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END

CASE 24 -- INFHOMMEDIA X-SECTS; COLLAPSE=Y; INFINITE SLAB MODEL; WITH SHOCK ABS
'
' NOTE THAT A BLANK LINE, OR A LINE WITH "LAST" TYPED IN COLUMNS 1-4,
' HAD TO BE PLACED BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  FOR ADDITIONAL COMMENTS ABOUT DATA ON NEXT TWO CARDS, SEE CASE [22].
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED TO
'  THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS REGION.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  EXTERNAL SHOCK ABSORBER ON END OF CASK (BALSA WOOD):
5 297.82  60  0
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION
' WOULD GO HERE IF USED. [SINCE THE TRANSVERSE DIMENSIONS (DY & DZ) ARE
' NOT SPECIFIED HERE, XSDRNPM WILL USE AN "INFINITE" SLAB MODEL WITH NO
' BUCKLING CORRECTION.  FOR 1-D AXIAL MODELS, THIS WILL YIELD CONSERVA-
' TIVE (BUT UNREALISTICALLY HIGH) DOSE RATES AT THE CASK SURFACE.]
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END
LAST
CASE 25 -- INFHOMMEDIA X-SECTS; COLLAPSE=Y; INFINITE SLAB; WITHOUT SHOCK ABS
'
' NOTE THAT A LINE WITH "LAST" TYPED IN COLUMNS 1-4, HAD TO BE PLACED
' BETWEEN THE PREVIOUS "END" CARD AND THE TITLE CARD FOR THIS FINAL CASE
'
DISC  REFLECTED
'
' DESCRIPTION OF EACH ZONE FOLLOWS:
' -------------------------------
'  THE +1 INDICATES THAT SOURCE SPECTRUM 1 COMES FROM AN ORIGEN-S FILE.
'  FOR ADDITIONAL COMMENTS ABOUT DATA ON NEXT TWO CARDS, SEE CASE [22].
1  137.16  50  +1       0  0.49811       60  2  2.60680E+6  7
1  182.88  50  +1       0  0.49811       60  2  2.60680E+6  7
```

Table S1.5.9 (continued)

```
'  THE -2 INDICATES THAT SOURCE SPECTRUM 2 IS ENTERED BELOW (AFTER ZONE DATA).
'  THE "0.0  0.0" INDICATES THAT SPECTRUM 2 HAS ALREADY BEEN NORMALIZED TO
'  THE CORRECT NUMBER OF NEUTRONS/S/CC AND PHOTONS/S/CC FOR THIS REGION.
2  219.02  40  -2       0  0.0           0.0  0.0
0  224.10   5   0
3  225.37   2   0
4  233.87  30   0
3  237.82   6   0
'  IF THE EXTERNAL AXIAL SHOCK ABSORBER WERE PRESENT IT WOULD BE NEXT.
'  IN THIS "ACCIDENT" SCENARIO, IT IS ASSUMED TO BE LOST OR DESTROYED.
'  NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' SOURCE SPECTRUM 1 IS BEING READ FROM AN ORIGEN-S FILE ON UNIT 60,
' THEREFORE WE DON'T NEED TO INPUT THAT DATA MANUALLY.  IF NEEDED,
' IT WOULD GO HERE, AS ILLUSTRATED IN CASE [15].
'
' SOURCE SPECTRUM 2 IS BEING ENTERED DIRECTLY AND GOES NEXT. THIS IS
' THE ACTIVATION SOURCE IN THE HARDWARE AT THE END OF THE ASSEMBLIES.
15Z  8Z  2.044E+6  1.094E+7  8Z
'
' OPTIONAL CONTROL PARAMETERS FOR THE XSDRNPM SHIELDING CALCULATION
' WOULD GO HERE IF USED. [SINCE THE TRANSVERSE DIMENSIONS (DY & DZ) ARE
' NOT SPECIFIED HERE, XSDRNPM WILL USE AN "INFINITE" SLAB MODEL WITH NO
' BUCKLING CORRECTION.  FOR 1-D AXIAL MODELS, THIS WILL YIELD CONSERVA-
' TIVE (BUT UNREALISTICALLY HIGH) DOSE RATES AT THE CASK SURFACE.]
'
READ XSDOSE
' ENTER RADIUS OF CASK USED BY THE XSDOSE CALC:
73.22
END
```

probability, and the moderating effect of adjacent materials may be represented in the Nordheim equation as a 1/E slowing-down source (unless one has specified no external moderator, as was the case here). With an infinite homogeneous media, the free-flight escape probability in the Nordheim equation is set to zero, and only the nuclides in the given material are assumed to have any moderating effect on the neutron spectrum used to weight the group-averaged, resonance self-shielded cross-section data. Because many neutron shielding materials do not contain resonance nuclides and because such shields tend to be many mean free paths thick, the infinite homogeneous media approximation is generally good if the final objective is to use the resulting cross-section data in a 1-D shielding analysis. Here, for example, cases 15, 16, and 22 all give identical results, cases 18 and 24 give identical results, cases 17 and 23 give identical results, and cases 19 and 25 give identical results (cf. Table S1.5.2).

The effect of collapsing the 13 thermal neutron groups in the 27n-18γ library down to one thermal sink group was also investigated (cf. cases 20 through 23). In all cases the external gamma and neutron dose rates appear to be unaffected, although that may not be the case if one had a strong thermal-neutron-absorbing/gamma-producing material like boron in the outer portion of the cask. It should be noted, however, that the 27n-18γ calculations ran 2.9 times longer than the collapsed 15n-18γ calculations.

Unlike the 1-D radial calculations where the buckling correction generally made very little difference in the external dose rate, the 1-D axial calculations generally require a buckling correction if the calculated dose rates at the surface are to be anywhere close to realistic. Even with a realistic buckling correction where DY and DZ are both set equal to the diameter of the cask, one can generally get only within 10 to 50% of the correct dose rate using a 1-D axial model. (See Table 7.4 of ref. 2 for more detailed comparisons against 3-D MORSE Monte Carlo results.) Without a buckling correction, however, the SS1 results at the surface may be off by an order of magnitude. Results for cases 16 and 18, or for cases 22 and 24 (cf. Table S1.5.2), show that the calculated neutron dose rate at the surface may vary from 15.28 to 132.0 mrem/h, depending on the buckling correction used in the XSDRNPM-S calculation, while the gamma dose rate may vary from 12.40 to 31.74 mrem/h. In addition to directly reducing the axial leakage of both neutrons and gammas, the transverse leakage also serves to reduce the subcritical neutron multiplication in the fueled portion of the cask. That, together with the longer mean free path of neutrons in the dry cask, causes the external neutron dose rate to be more sensitive to the buckling correction than the external gamma dose rates. In both cases, however, the axial representation of the cask as a series of 1-D slabs must be regarded as a very crude first-order geometric approximation, and the corresponding results should be treated accordingly. For more accurate results in the axial direction, one should use the multidimensional MORSE Monte Carlo code as embodied in the SAS4 control module (see Sect. S4).

S1.5.4 DISCUSSION OF THE COMBINED CRITICALITY/SHIELDING PROBLEM

Another sample problem, case 26, illustrates the application of the SAS1X capability to perform a combined 1-D criticality and shielding analysis by taking the leakage spectrum from an XSDRNPM criticality calculation and inputting it as a boundary source to subsequent shielding calculations. This problem models a sphere of homogenized fuel, clad, and moderator surrounded by 4.6 m (15 ft) of water. A critical radius search was performed with XSDRNPM in stand-alone mode to determine the critical size of the homogenized fuel/clad/moderator sphere surrounded by an infinite water reflector (30 cm). SAS1X was then used to analyze this problem. The criticality calculation in SAS1X modeled the homogenized fuel/clad/moderator sphere surrounded by 30 cm of water, identical to the XSDRNPM search case. The shielding case modeled the remainder of the 4.6 m (15 ft) of water surrounding the sphere. The SAS1X input deck for this case is presented in Table S1.5.10.

Table S1.5.10 Annotated input for case 26

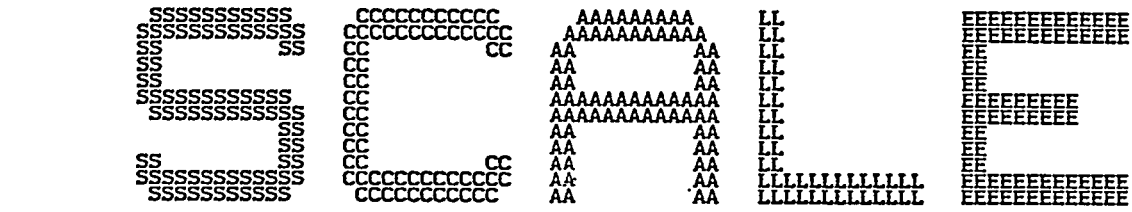
```
#SAS1X  PARM='SIZE=300000'
'
'THE SIZE PARAMETER MUST BE SPECIFIED BECAUSE OF THE LARGE NUMBER OF ZONES
'NECESSARY TO MODEL 15 FEET OF H2O REFLECTOR.
'
HOMOGENEOUS SPHERE OF FUEL, CLAD, & MODERATOR SURROUNDED BY 15 FT OF WATER.
27N-18COUPLE MULTIREGION
'
'MULTIREGION MUST BE SPECIFIED TO RUN COMBINED CRITICALITY/SHIELDING PROBLEM.
'
'MIX 1 IS THE HOMOGENIZED MIXTURE OF FUEL, CLAD, AND MOD
U-235   1  0  5.20215-4  END
U-238   1  0  3.77716-5  END
H       1  0  3.14930-2  END
O       1  0  1.72350-2  END

'MIX 2 IS THE WATER REFLECTOR FOR THE CRITICALITY CALCULATION
H2O    2  END
'
'MIX 3 IS THE WATER REFLECTOR FOR THE SHIELDING CALCULATION.
'THIS MUST BE A DIFFERENT MIXTURE THAN THE ONE USED IN THE CRITICALITY CALC,
'BECAUSE XSDRNPM PERFORMS CELL-WEIGHTING ON MIXTURES IN THE CRITICALITY CALC,
'AND SAS1X DOES NOT ALLOW THEIR USE IN THE SHIELDING CALCULATION.
'A TRACE OF ACTIVITIES IS INCLUDED IN ORDER TO OBTAIN THE CALCULATION OF
'ACTIVITIES FROM THE XSDRNPM SHIELDING CALCULATION.
H2O   3  END
ACTIVITIES 3 0  1.0E-24  END
END COMP
'
'THE CRITICALITY CALCULATION INPUT
SPHERICAL VACUUM END
1   18.5136
2   48.5136
 END ZONE
'ISN=16 IS SPECIFIED TO MATCH THE ANGULAR QUADRATURE IN THE SHIELDING CALC.
MORE DATA ISN=16  END MORE DATA
END
'
'THE SHIELDING CALCULATION INPUT
LAST
STORAGE POOL DOSE
SPHERICAL
'FIRST MIXTURE MUST BE VOID OF 1 INTERVAL WITH OUTER DIMENSION THAT MATCHES
'OUTER DIMENSION OF SHIELDING CALCULATION.
'FLAGS INDICATE BOUNDARY SOURCE WILL BE INPUT FROM XSDRNPM CRITICALITY CALC.
0  48.5136   1  1  0  0  0
3  475.71  427  0
 END ZONE
READ XSDOSE
END
```

S1.5.5 ILLUSTRATION OF OUTPUT

The SAS1X output for cases 1 and 2 is shown in Table S1.5.11, while the SAS1 output for cases 5 through 8 is shown in Table S1.5.12. These listings are limited to the output actually produced by the SAS1 control module with the PARM=CHK option (i.e., the XSDRNPM and XSDOSE output for each case is not listed). Annotated example output listings for XSDRNPM and XSDOSE may be found in Sects. F3.7 and F4.5, respectively. The bulk of the SAS1X or SAS1 output shown in Tables S1.5.11 and S1.5.12 is common to all control modules that use the SCALE Material Information Processor. Only the final subsections, labeled System Geometry" and "XSDOSE Data," are unique to the SAS1 control module and the 1-D shielding configuration specified by the user.

Table S1.5.11 SAS1X output for cases 1 and 2 with PARM=CHK



```
*********************************************************************************
*********************************************************************************
*********************************************************************************
*****                                                                       *****
*****                  PROGRAM VERIFICATION INFORMATION                     *****
*****                                                                       *****
*****                 CODE SYSTEM:    SCALE  VERSION:    4.1              *****
*****                                                                       *****
*********************************************************************************
*********************************************************************************
*****                                                                       *****
*****                                                                       *****
*****              PROGRAM:  SAS1X                                          *****
*****                                                                       *****
*****        CREATION DATE:  92.041                                         *****
*****                                                                       *****
*****              LIBRARY:  E.TZA27286.NEAD.PGMS77                         *****
*****                                                                       *****
*****                                                                       *****
*****      PRODUCTION CODE:  SAS1                                           *****
*****                                                                       *****
*****             REVISION:  1.6                                            *****
*****                                                                       *****
*****              JOBNAME:  USMSAS1X                                       *****
*****                                                                       *****
*****    DATE OF EXECUTION:  07/08/92                                       *****
*****                                                                       *****
*****    TIME OF EXECUTION:  15.02.00                                       *****
*****                                                                       *****
*****                                                                       *****
*********************************************************************************
*********************************************************************************
*********************************************************************************
```

Table S1.5.11 (continued)

```
CASES 1 & 2 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=NO

**** PROBLEM PARAMETERS ****

LIB  27N-18COUPLE LIBRARY
MXX             8 MIXTURES
MSC             9 COMPOSITION SPECIFICATIONS
IZM             3 MATERIAL ZONES
GE   LATTICECELL  GEOMETRY
MORE            0 0/1 DO NOT READ/READ OPTIONAL PARAMETER DATA
MSLN            0 FUEL SOLUTIONS

**** PROBLEM COMPOSITION DESCRIPTION ****

SC   UO2            STANDARD COMPOSITION
MX              1 MIXTURE NO.
VF         0.9017 VOLUME FRACTION
ROTH      10.9600 THEORETICAL DENSITY
TEMP       560.0 DEG KELVIN
            92234   0.03%
            92235   3.20%
            92236   0.02%
            92238  96.75%
END

SC   ZIRCALLOY     STANDARD COMPOSITION
MX              2 MIXTURE NO.
VF         1.0000 VOLUME FRACTION
ROTH       6.4400 THEORETICAL DENSITY
TEMP        560.0 DEG KELVIN
END

SC   SS304         STANDARD COMPOSITION
MX              3 MIXTURE NO.
VF         0.0217 VOLUME FRACTION
ROTH       7.9200 THEORETICAL DENSITY
END

SC   B4C           STANDARD COMPOSITION
MX              3 MIXTURE NO.
VF         0.0771 VOLUME FRACTION
ROTH       2.5200 THEORETICAL DENSITY
END

SC   SS304         STANDARD COMPOSITION
MX              4 MIXTURE NO.
VF         1.0000 VOLUME FRACTION
ROTH       7.9200 THEORETICAL DENSITY
END

SC   U(.27)METAL_  STANDARD COMPOSITION
MX              5 MIXTURE NO.
VF         1.0000 VOLUME FRACTION
ROTH      19.0500 THEORETICAL DENSITY
END

SC   H2O           STANDARD COMPOSITION
MX              6 MIXTURE NO.
VF         0.9440 VOLUME FRACTION
ROTH       0.9982 THEORETICAL DENSITY
END

SC   SS304         STANDARD COMPOSITION
MX              7 MIXTURE NO.
VF         0.1188 VOLUME FRACTION
ROTH       7.9200 THEORETICAL DENSITY
TEMP        560.0 DEG KELVIN
END

SC   N             STANDARD COMPOSITION
MX              8 MIXTURE NO.
VF         0.0012 VOLUME FRACTION
ROTH       1.0000 THEORETICAL DENSITY
TEMP        560.0 DEG KELVIN
END

**** PROBLEM GEOMETRY ****

CTP  SQUAREPITCH   CELL TYPE
PITCH      1.2598 CM CENTER TO CENTER SPACING
FUELOD     0.8357 CM FUEL DIAMETER OR SLAB THICKNESS
MFUEL           1 MIXTURE NO. OF FUEL
MMOD            8 MIXTURE NO. OF MODERATOR
CLADOD     0.9500 CM CLAD OUTER DIAMETER
MCLAD           2 MIXTURE NO. OF CLAD


ZONE SPECIFICATIONS FOR LATTICECELL GEOMETRY

                ZONE  1 IS FUEL
                ZONE  2 IS CLAD
                ZONE  3 IS MOD
```

```
CASES 1 & 2 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=NO

********** DATA LIBRARY INFORMATION **********

 UNIT NUMBER   DATA SET NAME                              VOLUME NAME   UNIT FUNCTION
 -----------   -------------                              -----------   -------------
      89       C.TZA27286.SCALE4.REV01.SCLIB              PSDE01        STANDARD COMPOSITION LIBRARY
      88       C.TZA27286.SCALE4.REV03.XN27G18            PSDE02        CROSS SECTION LIBRARY
      11       SYS92190.T150137.RA000.USMSAS1X.R0000012   SYSSA1        SHORT CROSS SECTION LIBRARY
      90       SYS92190.T150137.RA000.USMSAS1X.R0000021   SYSSA1        INPUT DATA DIRECT ACCESS

                          STANDARD COMPOSITION LIBRARY DATA

          UNIT NUMBER  :  89
          DATASET NAME :  C.TZA27286.SCALE4.REV01.SCLIB
          LIBRARY TITLE:  SCALE-4 STANDARD COMPOSITION LIBRARY
                          379 STANDARD COMPOSITIONS, 326 NUCLIDES
                          10 ELEMENTS WITH VARIABLE ISOTOPIC DISTRBUTIONS.
          CREATION DATE:  9/14/89

                            CROSS SECTION LIBRARY DATA

          UNIT NUMBER  :  88
          DATASET NAME :  C.TZA27286.SCALE4.REV03.XN27G18
          LIBRARY TITLE:  SCALE4 - 27 NEUTRON 18 GAMMA GROUP SHIELDING LIBRARY
                            BASED ON ENDF-B VERSION 4 DATA
                              COMPILED FOR NRC        1/27/89
                                LAST UPDATED          9/19/90
                                  L.M.PETRIE          ORNL

**** XSDRN MESH INTERVALS ****

  6 MESH INTERVALS IN ZONE  1
  4 MESH INTERVALS IN ZONE  2
  4 MESH INTERVALS IN ZONE  3
```

**** ADDITIONAL DATA ****

MIXING TABLE FROM STANDARD COMPOSITIONS DATA

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY	N.I.T. POINTER
1	92234	6.50065E-06	294
1	92235	7.14251E-04	295
5	592235	1.31783E-04	295
1	92236	3.55610E-06	296
1	92238	2.13233E-02	298
5	592238	4.80619E-02	298
1	8016	4.40952E-02	25
6	608016	3.15067E-02	25
2	40302	4.25156E-02	101
3	24304	3.78409E-04	47
4	424304	1.74286E-02	47
7	724304	2.07034E-03	47
3	25055	3.76992E-05	49
4	425055	1.73633E-03	49
7	725055	2.06259E-04	49
3	26304	1.28878E-03	52
4	426304	5.93579E-02	52
7	726304	7.05112E-03	52
3	28304	1.67633E-04	56
4	428304	7.72073E-03	56
7	728304	9.17146E-04	56
3	5010	1.67345E-03	19
3	5011	6.79370E-03	20
3	6012	2.11679E-03	21
6	1001	6.30133E-02	5
8	7014	5.24662E-05	23

COMPLETE MIXING TABLE

MIXTURE NO.	NUCLIDE NO.	ATOM DENSITY
1	92234	6.50065E-06
9	92234	2.24669E-06
1	92235	7.14251E-04
9	92235	2.46853E-04
5	592235	1.31783E-04
1	92236	3.55610E-06
9	92236	1.22903E-06
1	92238	2.13233E-02
9	92238	7.36956E-03
5	592238	4.80619E-02
1	8016	4.40952E-02
9	8016	1.52398E-02
6	608016	3.15067E-02
2	40302	4.25156E-02
9	40302	4.29267E-03
3	24304	3.78409E-04
4	424304	1.74286E-02
7	724304	2.07034E-03
3	25055	3.76992E-05
4	425055	1.73633E-03
7	725055	2.06259E-04
3	26304	1.28878E-03
4	426304	5.93579E-02
7	726304	7.05112E-03
3	28304	1.67633E-04
4	428304	7.72073E-03
7	728304	9.17146E-04
3	5010	1.67345E-03
3	5011	6.79370E-03
3	6012	2.11679E-03
6	1001	6.30133E-02
8	7014	5.24662E-05
9	7014	2.90360E-05

MMT	26	NUCLIDES FROM CROSS SECTION LIBRARY
IRES	10	RESONANCE NUCLIDES
IBL	1	LEFT BDY CONDITION 0/1/2/3 VACUUM/REFLECTED/PERIODIC/WHITE
IBR	3	RIGHT BDY CONDITION 0/1/2/3 VACUUM/REFLECTED/PERIODIC/WHITE
MS	26	ENTRIES IN THE MIXING TABLE
ISCT	3	ORDER OF SCATTERING
DY	0.0000	FIRST TRANSVERSE BUCKLING DIMENSION
DZ	0.0000	SECOND TRANSVERSE BUCKLING DIMENSION
VSC	0.0000	VOID STREAMING

Table S1.5.11 (continued)

RESONANCE DATA (3* ARRAY)

ID	TEMP	GEOM	LBAR	DANCOFF	INNER RAD.	NSUBO	ITA	M1	SIGMA1	IT1	M2	SIGMA2	IT2	LUMP VOL
92234	560.00	2	4.17850E-01	9.62085E-01	0.00000E+00	6.50065E-06	1	15.995	2.54370E+04	1	237.927	2.83849E+04	1	1.0000
92235	560.00	2	4.17850E-01	9.62085E-01	0.00000E+00	7.14251E-04	1	15.995	2.31511E+02	1	238.049	2.47936E+02	1	1.0000
592235	293.00	0	0.00000E+00	0.00000E+00	0.00000E+00	1.31783E-04	1	238.051	3.02705E+03	1	0.000	0.00000E+00	0	1.0000
92236	560.00	2	4.17850E-01	9.62085E-01	0.00000E+00	3.55610E-06	1	15.995	4.64995E+04	1	237.926	5.18970E+04	1	1.0000
92238	560.00	2	4.17850E-01	9.62085E-01	0.00000E+00	2.13233E-02	1	15.995	7.75476E+00	1	235.040	3.56663E-01	1	1.0000
592238	293.00	0	0.00000E+00	0.00000E+00	0.00000E+00	4.80619E-02	1	235.044	2.87904E-02	1	0.000	0.00000E+00	0	1.0000
40302	560.00	2	4.74980E-01	8.41087E-01	4.17850E-01	4.25156E-02	1	0.000	0.00000E+00	0	0.000	0.00000E+00	0	1.0000
25055	293.00	0	0.00000E+00	0.00000E+00	0.00000E+00	3.76992E-05	1	11.010	8.64998E+02	1	21.826	8.67379E+02	1	1.0000
425055	293.00	0	0.00000E+00	0.00000E+00	0.00000E+00	1.73633E-03	1	55.845	3.87325E+02	1	56.130	1.22934E+02	1	1.0000
725055	560.00	0	0.00000E+00	0.00000E+00	0.00000E+00	2.06259E-04	1	55.845	3.87325E+02	1	56.130	1.22934E+02	1	1.0000

NITAWL DATA

	NUCLIDE IDENTIFIER	THERMAL SCATTER TEMP.
1	92234	5.60000E+02
2	92235	5.60000E+02
3	592235	2.93000E+02
4	92236	5.60000E+02
5	92238	5.60000E+02
6	592238	2.93000E+02
7	8016	5.60000E+02
8	608016	2.93000E+02
9	40302	5.60000E+02
10	24304	2.93000E+02
11	424304	2.93000E+02
12	724304	5.60000E+02
13	25055	2.93000E+02
14	425055	2.93000E+02
15	725055	5.60000E+02
16	26304	2.93000E+02
17	426304	2.93000E+02
18	726304	5.60000E+02
19	28304	2.93000E+02
20	428304	2.93000E+02
21	728304	5.60000E+02
22	5010	2.93000E+02
23	5011	2.93000E+02
24	6012	2.93000E+02
25	1001	2.93000E+02
26	7014	5.60000E+02

CSAS(XSDRN) DATA

	ZONE BOUNDARIES	MIXTURE NUMBERS	SCATTER BY ZONE
1	0	1	3
2	4.17850E-01	2	3
3	4.74980E-01	8	3
4	7.10766E-01		

BONAMI DATA

	SIGMA H BY MIXTURE	TEMPERATURE BY MIXTURE
1	4.59691E-02	0
2	1.77062E-01	0
3	0	0
4	0	0
5	0	0
6	0	0
7	0	0
8	0	0

Table S1.5.11 (continued)

```
**** SYSTEM GEOMETRY ****
CASE 1 -- LATTICECELL X-SECT PROC, COLLAPSE=NO, SOURCE SPEC ENTERED BELOW
CS   CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER     1
MXZ           500 MIXTURE NO.
RZ          12.75 CM RIGHT BOUNDARY LOCATION
IMZ            20 MESH INTERVALS
ISZ            -1 SOURCE SPECTRUM NO.
MIXC            7 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.1799 VOLUME FRACTION FOR MIXC MATERIAL
XNN    5.9600E+02 NEUTRON SOURCE NORMALIZATION
XNG    2.5900E+10 GAMMA SOURCE NORMALIZATION

ZONE NUMBER     2
MXZ             3 MIXTURE NO.
RZ          21.72 CM RIGHT BOUNDARY LOCATION
IMZ             8 MESH INTERVALS

ZONE NUMBER     3
MXZ           500 MIXTURE NO.
RZ          38.05 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS
ISZ            -2 SOURCE SPECTRUM NO.
MIXC            7 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.1799 VOLUME FRACTION FOR MIXC MATERIAL
XNN    5.9600E+02 NEUTRON SOURCE NORMALIZATION
XNG    2.5900E+10 GAMMA SOURCE NORMALIZATION

ZONE NUMBER     4
MXZ             0 MIXTURE NO.
RZ          47.63 CM RIGHT BOUNDARY LOCATION
IMZ             5 MESH INTERVALS

ZONE NUMBER     5
MXZ             4 MIXTURE NO.
RZ          48.90 CM RIGHT BOUNDARY LOCATION
IMZ             2 MESH INTERVALS

ZONE NUMBER     6
MXZ             5 MIXTURE NO.
RZ          57.40 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS

ZONE NUMBER     7
MXZ             4 MIXTURE NO.
RZ          61.35 CM RIGHT BOUNDARY LOCATION
IMZ             6 MESH INTERVALS

ZONE NUMBER     8
MXZ             6 MIXTURE NO.
RZ          72.78 CM RIGHT BOUNDARY LOCATION
IMZ            16 MESH INTERVALS

ZONE NUMBER     9
MXZ             4 MIXTURE NO.
RZ          73.22 CM RIGHT BOUNDARY LOCATION
IMZ             1 MESH INTERVALS
' SOURCE FOR ZONE 1
   SOURCE SPECTRUM NO. -1 FROM CARDS
' SOURCE FOR ZONE 2
   SOURCE SPECTRUM NO. -2 FROM CARDS

   **** XSDOSE DATA ****
   NDETEC          0 NUMBER OF DETECTORS
                     (0 INDICATES DEFAULT DETECTOR LOCATIONS)
   NFACTR          0 NUMBER OF DOSE FACTOR ID NUMBERS
                     (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
   DIMEN1      73.22 PRIMARY DIMENSION, CM
   DIMEN2     595.64 SECONDARY DIMENSION,CM
   DOSE FACTOR ID NUMBERS 9029. 9504.

   DETECTOR NO.  1
   R= 7.3220E+01  Z= 2.9782E+02

   DETECTOR NO.  2
   R= 1.7322E+02  Z= 2.9782E+02

   DETECTOR NO.  3
```

Table S1.5.11 (continued)

```
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02

**** SYSTEM GEOMETRY ****

CASE 2 -- LATTICECELL X-SECT PROC, COLLAPSE=NO, SOURCE SPEC FROM ORIGEN-S FILE

CS   CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER     1
MXZ           500 MIXTURE NO.
RZ          12.75 CM RIGHT BOUNDARY LOCATION
IMZ            20 MESH INTERVALS
ISZ             1 SOURCE SPECTRUM NO.
MIXC            7 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.1799 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.8679E+05 ZONE VOLUME
NASS            1 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     2
MXZ             3 MIXTURE NO.
RZ          21.72 CM RIGHT BOUNDARY LOCATION
IMZ             8 MESH INTERVALS

ZONE NUMBER     3
MXZ           500 MIXTURE NO.
RZ          38.05 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS
ISZ             2 SOURCE SPECTRUM NO.
MIXC            7 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.1799 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.1215E+06 ZONE VOLUME
NASS            6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     4
MXZ             0 MIXTURE NO.
RZ          47.63 CM RIGHT BOUNDARY LOCATION
IMZ             5 MESH INTERVALS

ZONE NUMBER     5
MXZ             4 MIXTURE NO.
RZ          48.90 CM RIGHT BOUNDARY LOCATION
IMZ             2 MESH INTERVALS

ZONE NUMBER     6
MXZ             5 MIXTURE NO.
RZ          57.40 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS

ZONE NUMBER     7
MXZ             4 MIXTURE NO.
RZ          61.35 CM RIGHT BOUNDARY LOCATION
IMZ             6 MESH INTERVALS

ZONE NUMBER     8
MXZ             6 MIXTURE NO.
RZ          72.78 CM RIGHT BOUNDARY LOCATION
IMZ            16 MESH INTERVALS

ZONE NUMBER     9
MXZ             4 MIXTURE NO.
RZ          73.22 CM RIGHT BOUNDARY LOCATION
IMZ             1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

**** XSDOSE DATA ****

NDETEC          0 NUMBER OF DETECTORS
                  (0 INDICATES DEFAULT DETECTOR LOCATIONS)
NFACTR          0 NUMBER OF DOSE FACTOR ID NUMBERS
                  (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
DIMEN1      73.22 PRIMARY DIMENSION, CM
DIMEN2     595.64 SECONDARY DIMENSION,CM
DOSE FACTOR ID NUMBERS 9029. 9504.
```

Table S1.5.11 (continued)

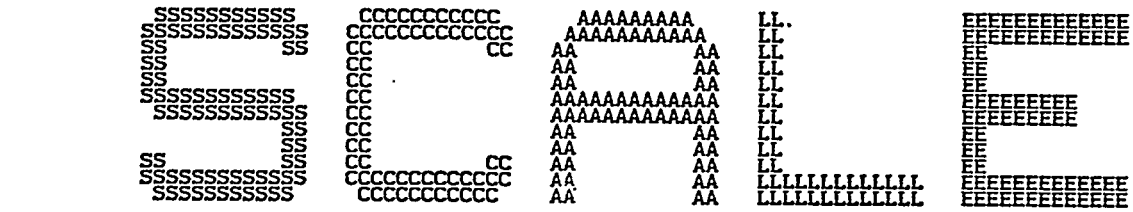
```
DETECTOR NO.  1
R= 7.3220E+01  Z= 2.9782E+02

DETECTOR NO.  2
R= 1.7322E+02  Z= 2.9782E+02

DETECTOR NO.  3
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02
```

Table S1.5.12 SAS1 output for cases 5-8 with PARM=CHK



```
PROGRAM VERIFICATION INFORMATION
CODE SYSTEM:    SCALE  VERSION:    4.1

PROGRAM:  SAS1
CREATION DATE:  92.041
LIBRARY:  E.TZA27286.NEAD.PGMS77

PRODUCTION CODE:  SAS1
REVISION:  1.6
JOBNAME:  USMSAS1F
DATE OF EXECUTION:  07/08/92
TIME OF EXECUTION:  15.09.56
```

Table S1.5.12 (continued)

```
CASES 5-8 (PREP) -- INFHOMMEDIUM USED FOR X-SECT PROCESSING, COLLAPSE=NO

**** PROBLEM PARAMETERS ****

LIB  27N-18COUPLE LIBRARY
MXX              6 MIXTURES
MSC              9 COMPOSITION SPECIFICATIONS
IZM              1 MATERIAL ZONES
GE   INFHOMMEDIUM GEOMETRY
MORE             0 0/1 DO NOT READ/READ OPTIONAL PARAMETER DATA
MSLN             0 FUEL SOLUTIONS

**** PROBLEM COMPOSITION DESCRIPTION ****

SC   UO2            STANDARD COMPOSITION
MX               1 MIXTURE NO.
VF          0.2555 VOLUME FRACTION
ROTH       10.9600 THEORETICAL DENSITY
TEMP         560.0 DEG KELVIN
             92234   0.03%
             92235   3.20%
             92236   0.02%
             92238  96.75%
END

SC   ZIRCALLOY     STANDARD COMPOSITION
MX               1 MIXTURE NO.
VF          0.0828 VOLUME FRACTION
ROTH        6.4400 THEORETICAL DENSITY
TEMP         560.0 DEG KELVIN
END

SC   SS304         STANDARD COMPOSITION
MX               1 MIXTURE NO.
VF          0.0214 VOLUME FRACTION
ROTH        7.9200 THEORETICAL DENSITY
TEMP         560.0 DEG KELVIN
END

SC   SS304         STANDARD COMPOSITION
MX               2 MIXTURE NO.
VF          0.0217 VOLUME FRACTION
ROTH        7.9200 THEORETICAL DENSITY
END

SC   B4C           STANDARD COMPOSITION
MX               2 MIXTURE NO.
VF          0.0771 VOLUME FRACTION
ROTH        2.5200 THEORETICAL DENSITY
END

SC   HE            STANDARD COMPOSITION
MX               3 MIXTURE NO.
VF          1.0000 VOLUME FRACTION
ROTH        1.0000 THEORETICAL DENSITY
END

SC   SS304         STANDARD COMPOSITION
MX               4 MIXTURE NO.
VF          1.0000 VOLUME FRACTION
ROTH        7.9200 THEORETICAL DENSITY
END

SC   U(.27)METAL   STANDARD COMPOSITION
MX               5 MIXTURE NO.
VF          1.0000 VOLUME FRACTION
ROTH       19.0500 THEORETICAL DENSITY
END

SC   H2O           STANDARD COMPOSITION
MX               6 MIXTURE NO.
VF          0.9440 VOLUME FRACTION
ROTH        0.9982 THEORETICAL DENSITY
END

**** PROBLEM GEOMETRY ****

**** INFINITE HOMOGENEOUS MEDIUM ****
MFUEL            1 MIXTURE NO. OF THE INFINITE HOMOGENEOUS MEDIUM
```

Table S1.5.12 (continued)

```
CASES 5-8 (PREP) -- INFHOMMEDIUM USED FOR X-SECT PROCESSING, COLLAPSE=NO

********** DATA LIBRARY INFORMATION **********

 UNIT
NUMBER        DATA SET NAME                                  VOLUME NAME   UNIT FUNCTION
------        -------------                                  -----------   -------------
  89    C.TZA27286.SCALE4.REV01.SCLIB                        PSDE01        STANDARD COMPOSITION LIBRARY
  88    C.TZA27286.SCALE4.REV03.XN27G18                      PSDE02        CROSS SECTION LIBRARY
  11    SYS92190.T150933.RA000.USMSAS1F.R0000012             SYSSA2        SHORT CROSS SECTION LIBRARY
  90    SYS92190.T150933.RA000.USMSAS1F.R0000021             SYSSA2        INPUT DATA DIRECT ACCESS

                        STANDARD COMPOSITION LIBRARY DATA
                        ---------------------------------

          UNIT NUMBER  :  89
          DATASET NAME :  C.TZA27286.SCALE4.REV01.SCLIB
          LIBRARY TITLE:  SCALE-4 STANDARD COMPOSITION LIBRARY
                          379 STANDARD COMPOSITIONS, 326 NUCLIDES
                          10 ELEMENTS WITH VARIABLE ISOTOPIC DISTRBUTIONS.
          CREATION DATE:   9/14/89

                           CROSS SECTION LIBRARY DATA
                           --------------------------

          UNIT NUMBER  :  88
          DATASET NAME :  C.TZA27286.SCALE4.REV03.XN27G18
          LIBRARY TITLE:  SCALE4 - 27 NEUTRON 18 GAMMA GROUP SHIELDING LIBRARY
                            BASED ON ENDF-B VERSION 4 DATA
                              COMPILED FOR NRC        1/27/89
                                LAST UPDATED          9/19/90
                                  L.M.PETRIE          ORNL
```

Table S1.5.12 (continued)

```
   **** ADDITIONAL DATA ****

MIXING TABLE FROM STANDARD COMPOSITIONS DATA

 MIXTURE    NUCLIDE       ATOM          N.I.T.
   NO.        NO.        DENSITY       POINTER
     1        92234   1.84216E-06          294
     1        92235   2.02405E-04          295
     5       592235   1.31783E-04          295
     1        92236   1.00773E-06          296
     1        92238   6.04260E-03          298
     5       592238   4.80619E-02          298
     1         8016   1.24957E-02           25
     6       608016   3.15067E-02           25
     1        40302   3.52114E-03          101
     1        24304   3.72536E-04           47
     2       224304   3.78409E-04           47
     4       424304   1.74286E-02           47
     1        25055   3.71141E-05           49
     2       225055   3.76992E-05           49
     4       425055   1.73633E-03           49
     1        26304   1.26877E-03           52
     2       226304   1.28878E-03           52
     4       426304   5.93579E-02           52
     1        28304   1.65031E-04           56
     2       228304   1.67633E-04           56
     4       428304   7.72073E-03           56
     2         5010   1.67345E-03           19
     2         5011   6.79370E-03           20
     2         6012   2.11679E-03           21
     3         2004   1.50456E-01           13
     6         1001   6.30133E-02            5

   COMPLETE MIXING TABLE

 MIXTURE    NUCLIDE       ATOM
   NO.        NO.        DENSITY
     1        92234   1.84216E-06
     1        92235   2.02405E-04
     5       592235   1.31783E-04
     1        92236   1.00773E-06
     1        92238   6.04260E-03
     5       592238   4.80619E-02
     1         8016   1.24957E-02
     6       608016   3.15067E-02
     1        40302   3.52114E-03
     1        24304   3.72536E-04
     2       224304   3.78409E-04
     4       424304   1.74286E-02
     1        25055   3.71141E-05
     2       225055   3.76992E-05
     4       425055   1.73633E-03
     1        26304   1.26877E-03
     2       226304   1.28878E-03
     4       426304   5.93579E-02
     1        28304   1.65031E-04
     2       228304   1.67633E-04
     4       428304   7.72073E-03
     2         5010   1.67345E-03
     2         5011   6.79370E-03
     2         6012   2.11679E-03
     3         2004   1.50456E-01
     6         1001   6.30133E-02


   MMT          26 NUCLIDES FROM CROSS SECTION LIBRARY
   IRES         10 RESONANCE NUCLIDES
   IBL           1 LEFT   BDY CONDITION 0/1/2/3 VACUUM/REFLECTED/PERIODIC/WHITE
   IBR           1 RIGHT BDY CONDITION 0/1/2/3 VACUUM/REFLECTED/PERIODIC/WHITE
   MS           26 ENTRIES IN THE MIXING TABLE
   ISCT          3 ORDER OF SCATTERING
   DY       0.0000 FIRST  TRANSVERSE BUCKLING DIMENSION
   DZ       0.0000 SECOND TRANSVERSE BUCKLING DIMENSION
   VSC      0.0000 VOID STREAMING

   RESONANCE DATA (3* ARRAY)

    ID   TEMP  GEOM   LBAR       DANCOFF    INNER RAD.   NSUB0      ITA  M1      SIGMA1      IT1  M2      SIGMA2      IT2 LUMP VOL
 92234 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 1.84216E-06   1  15.995 2.54370E+04   1 116.829 5.05486E+04   1   1.0000
 92235 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 2.02405E-04   1  15.995 2.31511E+02   1 115.481 4.49656E+02   1   1.0000
592235 293.00    0 0.00000E+00 0.00000E+00 0.00000E+00 1.31783E-04   1 238.051 3.02705E+03   1   0.000 0.00000E+00   0   1.0000
 92236 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 1.00773E-06   1  15.995 4.64995E+04   1 116.834 9.24129E+04   1   1.0000

 92238 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 6.04260E-03   1  15.995 7.75476E+00   1  73.123 7.11352E+00   1   1.0000
592238 293.00    0 0.00000E+00 0.00000E+00 0.00000E+00 4.80619E-02   1 235.044 2.87904E-02   1   0.000 0.00000E+00   0   1.0000
 40302 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 3.52114E-03   1  15.995 1.33079E+01   1 127.809 2.02510E+01   1   1.0000
 25055 560.00    0 0.00000E+00 0.00000E+00 0.00000E+00 3.71141E-05   1  15.995 1.26256E+03   1 116.926 2.50788E+03   1   1.0000
225055 293.00    0 0.00000E+00 0.00000E+00 0.00000E+00 3.76992E-05   1  11.010 8.64998E+02   1  21.826 8.67379E+02   1   1.0000
425055 293.00    0 0.00000E+00 0.00000E+00 0.00000E+00 1.73633E-03   1  55.845 3.87325E+02   1  56.130 1.22934E+02   1   1.0000
```

Table S1.5.12 (continued)

	NITAWL DATA		CSAS(XSDRN) DATA			BONAMI DATA	
	NUCLIDE IDENTIFIER	THERMAL SCATTER TEMP.	ZONE BOUNDARIES	MIXTURE NUMBERS	SCATTER BY ZONE	SIGMA H BY MIXTURE	TEMPERATURE BY MIXTURE
1	92234	5.60000E+02	0	1	3	0	0
2	92235	5.60000E+02	1.00000E+00			0	0
3	592235	2.93000E+02				0	0
4	92236	5.60000E+02				0	0
5	92238	5.60000E+02				0	0
6	592238	2.93000E+02				0	0
7	8016	5.60000E+02					
8	608016	2.93000E+02					
9	40302	5.60000E+02					
10	24304	5.60000E+02					
11	224304	2.93000E+02					
12	424304	2.93000E+02					
13	25055	5.60000E+02					
14	225055	2.93000E+02					
15	425055	2.93000E+02					
16	26304	5.60000E+02					
17	226304	2.93000E+02					
18	426304	2.93000E+02					
19	28304	5.60000E+02					
20	228304	2.93000E+02					
21	428304	2.93000E+02					
22	5010	2.93000E+02					
23	5011	2.93000E+02					
24	6012	2.93000E+02					
25	2004	2.93000E+02					
26	1001	2.93000E+02					

Table S1.5.12 (continued)

```
**** SYSTEM GEOMETRY ****
CASE 5 -- INFHOMMEDIUM X-SECTS; COLLAPSE=N; N-SHIELD PRESENT; ISN=16,ICM=4
CS   CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER     1
MXZ             1 MIXTURE NO.
RZ          12.75 CM RIGHT BOUNDARY LOCATION
IMZ            20 MESH INTERVALS
ISZ             1 SOURCE SPECTRUM NO.
MIXC            0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.8679E+05 ZONE VOLUME
NASS            1 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     2
MXZ             2 MIXTURE NO.
RZ          21.72 CM RIGHT BOUNDARY LOCATION
IMZ             8 MESH INTERVALS

ZONE NUMBER     3
MXZ             1 MIXTURE NO.
RZ          38.05 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS
ISZ             2 SOURCE SPECTRUM NO.
MIXC            0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.1215E+06 ZONE VOLUME
NASS            6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     4
MXZ             0 MIXTURE NO.
RZ          47.63 CM RIGHT BOUNDARY LOCATION
IMZ             5 MESH INTERVALS

ZONE NUMBER     5
MXZ             4 MIXTURE NO.
RZ          48.90 CM RIGHT BOUNDARY LOCATION
IMZ             2 MESH INTERVALS

ZONE NUMBER     6
MXZ             5 MIXTURE NO.
RZ          57.40 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS

ZONE NUMBER     7
MXZ             4 MIXTURE NO.
RZ          61.35 CM RIGHT BOUNDARY LOCATION
IMZ             6 MESH INTERVALS

ZONE NUMBER     8
MXZ             6 MIXTURE NO.
RZ          72.78 CM RIGHT BOUNDARY LOCATION
IMZ            16 MESH INTERVALS

ZONE NUMBER     9
MXZ             4 MIXTURE NO.
RZ          73.22 CM RIGHT BOUNDARY LOCATION
IMZ             1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

OPTIONAL PARAMETERS

ISN            16 ORDER OF ANGULAR QUADRATURE
ICM             4 OUTER ITERATION MAXIMUM
NDETEC          5 NUMBER OF DETECTORS
NFACTR          4 NUMBER OF DOSE FACTOR ID'S

**** XSDOSE DATA ****

NDETEC          5 NUMBER OF DETECTORS
                  (0 INDICATES DEFAULT DETECTOR LOCATIONS)
NFACTR          4 NUMBER OF DOSE FACTOR ID NUMBERS
                  (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
DIMEN1      73.22 PRIMARY DIMENSION, CM
DIMEN2     595.64 SECONDARY DIMENSION,CM
```

```
DOSE FACTOR ID NUMBERS 9029. 9504. 9027. 9503.

DETECTOR NO.  1
R= 7.3220E+01  Z= 2.9782E+02

DETECTOR NO.  2
R= 1.7322E+02  Z= 2.9782E+02

DETECTOR NO.  3
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02

DETECTOR NO.  5
R= 4.7322E+02  Z= 5.9564E+02

**** SYSTEM GEOMETRY ****

CASE 6 - INFHOMMEDIUM X-SECTS; COLLAPSE=N; N-SHIELD PRESENT; ISN=DEFAULT,ICM=10

CS   CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER      1
MXZ              1 MIXTURE NO.
RZ           12.75 CM RIGHT BOUNDARY LOCATION
IMZ             20 MESH INTERVALS
ISZ              1 SOURCE SPECTRUM NO.
MIXC             0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC         0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU            60 ORIGEN-S SOURCE UNIT NO.
NPOS             2 ORIGEN-S SOURCE POSITION
ZVOL    1.8679E+05 ZONE VOLUME
NASS             1 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER      2
MXZ              2 MIXTURE NO.
RZ           21.72 CM RIGHT BOUNDARY LOCATION
IMZ              8 MESH INTERVALS

ZONE NUMBER      3
MXZ              1 MIXTURE NO.
RZ           38.05 CM RIGHT BOUNDARY LOCATION
IMZ             30 MESH INTERVALS
ISZ              2 SOURCE SPECTRUM NO.
MIXC             0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC         0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU            60 ORIGEN-S SOURCE UNIT NO.
NPOS             2 ORIGEN-S SOURCE POSITION
ZVOL    1.1215E+06 ZONE VOLUME
NASS             6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER      4
MXZ              0 MIXTURE NO.
RZ           47.63 CM RIGHT BOUNDARY LOCATION
IMZ              5 MESH INTERVALS

ZONE NUMBER      5
MXZ              4 MIXTURE NO.
RZ           48.90 CM RIGHT BOUNDARY LOCATION
IMZ              2 MESH INTERVALS

ZONE NUMBER      6
MXZ              5 MIXTURE NO.
RZ           57.40 CM RIGHT BOUNDARY LOCATION
IMZ             30 MESH INTERVALS

ZONE NUMBER      7
MXZ              4 MIXTURE NO.
RZ           61.35 CM RIGHT BOUNDARY LOCATION
IMZ              6 MESH INTERVALS

ZONE NUMBER      8
MXZ              6 MIXTURE NO.
RZ           72.78 CM RIGHT BOUNDARY LOCATION
IMZ             16 MESH INTERVALS

ZONE NUMBER      9
MXZ              4 MIXTURE NO.
RZ           73.22 CM RIGHT BOUNDARY LOCATION
IMZ              1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

OPTIONAL PARAMETERS
```

Table S1.5.12 (continued)

```
ICM          10 OUTER ITERATION MAXIMUM

**** XSDOSE DATA ****
NDETEC        0 NUMBER OF DETECTORS
                (0 INDICATES DEFAULT DETECTOR LOCATIONS)
NFACTR        0 NUMBER OF DOSE FACTOR ID NUMBERS
                (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
DIMEN1     73.22 PRIMARY DIMENSION, CM
DIMEN2    595.64 SECONDARY DIMENSION,CM
DOSE FACTOR ID NUMBERS 9029. 9504.

DETECTOR NO.  1
R= 7.3220E+01  Z= 2.9782E+02

DETECTOR NO.  2
R= 1.7322E+02  Z= 2.9782E+02

DETECTOR NO.  3
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02

**** SYSTEM GEOMETRY ****
CASE 7 - INFHOMMEDIUM X-SECTS; COLLAPSE=N; NO N-SHIELD USED; ISN,ICM=DEFAULTS
CS   CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER     1
MXZ             1 MIXTURE NO.
RZ          12.75 CM RIGHT BOUNDARY LOCATION
IMZ            20 MESH INTERVALS
ISZ             1 SOURCE SPECTRUM NO.
MIXC            0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.8679E+05 ZONE VOLUME
NASS            1 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     2
MXZ             2 MIXTURE NO.
RZ          21.72 CM RIGHT BOUNDARY LOCATION
IMZ             8 MESH INTERVALS

ZONE NUMBER     3
MXZ             1 MIXTURE NO.
RZ          38.05 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS
ISZ             2 SOURCE SPECTRUM NO.
MIXC            0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   1.1215E+06 ZONE VOLUME
NASS            6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     4
MXZ             0 MIXTURE NO.
RZ          47.63 CM RIGHT BOUNDARY LOCATION
IMZ             5 MESH INTERVALS

ZONE NUMBER     5
MXZ             4 MIXTURE NO.
RZ          48.90 CM RIGHT BOUNDARY LOCATION
IMZ             2 MESH INTERVALS

ZONE NUMBER     6
MXZ             5 MIXTURE NO.
RZ          57.40 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS

ZONE NUMBER     7
MXZ             4 MIXTURE NO.
RZ          61.35 CM RIGHT BOUNDARY LOCATION
IMZ             6 MESH INTERVALS

ZONE NUMBER     8
MXZ             0 MIXTURE NO.
RZ          72.78 CM RIGHT BOUNDARY LOCATION
IMZ            16 MESH INTERVALS

ZONE NUMBER     9
MXZ             4 MIXTURE NO.
RZ          73.22 CM RIGHT BOUNDARY LOCATION
```

```
IMZ              1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

**** XSDOSE DATA ****

NDETEC           0 NUMBER OF DETECTORS
                   (0 INDICATES DEFAULT DETECTOR LOCATIONS)
NFACTR           0 NUMBER OF DOSE FACTOR ID NUMBERS
                   (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
DIMEN1       73.22 PRIMARY DIMENSION, CM
DIMEN2      595.64 SECONDARY DIMENSION,CM
DOSE FACTOR ID NUMBERS 9029. 9504.

DETECTOR NO.  1
R= 7.3220E+01  Z= 2.9782E+02

DETECTOR NO.  2
R= 1.7322E+02  Z= 2.9782E+02

DETECTOR NO.  3
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02

**** SYSTEM GEOMETRY ****

CASE 8 - INFHOMMEDIUM X-SECTS; COLLAPSE=N; NO N-SHIELD USED; ISN=DEFUALT,ICM=10

CS    CYLINDRICAL  COORDINATE SYSTEM

ZONE NUMBER      1
MXZ              1 MIXTURE NO.
RZ           12.75 CM RIGHT BOUNDARY LOCATION
IMZ             20 MESH INTERVALS
ISZ              1 SOURCE SPECTRUM NO.
MIXC             0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC         0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU            60 ORIGEN-S SOURCE UNIT NO.
NPOS             2 ORIGEN-S SOURCE POSITION
ZVOL    1.8679E+05 ZONE VOLUME
NASS             1 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER      2
MXZ              2 MIXTURE NO.
RZ           21.72 CM RIGHT BOUNDARY LOCATION
IMZ              8 MESH INTERVALS

ZONE NUMBER      3
MXZ              1 MIXTURE NO.
RZ           38.05 CM RIGHT BOUNDARY LOCATION
IMZ             30 MESH INTERVALS
ISZ              2 SOURCE SPECTRUM NO.
MIXC             0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC         0.0000 VOLUME FRACTION FOR MIXC MATERIAL
NSOU            60 ORIGEN-S SOURCE UNIT NO.
NPOS             2 ORIGEN-S SOURCE POSITION
ZVOL    1.1215E+06 ZONE VOLUME
NASS             6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER      4
MXZ              0 MIXTURE NO.
RZ           47.63 CM RIGHT BOUNDARY LOCATION
IMZ              5 MESH INTERVALS

ZONE NUMBER      5
MXZ              4 MIXTURE NO.
RZ           48.90 CM RIGHT BOUNDARY LOCATION
IMZ              2 MESH INTERVALS

ZONE NUMBER      6
MXZ              5 MIXTURE NO.
RZ           57.40 CM RIGHT BOUNDARY LOCATION
IMZ             30 MESH INTERVALS

ZONE NUMBER      7
MXZ              4 MIXTURE NO.
RZ           61.35 CM RIGHT BOUNDARY LOCATION
IMZ              6 MESH INTERVALS

ZONE NUMBER      8
MXZ              0 MIXTURE NO.
RZ           72.78 CM RIGHT BOUNDARY LOCATION
```

Table S1.5.12 (continued)

```
IMZ             16 MESH INTERVALS

ZONE NUMBER      9
MXZ               4 MIXTURE NO.
RZ            73.22 CM RIGHT BOUNDARY LOCATION
IMZ               1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.2 DAYS

OPTIONAL PARAMETERS

ICM           10 OUTER ITERATION MAXIMUM

**** XSDOSE DATA ****

NDETEC            0 NUMBER OF DETECTORS
                    (0 INDICATES DEFAULT DETECTOR LOCATIONS)
NFACTR            0 NUMBER OF DOSE FACTOR ID NUMBERS
                    (0 INDICATES DEFAULT ID FOR ANSI STANDARD)
DIMEN1       73.22 PRIMARY DIMENSION, CM
DIMEN2      595.64 SECONDARY DIMENSION,CM
DOSE FACTOR ID NUMBERS 9029. 9504.

DETECTOR NO.  1
R= 7.3220E+01  Z= 2.9782E+02

DETECTOR NO.  2
R= 1.7322E+02  Z= 2.9782E+02

DETECTOR NO.  3
R= 2.7322E+02  Z= 2.9782E+02

DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02
```

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Computing Applications Division

SAS2H: A COUPLED ONE-DIMENSIONAL DEPLETION AND SHIELDING ANALYSIS MODULE

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ABSTRACT

The SAS2 control module was originally developed for SCALE to provide a sequence that generated radiation source terms for spent fuel and subsequently utilized these sources within a one-dimensional (1-D) radial shielding analysis of a shipping cask. One of the principal uses of SAS2 over its history has been fuel depletion analyses to obtain radiation and heat generation sources and spent fuel isotopics to be used in subsequent analyses. This document describes the new, significantly enhanced version of the SAS2 control module which is denoted as SAS2H. For each time-dependent fuel composition, SAS2H performs 1-D neutron transport analyses (via XSDRNPM) of the reactor fuel assembly using a two-part procedure with two separate lattice-cell models. The first model is a unit fuel-pin cell from which cell-weighted cross sections are obtained. The second model represents a larger unit cell (e.g., an assembly) within an infinite lattice. The larger unit cell zones can be structured for different types of BWR or PWR assemblies containing water holes, burnable poison rods, gadolinium fuel rods, etc. The fuel neutron flux spectrum obtained from the second (large) unit cell model is used to determine the appropriate nuclide cross sections for the specified burnup-dependent fuel composition. The cross sections derived from a transport analysis at each time step are used in a point-depletion computation (via ORIGEN-S) that produces the burnup-dependent fuel composition to be used in the next spectrum calculation. This sequence is repeated over the operating history of the reactor. Optionally, a 1-D cask shielding analysis is performed after the depletion portion of the sequence is completed. This document presents input requirements, computational procedures, applications and uncertainties, subroutine descriptions, and sample problems for the SAS2H sequence.

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S2.1 INTRODUCTION

The Shielding Analysis Sequence No. 2 (SAS2) control module was originally developed for the SCALE code system to provide a sequence that generated radiation source terms for spent fuel and subsequently utilized these sources within a one-dimensional (1-D) shielding analysis of a shipping cask. Although the shielding portion of the sequence can still be optionally accessed, the principal use of SAS2 over its history has been fuel depletion analysis to obtain radiation sources, decay heat, and spent fuel isotopics. The sequence can be halted after the depletion/decay portion is complete. When calculation of radiation sources was the prime objective, a unit fuel-pin cell could be used to obtain the burnup-dependent flux spectrum necessary to prepare burnup-dependent cross sections during the reactor depletion analysis. This simple procedure has been shown to produce conservative actinide inventories for pressurized-water reactor (PWR) spent fuel and does not provide the flexibility required for depletion of boiling-water reactor (BWR) fuel. Thus, the original SAS2 sequence was considerably enhanced to produce the SCALE-4 version which is denoted SAS2H.

The criteria applied in developing SAS2 were the following:

1. to predict spent fuel characteristics for spent fuel assemblies having a specified reactor history;
2. to predict radiation dose rates for a radial model of a shipping cask containing spent fuel with the calculated characteristics;
3. to permit the user to supply a minimal quantity of input in the relatively convenient format of the SCALE system;
4. to apply standard analytical models that represent the physics of the system being analyzed (within the 1-D transport limits of the problem);
5. to apply acceptable and documented data bases that can be updated in the future; and
6. to automate the use of known methods of calculating some of the input parameters and the selection of appropriate control options for the various codes applied in the analysis.

Using a prescribed reactor history and cooling time, the SAS2H module is able to determine the spent fuel characteristics (isotopics, heat generation, and radiation sources) and then subsequently compute the neutron and gamma dose rates at various distances from a specified shipping cask. The fuel region in the cask may be either dry or filled with water. A 1-D transport treatment is applied in the burnup-dependent flux calculation of the fuel assembly and the shielding analysis of the shipping cask. A matrix exponential expansion model is used to solve the nuclide generation and depletion rate equations.

The neutron transport analysis of the reactor fuel assembly for each time-dependent fuel composition is basically a two-part procedure in which two separate unit-cell-lattice calculations are performed, determining the neutron spectrum and, subsequently, the nuclide cross sections. Even though the flux in the axial direction of the assembly is assumed to be constant, the two-part procedure more nearly characterizes the major two-dimensional (2-D) effects than the one-step procedure applied in the SCALE-3 version of SAS2. For example, in addition to simulating the fuel pins in the method used in earlier versions, the model may include either the guide tubes or burnable poison pins that may be a part of various types of assemblies. Also, the model description may contain the fuel-element casing and the channel moderator, which may significantly affect the flux, particularly in a BWR. At specified times during the burnup, the cross sections are updated using resonance processing codes and 1-D transport analyses. These updated cross sections are used in the depletion computation that produces the time-dependent fuel composition to be used for the next cross-section update. This sequence is repeated over the operating history of the reactor.

Nuclide compositions are computed for a specified reactor assembly, which is allowed to decay for a given cooling time after discharge. The subsequent gamma source includes radiation from fission products, activation products of both the fuel and structural materials, and (n,γ) reactions resulting from neutrons produced by some of the heavy isotopes. The neutron source includes neutrons from spontaneous fission and

isotopes. The final dose rates are calculated in the shielding analysis by applying these sources in a specific radial model of a shipping cask.

Only basic data are required to perform the SAS2 evaluation of a shipping cask. These data, briefly, include:

1. the material zone dimensions of the shipping cask, the fuel-pin cell, and the larger unit cell representation of the fuel assembly;
2. the material densities of the fresh fuel assembly and the shipping cask;
3. the material temperatures;
4. the specific power, exposure time and shutdown time of the fuel assembly in each appropriate cycle of the reactor history;
5. various control parameters used to select libraries, optional parameters preferred over the defaults, the level of printout, and modifications to the transport computations (e.g., the fineness of mesh intervals or the problem convergence criteria);
6. other optional data such as dose detector distances that differ from default values or light-element weights per assembly; and
7. an optional input method, where the shorter and easier input description of the larger unit cell normally supplied to SAS2H is replaced by user input of the actual data used by the codes (e.g., the 1$ or the 35* arrays in XSDRNPM, Sect. F3) in performing the second cell computation.

The SAS2 control module converts the user input to data required by the functional modules, which are used in the execution of the case. The SCALE system driver (reported in Sect. M1) invokes the execution of the various codes requested by SAS2 and then returns control to SAS2. Pertinent results computed by one functional module are used in generating input data for subsequent modules. Passes through the functional modules are repeated until the case is completed.

The model and the methods or techniques involved in the SAS2 control module are discussed in the following section. Then, the general structure and subroutine descriptions are presented. Finally, the input requirements are described, and sample cases are presented.

S2.2 METHOD AND TECHNIQUES

The method followed by SAS2 in performing the fuel depletion and analysis of a spent fuel shipping cask is presented here. The procedure, basically, is a combination of techniques by which data are prepared for the execution of the various SCALE functional modules required for the problem.

S2.2.1 OVERVIEW OF MODULES AND LIBRARIES

Six different codes plus several routines in the SCALE subroutine library are utilized by the SAS2 control module. The basic functions of the six functional modules, as applied by SAS2, are described below. References are given to sections in the SCALE manual or other reports that describe the codes in detail.

BONAMI applies the Bondarenko method of resonance self-shielding for nuclides that have Bondarenko data included with their cross sections. BONAMI is described in Sect. F1, and the Bondarenko methods and applicability are discussed in Sects. M7.2 and M7.A.

NITAWL-II performs the Nordheim resonance self-shielding corrections for nuclides that have resonance parameters included with their cross sections. NITAWL-II is described in Sect. F2, and the Nordheim Integral Treatment is also discussed in Sects. M7.2 and M7.A.

XSDRNPM performs a 1-D discrete-ordinates transport calculation based on various specified geometries requested in the data supplied by SAS2H. The code, as applied by SAS2H, has three particular functions:

1. to produce cell-weighted cross sections for fuel depletion calculations;
2. to determine cell-weighted cross sections for spent fuel assemblies in a specified shipping cask; and
3. to compute the angular flux data for the specified shipping cask, which are then applied by XSDOSE in computing dose rates.

XSDRNPM is described in Sect. F3 and Ref. 1. Also, the automatic quadrature generator, the unit cell mesh generator, and convergence criteria applied by the code are presented in Sect. M7.2.5.

COUPLE updates the cross-section constants included on an ORIGEN-S nuclear data library with data from the cell-weighted cross-section library produced by XSDRNPM. Also, the weighting spectrum computed by XSDRNPM is applied to update all nuclides in the ORIGEN-S library that were not specified in the XSDRNPM analysis. COUPLE is described in Sect. F6.

ORIGEN-S performs both nuclide generation and depletion calculations for the specified reactor fuel history. Also, the code computes the neutron and gamma sources generated by the fuel assembly. ORIGEN-S is described in Sect. F7.

XSDOSE applies the angular flux at the surface of a shipping cask, as produced by XSDRNPM-S, to compute dose rates at specified detector positions outside the shipping cask. XSDOSE is described in Sect. F4.

Other subroutine packages applied by SAS2 are

1. the SCALE Free-Form Reading Routines (Sect. M3);
2. the Material Information Processor of the SCALE system (Sect. M7); and
3. the SRCALC subroutine package for computing neutron sources. SRCALC is a separate utility code that has also been incorporated into ORIGEN-S. The routine was originally written for SAS2 (Sect. S2.2.7).

Data libraries that are utilized by SAS2 include:

1. SCALE Cross-Section Libraries (Sect. M4);
2. the SCALE Standard Composition Library (Sect. M8);

3. an ORIGEN-S Binary Working Library (Sects. M6.1.2 and M6.7); and
4. an ORIGEN-S Master Photon Binary Data Base (Sect. M6).

S2.2.2 GENERAL DESCRIPTION OF METHOD

Three areas require the knowledge and attention of cask shielding analysts—radiation source generation, radiation transport and dose evaluation, and proper utilization of cross-section data. Several different codes may be required to determine an adequate radiation source and subsequently calculate the required dose. The complexity of the radiation transport analysis that is applied can vary widely depending on the desired accuracy, the level of geometry detail to be included, and computer time limitations. The SAS2 control module provides an automated sequence to generate the radiation source, perform a 1-D radiation transport analysis through the side of a cask, and evaluate the dose at selected points away from the cask. The complete shielding analysis is performed with a single set of input specifications.

The method applied by SAS2 starts with the data describing a fuel assembly as it is initially loaded into a particular reactor. The composition, temperatures, geometry, and time-dependent specific power of the fuel assembly are required. For each time-dependent fuel composition, the new SAS2H sequence performs 1-D neutron transport analysis (via XSDRNPM) of the reactor fuel assembly using a two-part procedure with two separate unit-cell-lattice models. The first model is a unit fuel-pin cell from which cell-weighted cross sections are obtained. The second model represents a larger unit cell (e.g., an assembly) within an infinite lattice. The larger unit cell zones can be structured for different types of BWR or PWR assemblies containing water holes, burnable poison rods, gadolinium fuel rods, etc. Problem-dependent resonance self-shielding of the cross sections is performed using the BONAMI and NITAWL modules.

The neutron flux spectrum obtained from the second (large) unit cell model is used to determine the appropriate nuclide cross sections for the specified burnup-dependent fuel composition. The cross sections derived from a transport analysis at each time step are used in a point-depletion computation (via ORIGEN-S) that produces the burnup-dependent fuel compositions to be used in the next spectrum calculation. This sequence is repeated over the operating history of the reactor. Ultimately, the nuclide inventory (actinides, fission products, and light elements) is computed at the burnup corresponding to the discharge of the assembly from the reactor.

The buildup and decay of the nuclides in the fuel assemblies are subsequently computed by ORIGEN-S for the cooling time (from discharge) of interest for the assemblies. The gamma source spectrum, in the required energy group structure, is computed from photon-intensity data for nuclides present in the final compositions of the fuel, its activation products, the fission products, and the activation products of the clad and structural materials. Also, the neutron source spectrum, in the appropriate energy group structure, is derived from actinide nuclide data for neutron emission during spontaneous fission and neutron production by the interaction of alpha particles with the ^{17}O and ^{18}O atoms in the fuel. The heat generation rate (total and by nuclide) is also computed in the final ORIGEN-S case.

The shielding analysis of the shipping cask is performed in three parts. First, cell-weighted cross sections are computed for the fuel-pin lattice representation of the given assemblies, either moderated or dry, within the specified shipping cask. For a dry cask calculation, cell-weighting of the fuel cross sections is usually not necessary and can be optionally skipped in order to reduce the overall computing time requirements. Second, applying processed cross-section data of other zone materials in the shipping cask, together with the cell-weighted fuel cross sections and zone-averaged fixed sources of the fuel zone, angular neutron and photon fluxes are computed for the system. The use of coupled neutron-photon cross sections in the fixed-source transport calculation accounts for secondary gamma production during the radiation transport. Third, a multidimensional treatment is applied to the angular leakage fluxes to compute gamma and neutron dose rates at specified detector locations outside of the shipping cask.

The SAS2 module allows the following data sets to be saved: ORIGEN-S reactor cross-section libraries, unformatted nuclide concentrations and radiation sources, formatted nuclide atom densities and assembly sources, and case restart data. These data sets are used as interfaces to ORIGEN-S (Sect. F7),

PLORIGEN (Sect. F15), SAS1 (Sect. S1), SAS4 (Sect. S4), restarts of SAS2, and other codes. The data sets are described further in the input/output requirements of Sect. S2.5.5.

The above description is a brief summary of the entire SAS2H procedure. The following subsections S2.2.3-S2.2.9 discuss the various parts of the procedure in more detail.

S2.2.3 PREPARATION OF FUEL CROSS SECTIONS

The previous section provided a brief description of the entire SAS2H procedure. A diagram of the basic flow path invoked by SAS2H and the SCALE driver is shown in Fig. S2.2.1. Appropriate parameters are returned to the SCALE driver to properly invoke the functional modules in the SAS2H method. The upper part of Fig. S2.2.1 shows the basic flow for the neutronics-depletion analysis "passes" that create a cross-section library at specified burnup intervals. First, in path A, BONAMI, NITAWL-II, and XSDRNPM are invoked to produce the cell-weighted cross sections of the fuel zone. The second return to the driver for path B of the reactor pass invokes all five functional modules. The compositions for the first reactor library pass are simply the nuclide mixtures of the new, or freshly loaded, fuel assembly. After completing the neutronics code computations, execution continues with COUPLE updating an ORIGEN-S working library with data on the XSDRNPM weighted working library. The ORIGEN-S execution is invoked to compute the time-dependent densities of the nuclides in the fuel and burnable poison, if present, for the specified power and exposure times. Finally, SAS2 is invoked for the next control function in the procedure.

The neutronics models used in path A and path B of the computational flow are discussed below in Sect. S2.2.3.1. Then Sect. S2.2.3.2 provides more information on the procedures used to process data for the neutronics-depletion analysis.

S2.2.3.1 Description of the Neutronics Models

The flow chart of Fig. S2.2.1 indicates two computational paths (path A and path B) for the neutronics portion of the depletion analysis. Although the neutronics modules used in these sequential flow paths are similar (both access BONAMI/NITAWL/XSDRNPM), the models analyzed are quite different. The model used in path A is similar to that used in earlier SAS2 versions, through SCALE-3, inclusively. The addition of flow path B and its model produces the new version of SAS2 that is denoted SAS2H.

Basically, the model used in path A represents the fuel by an infinite lattice of fuel pins. Cross sections are processed using a resonance self-shielding calculation followed by a discrete-ordinates 1-D transport computation of the neutron flux in a unit cell with white boundary conditions. The cell-weighted cross sections produced by this path A model are then applied to the fuel region of the path B model. The model used in path B is a larger unit cell model used to represent part or all of an assembly. The concept of using cell-weighted data in the 1-D XSDRNPM analysis of path B is an approximate method for evaluating 2-D effects found in fuel-pin lattices containing different types of rods or water "holes." The path B model is used by SAS2H to calculate an "assembly-averaged" fuel region flux that considers the effects due to the path A model and channel moderation, if present.

The path B model represents a larger unit cell within an infinite lattice. Two examples of the larger unit cells are depicted in Fig. S2.2.2, where diagram (a) applies to a PWR control rod assembly and diagram (b) applies to a BWR burnable poison assembly. Variations to diagram (b) (e.g., omitting the casing and channel moderator) would apply to different types of BWR or PWR assemblies. The essential rule in deriving the zone radii is to maintain the relative volumes for all zones in the actual assembly. The control region of the larger cell can be modeled as an assembly guide tube, a burnable poison rod containing no fuel, an orifice rod, an axial peaking rod, a fuel rod containing a burnable poison, or almost any other pin-cell type rod. The moderator of the path A model is included with an outer radius equal to the unit cell radius. Then a fuel region surrounds the moderator with a radius that maintains volume conservation of fuel and moderator for the entire assembly. Also, the fuel assembly housing material, or casing, and channel moderator between assemblies may be added by conserving volumes. Assembly rod spacers and other hardware that may be

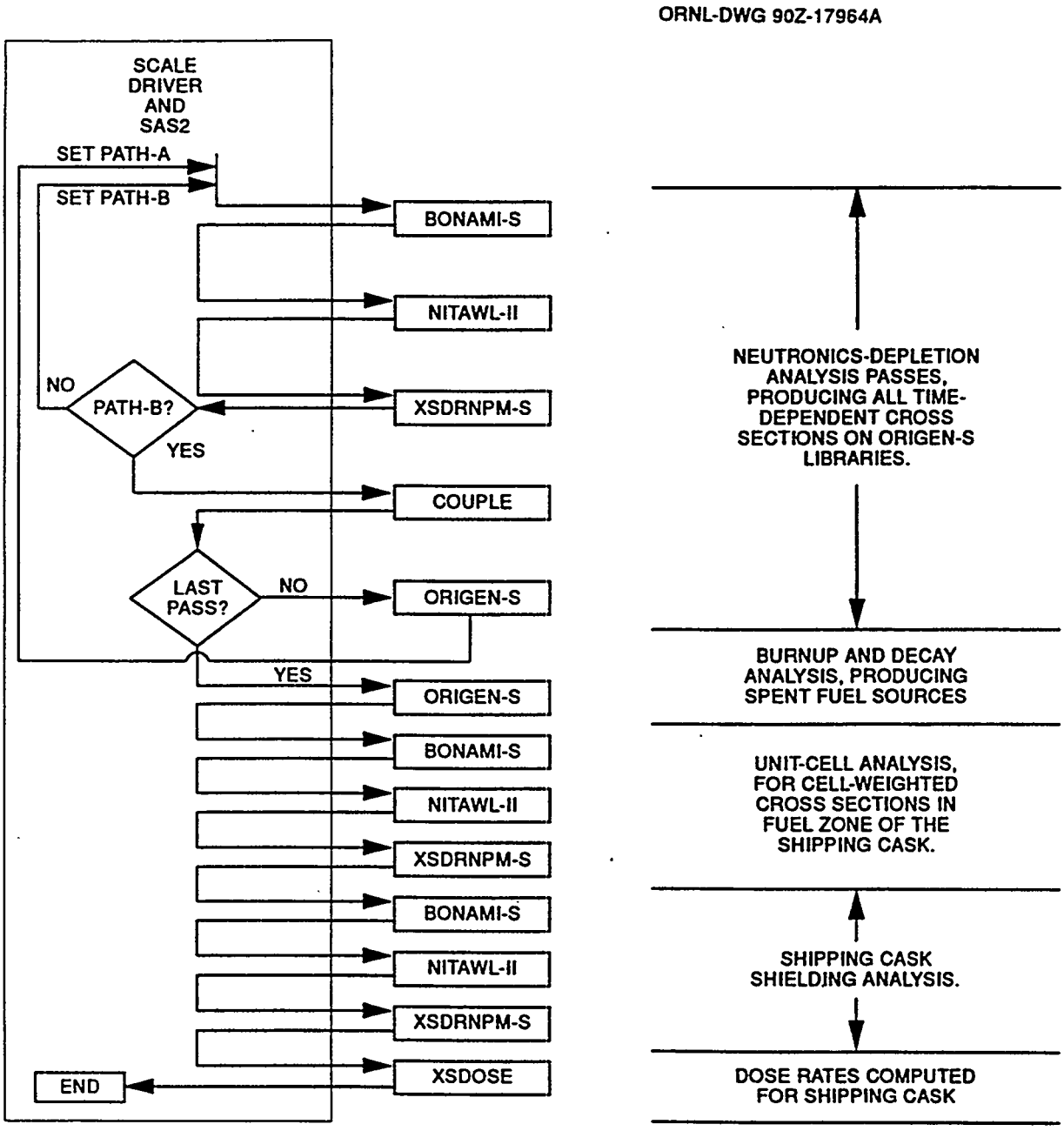

Figure S2.2.1. Computational flow chart for the SAS2H procedure

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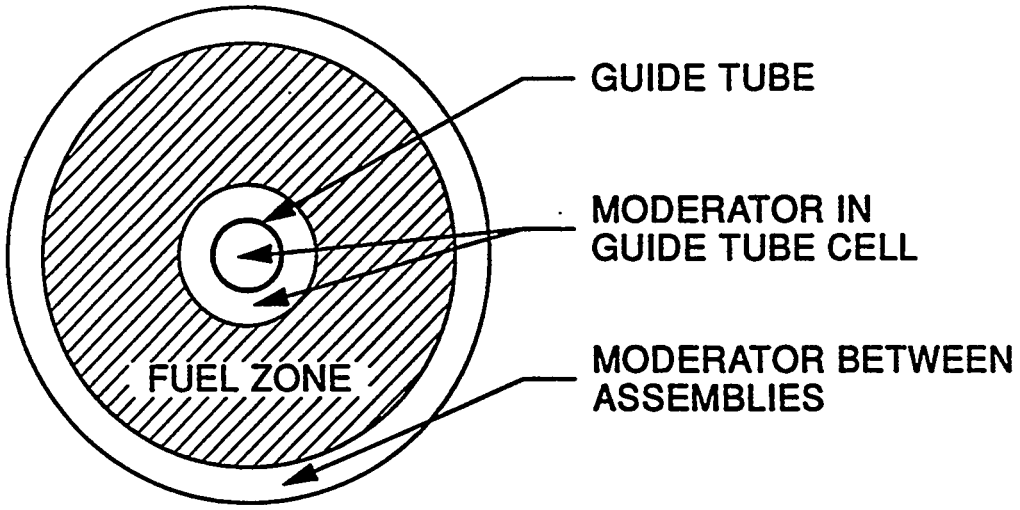
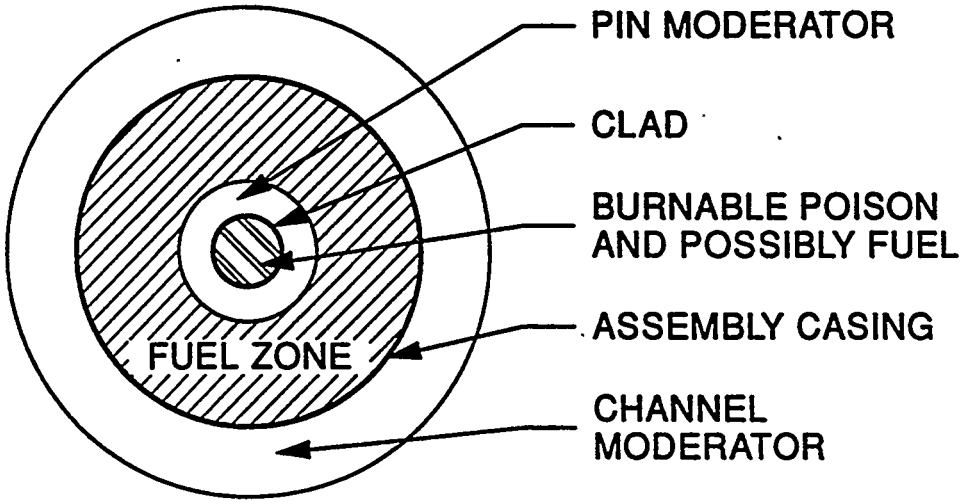


(a) FOR PWR CONTROL ROD ASSEMBLY, AFTER CONTROL RODS WITHDRAWN.



(b) FOR BWR BURNABLE POISON ASSEMBLY WITH LARGE CHANNEL ZONE.

Figure S2.2.2 Examples of larger unit cell for the model used in the path B portion of SAS2H

present are usually ignored. However, if their effects are estimated to be significant, they may be input by using zone average or effective densities.

Although there is a distinct improvement in the geometry applied by SAS2H over that of earlier versions, there still remain geometrical approximations. In designing assemblies there appears to be an attempt to have control rods or burnable poison pins separated at equal distances. But, in practice, these distances are not exactly equal, as assumed in the model. Also, when there is a channel moderator, the simulation places part of it as the outer zone of each larger unit cell (which may only represent a portion of the assembly) instead of placing all of it around the whole assembly. However, in either of these cases, the approximations in the placement of the moderator, burnable poison, or assembly casing appear to be significantly less than in models depicting those materials (with volume conservation) in an extra zone around each fuel-pin cell. In these cases, a neutron leaving a fuel pin may be scattered by the extra moderator before entering the adjacent cell, whereas in the SAS2H model and in actual assemblies the neutron would normally cross at least two fuel-pin cells before interacting with the extra moderator or poison.

S2.2.3.2 Data Processing Procedures

To prepare the fuel cross-section library for ORIGEN-S, the SAS2H sequence uses several SCALE functional modules. Fundamentally, the chief function of the SAS2 control module is to convert user input data, plus data available within the SCALE system into the input required by these functional modules and subsequently write the input on the interface units read by the codes. To assist in this process, SAS2H uses the Material Information Processor (see Sect. M7) and another neutronics data processor similar to the Material Information Processor.

Isotopic and other material densities, required by the codes, are prepared by the Material Information Processor from both the user input (e.g., volume fractions) and the contents of the Standard Composition Library. The mixture compositions of the reactor-loaded fuel assembly (i.e., fresh fuel isotopics) and the shipping cask materials are specified in the user input, representing a "total problem" composition description. The spent fuel composition is excluded, since it is computed in the SAS2H procedure. The first three input mixtures are used to describe the fuel-pin unit cell of the path A model, while all other mixtures apply to either the larger unit cell of the path B model or the shipping cask. This method produces a single "input mixing table." The term "mixing table" pertains to the grouping of composition data for nuclides into three corresponding sets that define the nuclide identification (ID) number, the mixture number, and the number density of the nuclide in the mixture. A "master mixing table" for the problem is derived from the input mixing table plus trace densities (1×10^{-20} atoms/b-cm) of those actinides that are both on the specified neutron cross-section library and in the Block Data list for the COMMON/FUELID/ (listed in Table S2.2.1). Trace amounts of these selected nuclides are automatically included by SAS2 to ensure appropriate cross sections are available for important nuclides that build up in the fuel during depletion. Additional trace nuclides can be input by the user.

For the fuel-pin cell model (path A of Fig. S2.2.1), the input data files for BONAMI, NITAWL-II, and XSDRNPM are prepared as described in Sect. M7. The cell-weighting option is used with the fuel-pin cell model to produce cross sections appropriate for the region denoted as the fuel zone in the larger unit cell of the path B model. The interface data sets for the three neutronics codes pertaining to the path B model are then developed by techniques that are either similar to those used for the fuel pin cell or, at least, reasonably appropriate for this type of analysis.

Two geometry-dependent parameters are computed by the Material Information Processor for the fuel-pin model of path A that are prepared differently by SAS2 for the larger unit cell model of path B. The first parameter is the effective escape cross-section input to account for heterogeneous effects in BONAMI (see Sect. F1.2.1). If the zone contains fuel and is the most central zone, the value is taken from the fuel zone of path A. If this is not true, the effective escape cross section is taken to be the reciprocal of the mean chord length for the zone or $0.5/(r_i - r_{i-1})$ for the i^{th} zone, where r_i are zone radii and $r_0 = 0$. The second parameter computed differently in the path B procedure is the Dancoff factor (see Sect. M7.2.5.3 for a definition)

Table S2.2.1 List of fuel nuclides automatically included by SAS2 for inclusion in neutronics processing[a] when on SCALE library

Xe-135	Pu-240
Cs-133	Pu-241
U-234	Pu-242
U-235	Am-241
U-236	Am-242m
U-238	Am-243
Np-237	Cm-242
Pu-238	Cm-243
Pu-239	Cm-244
	1/v-absorber[b]

[a]Unless overridden by user input, these nuclides are added to the initial fuel mixture with a number density of 10^{-20} atoms/b-cm.

[b]Used to calculate the THERM parameter applied in ORIGEN-S (see Sect. F7.6.12).

used in NITAWL-II for the resonance nuclides not in the fuel zone. If the zone is interior to the fuel zone, the contribution to the Dancoff correction from neutrons escaping outward from the zone is neglected since their probability of colliding or interacting with the large fuel zone is rather high. Thus, the Dancoff factor for resonance nuclides in a zone interior to the fuel zone is computed based on the volume-weighted nuclide densities in zones interior to the zone containing the resonance nuclide. For nuclides in zones exterior to the fuel zone, the Dancoff factor is not likely to affect final results and is set to zero. The path B model also uses the cell-weighted cross-section option and collapses the cross sections as required in updating an ORIGEN-S library.

After the neutronics code interfaces are completed, SAS2 generates interface files for codes that couple burnup-dependent densities into the model for producing time-dependent cross sections. First, an interface data set is produced for COUPLE, which updates cross-section constants on libraries input to ORIGEN-S. Finally, an input data set for ORIGEN-S is developed to execute a depletion case in which computed densities of the fuel are saved in a data set at prescribed time intervals. More about the meaning of these intervals will be discussed in the next section.

S2.2.4 FUEL IRRADIATION ANALYSIS TO PRODUCE TIME-DEPENDENT CROSS SECTIONS

The fuel cross sections vary with burnup because of the change in nuclide concentration and because of the resulting shift in the energy spectrum of the neutron flux. The neutronics-depletion procedure of Fig. S2.2.1, as discussed in Sect. S2.2.3, is applied repeatedly by SAS2H to produce cross-section libraries for the irradiation intervals requested in the input. This subsection discusses the "bootstrapping" method by which SAS2H repeatedly "passes" through the neutronics-depletion procedure. The major data differences for the sequential "passes" are in the nuclide densities and reactor history parameters. Note that each "pass" through the procedure involves (1) preparation of new data interfaces by SAS2, (2) return of control to the SCALE driver for execution of the three codes in the path A model, (3) SAS2 preparation of the code interfaces for the path B model, (4) another return to the SCALE driver for execution of the five codes in the path B model, and (5) return to SAS2.

The user input specifies the number of cycles (e.g., the number of years the assembly resides in the reactor), the number of libraries to make per cycle, the specific power in each cycle, and both the total

operation time and downtime of each cycle. Thus, the irradiation-time interval associated with each library is derived from the input. With the exception of the initial fresh-fuel library, each cross-section library is based on number densities obtained for the midpoint of the irradiation-time interval. The midpoint number densities for an irradiation interval are computed from an ORIGEN-S case that uses the library from the previous irradiation interval.

The procedure is illustrated schematically in Fig. S2.2.3 for a two-cycle case where two libraries per cycle are requested. The first step is to produce the "PASS 0" library prepared using the fresh-fuel isotopics. This initial library is used in the first ORIGEN-S case to generate number densities at the midpoint of the first irradiation interval. Next, the SAS2 module (1) computes density-dependent parameters for the resonance calculations, (2) increments the required data set unit numbers, (3) adds "PASS 1" to the ORIGEN-S library title, (4) updates the ORIGEN-S input for the second case to save number densities for the starting point and the midpoint of the second irradiation interval, and (5) rewrites all code interfaces using the new data. Then, the "PASS 1" library is produced by invoking execution of the five codes in both path A and path B of Fig. S2.2.1 a second time with the new input interfaces. Each additional pass applies the same procedure as used for "PASS 1." The midpoint densities are applied to the neutronics analysis to produce a new library. The depletion computation applies this library and the densities calculated for the start of the pass. A decay computation with zero power is applied for reactor downtime, if specified for the end of a cycle, before deriving densities for the next pass. All ORIGEN-S libraries are saved, starting with the "PASS 1" library. The last pass is the only one in which there is a major difference in the procedure. After the completion of COUPLE in the final pass, the required libraries have been produced. The final ORIGEN-S case corresponding to the last pass uses all the libraries and runs through the entire reactor history input the SAS2 module. This final case is described in detail in Sect. S2.2.5. Starting with SCALE 4.2, all the cross-section data libraries produced during all passes are combined into the final multi-burnup-dependent ORIGEN-S binary library made by the case.

The time-dependent number densities applied in the neutronics analysis are obtained by different methods. Number densities for the heavy nuclides of the fuel, together with their activation products and fission products, are all computed by ORIGEN-S. In addition, ORIGEN-S calculates the depletion of most light elements, including the burnable poisons boron, gadolinium, and cadmium, and most isotopes of the specified structural materials. However, the densities of alloys or elements in the clad, moderator, or structural materials, and oxygen in the fuel remain constant. The use of time-dependent densities for structural materials or clad light elements in place of constant densities is probably not very significant in the neutronics analysis of light-water reactors (LWRs), except for the isotopes of burnable poisons. In general, within a single subcase to ORIGEN-S, a depleted density may be computed for only one initial density of each nuclide. Thus, light-element nuclide depletion (typically of a burnable poison) is restricted to either those nuclides in mixtures outside of the fuel zone of the larger unit cell or those in the fuel and clad. Detailed selection conditions are presented in Data Note A of Sect. S2.5.4. Note two exceptions to the point-depletion limitation of ORIGEN-S within SAS2H concerning light-element (LE) nuclides. Some of the fission-product (FP) nuclides are on both the FP library and the LE library. Such a nuclide input as a trace in the fuel mixture is computed as being produced from fissioning for densities in the fuel. In the case where the fission-product nuclide is input in both the clad and the fuel, only the computation for production and depletion in the fuel is calculated, and the clad density is kept constant. The same nuclide (the FP in the fuel) input in a nonmoderator zone outside of the fuel zone of the path B model (see Fig. S2.2.2) may also undergo a LE depletion calculation. The other exception to the single depletion restriction concerns a LE nuclide (not in the FP library) contained in both the fuel and the clad. A single depletion of a properly combined density for the nuclide is applied by SAS2H to subsequently derive the individual depleted densities in both of the materials. Many of the LE depletion capabilities of SAS2H have a more significant value in certain product or research reactor designs rather than in the usual LWR designs.

The moderator (water) density does not change from the initial material specification unless requested by the user. The fraction of the first-cycle (initial material specification) density of the water or soluble boron may be specified by the user for each cycle. Also, the moderator boron concentration is automatically changed during the passes of a cycle, if more than one library per cycle is requested. The boron density is assumed to

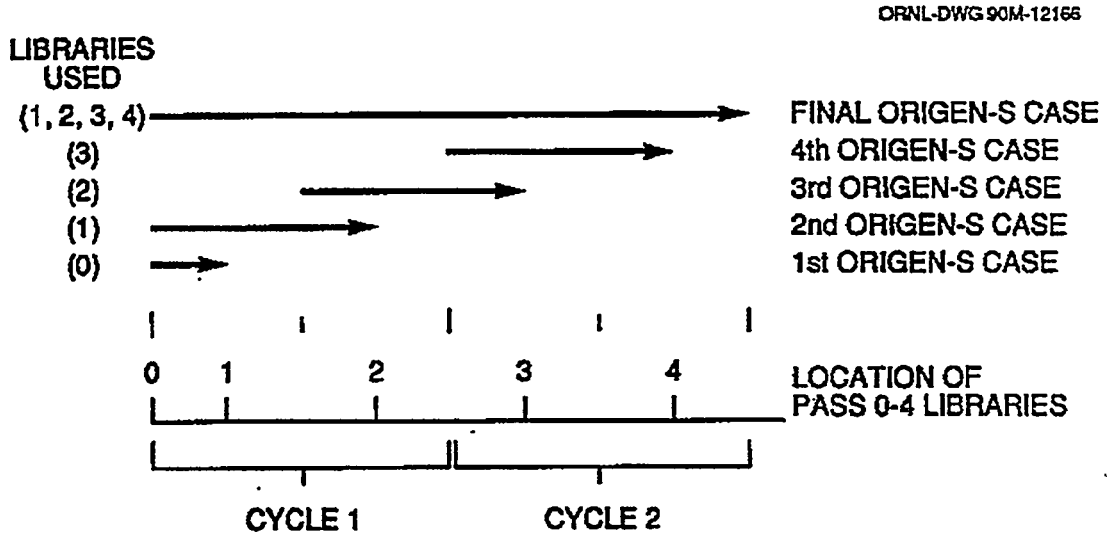


Figure S2.2.3 Schematic of successive ORIGEN-S cases used to produce the burnup-dependent number densities

vary linearly from 1.9 to 0.1 times its average (input) density during the time interval of the cycle. The value applied is determined from linear interpolation to the midpoints of each library time interval. This method is applied to somewhat approximate a typical decrease in the boron as a function of time for each cycle. Thus, if multiple libraries are requested per cycle, the user should ensure that the linear fit is appropriate for the cycle history. Alternatively, a user can increase the number of cycles requested, request only one library per cycle, and input a boron fraction that best models the actual amount of soluble boron in the reactor.

The pin-cell zone temperatures also may be changed at different cycles. Note that all temperatures are changed to the same value, which is input to BONAMI and NITAWL-II. This feature is not applicable to periods during normal reactor exposure operations. Usually the fuel temperature change is either small or none between cycles. However, SAS2 has been used to compute (via XSDRNPM) the infinite multiplication factor (k_∞) for cold spent fuel at various burnup or decay times by applying an irradiation pulse and reducing the system temperature.

S2.2.5 FINAL DEPLETION AND DECAY ANALYSES

The ORIGEN-S case in the final pass of the reactor irradiation period has a different function than that of previous passes. Prior to the final pass, the purpose of the neutronics depletion method was to produce a set of time-dependent cross-section ORIGEN-S working libraries that apply to the specified fuel assembly at various points during its irradiation history. Now, these libraries, which are ultimately combined into a multi-burnup-dependent ORIGEN-S binary library, and the initial nuclide densities form the input to the final ORIGEN-S depletion case. The user may observe from the SAS2 printout that densities in the previous ORIGEN-S cases are in atoms/b-cm, while the quantities input in the final case are given in total

grams per assembly. A short (zero time) decay subcase is applied, in order to list input grams, simply to aid as a problem definition check. During depletion calculations, ORIGEN-S prints results only in units of gram-atoms per fuel input (e.g., gram-atoms/assembly for the final SAS2 application).

A separate depletion subcase is performed, in turn, for each of the input ORIGEN-S working libraries. All the nuclides in the library on unit number 21 (the large ORIGEN-S binary library) are available in the analysis. These include over 1600 nuclides (for details see Sects. M6, F6.5, and F7.6.3). All chains are automatically provided in the library processing by ORIGEN-S and COUPLE. Cross-section constants are either updated directly from XSDRNPM output, or for those nuclides not included in the pin-cell analysis, from broad-group flux weight factors (Sects. F6.2.1 and F6.4.2).

First, in the procedure given here, the nuclide generation and depletion computation using the "PASS 1" library is performed. The first-cycle power and "PASS 1" time interval are applied. Four equal-size time steps are used during the irradiation time, followed by a single downtime interval. If no downtime was specified, a zero-time interval is applied. Next, a similar computation is performed using the compositions determined at the end of the "PASS 1" calculation and the cross-section data on the "PASS 2" library. The analysis proceeds with each succeeding library and corresponding assembly power and time interval. Ultimately, the discharge composition of the fuel assembly is determined. Finally, a decay-only subcase (six equal-size time steps) is computed for the requested spent fuel cooling time. These calculated compositions are applied in both the final shipping cask analysis and the determination of neutron and gamma sources.

The user may note that while light-element inventory in kilograms/assembly may be specified in the input description, there is no corresponding input for the fuel. In addition to standard composition and unit cell specification data, the number of fuel pins per assembly and the fuel length of the pins are the only fuel data required by SAS2. The code simply computes fresh-fuel nuclide inventories from this density and geometry data. The assembly light elements, converted to proper units, are applied in both the cross-section processing and the final ORIGEN-S cases. Their composition has a small effect upon the conversion of input power to the flux applied in the computation because ORIGEN-S uses a recoverable energy per fission that includes energy from the (n,γ) reactions for all specified nuclides. Also, the contribution to the gamma source by the light elements (e.g., cobalt) may be significant and is computed by ORIGEN-S. When an element or nuclide is input both as a standard composition specification and a light element in kilograms/assembly, the standard composition density is used only in the ORIGEN-S cases for cross-section processing, and the light-element data are used in the final ORIGEN-S case to derive final spent fuel results.

S2.2.6 THE GAMMA SOURCE SPECTRUM

The last subcase (decay portion) of the ORIGEN-S case described in Sect. S2.2.5 invokes the option for computing the gamma source spectrum of the spent fuel assembly. The spectrum is calculated for the photon energy group structure present on the cross-section library specified for use in the shipping cask shielding analysis.

The code first converts inventories of all nuclides of the cooled fuel assembly to disintegrations per second. Then, applying the ORNL Master Photon Data Base,[2] it sums individual nuclide photon spectra to determine the total gamma source spectrum. The intensity of a line at energy E, from the data base, is normalized to E_{ave}, the average energy of the group, using direct multiplication by the factor E/E_{ave}, with one exception. In cases where $E - E_1$ or $E_2 - E$ is less than 0.03 $(E_2 - E_1)$, where E_1 and E_2 are the boundaries of a group, one-half the initial intensity is applied to each of the two groups having the boundary near the line. These procedures maintain the conservation of energy rather than photon intensity, which should give a more correct computation of dose rates in the shielding analysis. As a final correction, the ratio of total nuclide gamma energy (from data in the ORIGEN-S working library) to the gamma energy of only those nuclides having line data, is multiplied times the spectrum computed from the data base. Later, the spectrum is converted to a uniform volumetric photon source for the shielding analysis.

The ORNL Master Photon Data Base[2] includes photon intensity and energy data for the following physical processes: X-rays and gamma rays emitted during radioactive decay of 427 nuclides, or more, taken

from the Evaluated Nuclear Structure Data File (ENSDF);[3-5] prompt fission gamma rays from spontaneous fission of heavy nuclides; gamma rays from the fission products produced in spontaneous fission; gamma rays from (α,n) reactions for heavy-metal dioxides; and bremsstrahlung production from beta and positron deceleration in UO_2 and water using beta energy data from ENSDF (see Sect. M6).

S2.2.7 THE NEUTRON SOURCE SPECTRUM

An energy-dependent neutron source is required for computing neutron dose rates in the shielding analysis. Since ORIGEN-S did not calculate neutron source spectra at the time SAS2 was written, the procedure for computing neutron spectra described here was developed for SAS2. Also, substantially improved spontaneous fission and (α,n) reaction yield data were applied. The data and method originally used in ORIGEN[6] overpredicted the (α,n) yields by a factor of approximately 2. Presently, the model described here is used in ORIGEN-S and supplied to SAS2, in place of making the calculation in SAS2.

The major part of the neutron source is produced from spontaneous fission of the heavy nuclides. Data required to compute the neutron production rate from this process include the spontaneous fission half-life, the average neutron yield per spontaneous fission, ν_{sf}, and the concentration for each contributing nuclide. Spontaneous fission half-lives for the more significant nuclides are those from the ORIGEN-S card-image actinide decay data library[7] (see ORIGEN-S Data Libraries, Sect. M6). For several less important nuclides, unmeasured half-lives are taken from Ref. 8. These data were estimated with a correlation between measured data and so-called fissility parameters.[9] The ν_{sf} data are taken from Ref. 8. Measured values are available for 21 nuclides, including the most significant. An equation, derived[8] to compute ν_{sf}, produces values which are within two experimental standard deviations for all except three nuclides. This equation is applied by the model for nuclides that do not have measured data.

A significant neutron source is produced from $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions in the UO_2 and other oxygen compounds of the spent fuel. Thin target cross sections[10] for these reactions and alpha stopping power data were applied to compute neutron yields of the fuel material. Measurements[10] of thin target cross sections for the $^{17}O(\alpha,n)$ and $^{18}O(\alpha,n)$ reactions produced improvement over earlier data.[11] Thick target energy-dependent (α,n) yields for $^{238}U^{NAT}O_2$ were computed,[10] having estimated accuracies within 10%. These data are applied by ORIGEN-S to the various alpha energies of the actinide nuclides. Although alpha energies are not explicitly given in the ORIGEN-S decay data base (Sect. M6), these data were derived from the same sources as those used to produce the decay data base. ENDF/B-VI data[12] were used for a large majority of the actinides. Evaluated Nuclear Structure Data File (ENSDF) data[3,4] were used, if available, for those not in ENDF/B-VI. Then, for the remaining actinides (of lesser significance), available alpha-energy data from the *Table of Radioactive Isotopes*[13] were applied. All the yields, energies, and associated data are edited during the execution of the neutron source option if the edit of the actinide library option is requested. These data, which are not contained in the ORIGEN-S library, are supplied in the Block Data COMMON/SPECDT/.

The isotopes ^{242}Cm and ^{244}Cm characteristically produce all except a few percent of the spontaneous fission and (α,n) neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the (α,n) reaction of alphas from ^{238}Pu, which is approximately 1 to 2% of the source. Neutron energy spectra of both the spontaneous fission and (α,n) reactions have been determined for the curium isotopes[14,15] and ^{238}Pu.[16] The measured spontaneous fission neutron spectrum of ^{244}Cm was found to be quite similar to that from ^{235}U and ^{252}Cf. Thus, the spectrum for ^{242}Cm was computed[15] from these measurements. The (α,n) neutron spectra were determined by extrapolating the neutron spectrum from Po-α-O source measurements[17] to the alpha energies of ^{242}Cm, ^{244}Cm, and ^{238}Pu. The energy distribution of the spontaneous fission neutron spectrum is computed from the spectra for ^{242}Cm and ^{244}Cm described above, using the calculated concentrations of those two isotopes. This spectrum is then renormalized to include the total neutron source from all spontaneously fissioning isotopes. A similar calculation, using the data for all three isotopes, is performed for the (α,n) neutron spectrum. The spectra are collapsed from the energy group structure of the data to that of the SCALE library requested for the shipping cask computation. The procedure assumes uniform distribution within each group and simply sums the quantities based upon energy

fractions common to both groups in the two group structures. The total neutron source spectrum is then computed as the sum of the spontaneous fission and (α,n) spectra.

Neutrons produced by photofission and photoneutron reactions are not included in the source term computed by SAS2. Cross sections for these reactions have been reported for several heavy nuclides[18] (e.g., ^{238}U) and for the light nuclides:[19] ^{2}H, ^{6}Li, ^{NAT}Li, ^{9}Be, and ^{13}C. The photon reaction energy thresholds in these data are 1.67 MeV for ^{9}Be, 2.23 MeV for ^{2}H, and approximately 5 MeV for the other nuclides. The gamma source energy range in spent fuel for significant intensities is 0 to 10 MeV, with only a somewhat minor fraction >5 MeV. Cross sections for the light nuclides are <2.5 millibarns for energies <10 MeV. Since the effective photoneutron cross sections (i.e., in the range 5 to 10 MeV) of nuclides of intermediate mass[20] are smaller than that of ^{238}U, relatively fewer neutrons would be produced from these nuclides. Calculations, applying the photon flux computed for typical PWR spent fuel, various time-dependent gamma sources derived by ORIGEN-S cases, and the referenced cross-section data, indicate the quantitative significance of the photon reactions. The contributions from photofission and photoneutron reactions with ^{238}U are approximately 0.1% of the neutron source at a 1-day cooling time, approximately 0.01% at 90 days, and less at later times. Calculations, considering masses equal to that of ^{238}U, produce comparable results for ^{6}Li and an appreciable decrease for ^{13}C. However, due to the quantity of photon emission in the 2.5- to 3.0-MeV range, sources from ^{2}H and ^{9}Be may require consideration. Approximately 1 kilogram of either of these two isotopes in the fuel region of the shipping cask may produce a significant part of the neutron source and dose rate. The evaluation of a dry shipping cask, where the neutron and gamma dose rates tend to be near the same magnitude, may require an additional analysis of photoneutrons if appreciable quantities of ^{2}H and ^{9}Be are present. One source of ^{2}H is the 0.015 atom % deuterium in natural hydrogen in the water coolant of various shipping casks. Fortunately, when the reduction in neutron dose from the effect of water is taken into account, the estimated ^{2}H neutron source fraction is <1% at 1-day cooling time and less significant at later times. However, SAS2 may not produce an adequate neutron source for systems containing large quantities of ^{9}Be intermixed with the fuel.

Given the concentrations of heavy-element nuclides in spent fuel, the major uncertainty in the computed neutron source strength is in the neutrons produced by spontaneous fission of ^{242}Cm and ^{244}Cm. The uncertainties in ν_{sf} for these isotopes is reported[8] to be 3 to 4% and the reported[7] uncertainty of the spontaneous fission half-life is 10% for ^{242}Cm and 0.1% for ^{244}Cm. Thus, over a 10-year cooling time the combined uncertainty in the computed neutron source from the spontaneous fission is in the range 4 to 8%, with a decrease as a function of time resulting from the 163-day half-life of ^{242}Cm. By considering the uncertainty of the thick target (α,n) yield data,[10] the possible error in applying $^{238}UO_2$ stopping powers for other nuclides of the spent fuel, and the fact that the computed (α,n) source is 10% of the total, it is estimated that the total neutron source has an additional uncertainty of about 2%. This total uncertainty (<10%) in the complete neutron source strength is less significant than inaccuracies arising from the neutron spectrum data, the concentration predictions and the neutronics analysis which are ultimately applied by SAS2 in computing the neutron dose rate.

S2.2.8 DOSE RATES FROM THE SHIELDING ANALYSIS OF THE SPENT FUEL SHIPPING CASK

Two additional passes through SAS2 are required after the final ORIGEN-S calculation is performed. These passes prepare data for the shielding analysis and the computation of dose rates outside the spent fuel shipping cask. The purpose of the first pass is the cell-weighted calculation of the fuel-pin lattice cross sections within fuel zones in the cask. During the second pass, the cross sections for other zones of the shipping cask are processed and the transport calculation for the entire shipping cask is performed to get the neutron and photon angular flux at the surface of the cask. Alternatively, the user can request the cell-weighting pass be skipped because the cell-weighting feature changes dose results insignificantly when used for a cask in which the fuel zones are dry. Finally, gamma and neutron dose rates are computed at either specified or default detector locations outside of the shipping cask.

The cell-weighted cross-section calculation is optionally provided for the user who desires to correct the spent fuel cross sections by a self-shielding resonance treatment and weight the cross sections in accordance with flux magnitudes of the unit-cell zones. SAS2 prepares the data similar to that used in the Path A model of the irradiation analysis. The fuel zone nuclide densities of the unit cell are those calculated by the last ORIGEN-S case (i.e., that of the cooled spent fuel). The moderator zone densities, for the cask cooled with water, are computed by using a routine from the LEOPARD code[21] and applying the user input temperature and pressure of the cask. The cask input temperature is also used to change the fuel temperature from that applied in the irradiation cases. The XSDRNPM-S case is supplied the following: the fixed gamma and neutron sources, buckling parameters for the cask fuel zone (the largest radius of multiple fuel zones), and print options or control parameters supplied by the user input. The SCALE library specified in the input may contain either neutron-photon or only neutron or photon cross sections, producing corresponding type dose rates. The BONAMI-S, NITAWL-II, and XSDRNPM-S functional modules are invoked by the driver during the pass to attain the final objective (i.e., the production of the cell-weighted working library).

During the final pass, SAS2 completes preparation of other data required for the shielding analysis. Important considerations here pertain to data describing both the materials and geometry of the shipping cask, and the type of cross-section treatments to apply for these materials. The convention used in SAS2 input assumes that standard compositions identified by mixture numbers >3 may apply to the shipping cask materials other than the fuel pin cell. (Note: the fuel assembly, as defined here, includes the moderator of the unit cell used in the optional cell-weighting case.) Other materials, such as the fuel basket and water between the assemblies, may be specified as extra material in a fuel zone. The user specifies the radial dimensions of all zones and the number of fuel assemblies per fuel zone. Then, SAS2 converts all unit-cell densities from the cell-weighted case to homogenized densities of a fuel zone by applying the conservation of mass. The source densities are similarly computed, conserving the total source. The light elements input for the depletion analysis by ORIGEN-S, other than that specified in mixtures 1 and 2 (e.g., O in UO_2 or Zr in clad), are not applied unless specified again with a mixture number >3. Thus, all densities are supplied from either the spent fuel composition computed by ORIGEN-S, or the master mixing table described in Sect. S2.2.3, and only nuclides in the mixing table are used. In addition to the mixing tables applied by the shielding analysis codes, other specifications are used as presented in the following paragraphs.

The BONAMI-S case applies an infinite homogeneous geometry in the treatment of nuclides having Bondarenko data with their cross sections. Material from all of the zones, except the cell-weighted nuclides, are considered.

The NITAWL-II case applies the infinite homogeneous medium Nordheim integral method, as required, for all materials not in a fuel zone. Any materials added to the cell-weighted nuclides of a fuel zone are considered for the resonance treatment in the analysis of a "dry" shipping cask. This resonance computation is omitted in the case of a "wet" cask, because the assumption that the water is homogeneous produces more unsatisfactory results than the application of the unprocessed cross sections of the nuclides (e.g., those of the fuel basket). Also, the NITAWL-II case merges the cross sections from the other zones with those that have been cell weighted, to produce the working library needed by XSDRNPM-S.

The XSDRNPM-S case performs the transport shielding analysis for the fixed volumetric sources and the multiregion geometry of the shipping cask. In addition to the application of data described above in this section, the spatial intervals of all zones are developed from the mesh generator discussed in Sect. S2.2.9. Since fission cross sections of fuel nuclides are supplied, both neutron multiplication and attenuation are computed. Secondary gamma production is computed from (n,γ) transfer data on the neutron-photon library applied. The attenuated neutron and photon flux is ultimately calculated, producing the angular flux at the shipping cask surface.

The final functional module executed in the last pass through SAS2 is XSDOSE. This module performs the required numerical integration of the angular flux over the finite surface of the cylindrical shipping cask to compute the scalar flux at specified detector locations. Flux-to-dose-rate conversion factors on the SCALE cross-section libraries are applied in the ultimate calculation of the desired gamma and neutron dose rates predicted for the case. The standard, or default conversion factors are those derived (in multigroup

format) from the American National Standard Institute Neutron and Gamma-Ray Flux-to-Dose-Rate Factors.[22] The dose rates that are automatically evaluated by SAS2 are at locations on the midplane of the shipping cask at distances of 0, 1, 2, and 4 m from the surface, unless specified differently in the user input.

S2.2.9 THE SHIELDING GEOMETRY MESH GENERATOR

The user input to SAS2 does not require mesh interval input for the Geometry of the problem. The automatic mesh generator derived (see Sect. M7.2.5.6) for the Material Information Processor is applied in all unit fuel cell calculations in SAS2. A modified version of this mesh generator, applied to the multiregion geometry in the shipping cask analysis, is described here.

Three additional considerations for the shielding analysis problems are

1. the application is for the treatment of both neutrons and photons,
2. the zones may be thick in comparison with mixture diffusion lengths, and
3. the uncollided flux tends to be reduced by the inverse square law.

The first parameters computed in the algorithm of the mesh generator are the total neutron cross sections of neutron shielding zones, Σ_T, the epithermal asymptotic diffusion lengths of neutrons within fuel zones, L, and an analogous variable for photons, L_g. The estimates of L and L_g for a mixture of K nuclides in the zone included by radii r_{i-1} and r_i are derived from:

$$(1/L)^2 = 3\,\Sigma_a\Sigma_t(1-\bar{\mu})(1-4\,\Sigma_a/5\Sigma_t)\ , \tag{S2.2.1}$$

$$1/L_g = \sum_{j=1}^{K}(10^{-10}M_j^5 + M_j/10)N_j\ , \tag{S2.2.2}$$

where,

j = nuclide identifier in the mixture of zone i,
Σ_a = macroscopic absorption cross section of zone i,
Σ_t = macroscopic total cross section in zone i,
$\bar{\mu}$ = average cosine of scattering angle per collision in zone i,
M_j = atomic mass of nuclide j,
N_j = atom density of nuclide j.

The method described here produces the smallest intervals near the inner boundary, with increasing sizes in the first one-fourth of the zone thickness. Then, equal size intervals are applied along the remainder of the radial distance across the zone, except that the outer two intervals are reduced to half the size.

The number of intervals, Y, in the first one-fourth of the zone of thickness, d, is computed from the following definitions and set of equations:

$a = 2L/d$
$b = 6L_g/d$
$Y_1 = [1+9/(10^a - 1]_{\text{truncated}}$ for inner zones including the outer fuel zone
$Y_1 = 0.5\,d\Sigma_t$, for zones beyond the fuel zone

$$Y_2 = [1+9/(10^b - 1)]_{\text{truncated}}$$
$$Y = \max(Y_1, Y_2) \qquad \text{(S2.2.3)}$$

For each zone, let r_n be mesh radii for $n = 1$ to Y and r_o be the inner radius of the zone. Then, r_n is the smaller of 1.14 r_{n-1} and that derived by

$$r_n = r_{n-1} + 0.25\, d \log_{10}[1 + 9(10Y - 9n)] \,. \qquad \text{(S2.2.4)}$$

A constant size interval, S, approximately equal to the maximum interval size computed by Eq. (S2.2.4), is determined by:

$$Z = [0.75\, d/(r_Y - r_{Y-1})]_{\text{truncated}}$$
$$S = 0.75\, d/Z. \qquad \text{(S2.2.5)}$$

All the mesh radii beyond the first one-fourth of a zone are computed from S, of Eq. (S2.2.5), except for the additional split in the last interval using S.

The mesh interval sizes may be changed from those generated by the above method, through the specification of SZFCASK in the user input. Sizes are approximately the value of SZFCASK times their default values, which are produced by SZFCASK= 1.

S2.3 APPLICATIONS, LIMITATIONS, AND UNCERTAINTIES

The SCALE-4 version of SAS2, referred to sometimes as SAS2H, has eliminated much of the conservatism inherent in earlier SAS2 versions, particularly, at long cooling times. Earlier SAS2 versions used an infinite lattice pin-cell model for the neutronics analysis and so only variations in lattice design and composition could be considered. With the SAS2H model, the presence of water holes, control rods, burnable poison rods, orifice tubes, and other assembly design features can be considered in an approximate fashion. This new capability allows actinide concentrations to be more accurately computed by the SAS2H procedure and, thus, leads to a more accurate evaluation of source terms and dose rates at long cooling times (>10 years) where actinide contributions are more important. However, the SAS2H procedure still requires only a relatively simple input description.

Even though numerous improvements have been made in the SAS2 control module, definite assumptions and limitations remain. The neutron flux and compositions are assumed to be constant in the axial direction of the assembly. Although this is a relatively small approximation in the PWR case, there is a large enough axial change in BWR fuel moderator density that a prior determination of a power-weighted moderator density is recommended. Other major limitations to the SAS2 module are in the final dose rate computations. Dose rates cannot be calculated for the ends of the cask or for any drain or instrumentation ports that may be included in a cask design. Techniques are available, however, for using ORIGEN-S and the neutronics modules in order to estimate the photon source in the assembly end fittings. These sources can subsequently be used in other shielding analysis codes (e.g., SAS4 sequence of SCALE) to obtain end dose rates.

Even though the end product from SAS2 is to compute shipping-cask dose rates, it has a much wider application. First, it has the capability of updating the cross-section constants on time-dependent ORIGEN-S libraries. Then, from these libraries, ORIGEN-S may compute nuclide inventories, cooling-time-dependent decay heat powers, neutron and gamma source strengths, and neutron and gamma source spectra. The intermediate results printed in the ORIGEN-S cases of SAS2 may be useful since the accuracies of the dose rates computed by SAS2 depend, in part, upon the accuracy of intermediate ORIGEN-S results.

The purpose of this section is to discuss the limitations and uncertainties in SAS2H as they affect the intermediate results (i.e., nuclide inventories, decay heat, etc.).

S2.3.1 NUCLIDE INVENTORIES

With the development of the SAS2H version in SCALE-4, the nuclide inventory comparisons with measurements referred[23] to in the SCALE-3 documentation of SAS2 no longer apply. Nuclide inventory results computed by SAS2H have been compared with measurements[24] and reported[25] for fuel rod sample D01-G10-4 irradiated in the Turkey Point Unit 3 (PWR) reactor. SAS2 versions from both SCALE-3 and SCALE-4 were used, and both cases applied the same SCALE ENDF/B-IV 27-group cross-section library. The differences of calculated minus measured values before and after the new SAS2H version changed from 3% to -5% for $^{235}U/^{238}U$, from 19% to 3% for $^{239}Pu/^{238}U$, and 13% to -1% for total $Pu/^{238}U$. Preliminary (unreported) cases, using the new version and the same libraries for comparisons with other spent fuel measurements, indicate less ^{235}U differences and either the same or slightly higher ^{239}Pu differences. Also, there were indications that changing to ENDF/B-V cross sections tend to reduce the computed ^{239}Pu inventory (approximately 4%).

The most important actinide nuclide for which inventories are computed, in regard to contribution to final dose rates, is ^{244}Cm. At cooling times of general interest (<20 years), the actinides contribute only a small fraction to the photon dose rates of typical casks. Of course, actinides produce all the neutron dose rates. The reduction in computed quantities of ^{244}Cm in changing to the SCALE-4 version has been at least as great as the decrease in Pu. Some calculations indicate that the SCALE-4 version with ENDF/B-IV data might even underpredict ^{244}Cm, although the evidence presently remains indefinite. Experimental errors in

^{244}Cm densities, when quoted, have always been at least ±20%. Thus, both the quantity and quality of ^{244}Cm experimental determinations limit the degree to which ^{244}Cm can be validated.

The effect of including additional fission products in the depletion analysis should be considered by the user. SAS2 input requires the composition of the initial fresh fuel. However, time-dependent cross sections are produced for only the fuel nuclides included in the input to the neutronics codes. Thus, in order to update cross sections for important nuclides that are generated during depletion but are not present in the initial composition, the trace density of 10^{-20} atoms/b-cm is usually included for each nuclide. The most significant actinides, together with ^{135}Xe and ^{133}Cs, are always added by the code (see Table S2.2.1). Also, the user may add other fission products included in the SCALE cross-section library. Since these nuclides are applied in the neutronics computation and influence the neutron flux, their inclusion in the case may somewhat change the calculated actinide inventories.

As discussed in Sect. S2.2.3, the SAS2H neutronics model attempts to provide a simple, yet accurate, model of the neutronic characteristics within a fuel assembly. Besides the geometry model, other simplifying approximations within SAS2H are

1. axial uniformity;
2. densities within the fuel pin are considered uniform with space;
3. a constant temperature is applied in each zone of the unit cell; and
4. a single fuel-pin unit cell type is assumed (i.e., all assembly pins are assumed to have a constant enrichment and pitch.

These simplifying approximations can somewhat affect the neutronics variables within fuel pins. In addition, the substantially different burnups and assembly enrichments that exist across a reactor core can influence the neutronic characteristics of a particular assembly. However, as noted above, preliminary validation of SAS2H against measured isotopic data indicates acceptable actinide inventories are obtained with SAS2H. To obtain more accurate results for actinide inventories in neutronically complex systems may require application of a multidimensional neutronics model. Even though the acceptability of actinide inventories computed by SAS2 depends upon both the reactor characteristics and the intended application, fission product inventories, with the exception of two or three important isotopes, are not significantly dependent upon cross-section calculations. The total fission product inventory computed for a given burnup is expected to be highly accurate, since it depends directly upon a relatively accurate calculation of removable energy per fission. Also, little difference in fission product inventory is expected in between the SCALE-3 and SCALE-4 versions of SAS2.

S2.3.2 DECAY HEAT POWERS

Next, consider decay heat power computed by ORIGEN-S and the SAS2H-produced libraries. The part of the power from actinides is 3 to 5% during the first 30 days of cooling time and increases to 15 to 25% at 10 years, for most LWR fuel after burnup exposure in the range of 25 to 50 GWd/MTU. Thus, the uncertainties in nuclide compositions of actinide nuclides convert to a much lower percentage of the total decay heat power. More uncertainty exists in fission-product power at discharge and immediately thereafter than at later cooling times. The 1σ uncertainty of fission product power at the later times, excluding that from ^{134}Cs, is estimated[23] to be approximately 3%. At cooling times where the actinide power is less than 10% of the total (i.e., cooling times less than 0.5 to 2 years for most cases,[23] the total decay heat power uncertainty is about 4.5%. There is an increase, thereafter, because the uncertainty in ^{244}Cm and other actinide inventories have an increased importance.

Relatively good agreement was indicated in comparisons of decay heat power computed by the SCALE-3 version of SAS2[23,26] and three measurements of reactor assemblies with cooling times near 2.5 years.[27] This older version of SAS2 overpredicted the power within 5.6%. Also, the total fission product power from ^{235}U and ^{239}Pu, excluding that resulting from (n,γ) reactions, was computed by both the earlier

SAS2/ORIGEN-S and the ANSI Standard[28] method. The maximum differences were 3.5% for ^{235}U and 2.6% for ^{239}Pu, with the larger values computed by the ANSI method. The data in the ANSI method were principally derived from ENDF/B-IV data, and that for the SAS2/ORIGEN-S method were primarily from ENSDF[2,3] data. The average beta energy is derived from a more accurate method[29] for ENSDF data than that applied[30,31] for ENDF/B-IV data, which accounts for a major part of the differences.

With the availability of additional calorimetric measurements of spent fuel assembly heat rates, a more thorough validation of the calculated decay heat power has been performed[32] for the new SAS2H version within SCALE-4. In this study, calculated and measured results were compared for ten PWR and ten BWR spent fuel assemblies. The fuel was from three reactors: Point Beach Unit 2 PWR, Turkey Point Unit 3 PWR, and Cooper Nuclear Station BWR. A summary of percentage differences in comparisons of measured and calculated spent fuel decay heat rates for all cases and assemblies is presented in Table S2.3.1. The average heat rate computed was less than the measured for the BWR assemblies, and the opposite was true for the PWR assemblies. The final average difference for all 20 spent fuel assemblies was 0.4 ± 1.4%. At a confidence level associated with two standard deviations, the percentage differences lie in the range -2.4 to 3.2%. Thus, at the 2σ confidence level and for the design and operating parameters of the given assemblies, the nonconservative (negative decay heat) error in computed decay heat rates does not exceed 2.4% plus any nonconservative bias in the measurements. Detailed results and discussion on the measured and calculated decay heat rates are presented in Ref. 32.

Table S2.3.1 Summary of decay heat rate comparisons

Type of summary	Number	% difference[a] ± std dev
Summary by cases:		
Average Point Beach case	6	3.6 ± 2.3
Average Turkey Point case	8	0.1 ± 1.3
Average PWR case	14	2.1 ± 1.4
Average BWR case	25	-1.4 ± 1.7
Average PWR and BWR av-case		0.3 ± 1.1
Summary by assemblies:		
Average Point Beach assembly	6	3.0 ± 1.9
Average Turkey Point assembly	4	-0.7 ± 1.7
Average PWR assembly	10	1.5 ± 1.3
Average BWR assembly	10	-0.7 ± 2.6
Final average, all assemblies	20	0.4 ± 1.4

[a](Calculated/measured - 1)100%.

S2.3.3 GAMMA SOURCE SPECTRA

The accuracy of gamma source spectra is dependent upon the energy. Photon rates computed for fission products tend to be more accurate than those for actinides, since the calculation of their inventories have less uncertainty. Even though the uncertainty of fission product photon rates of some groups may be comparable with that of their decay heat power, there could be a tendency for the spectra uncertainties to be somewhat greater because when fewer nuclides dominate the emission for the energy group, it becomes less likely that opposite biases in data will have a cancellation effect. Note that shortly after discharge and thereafter, the photon emission rates in the higher energy range are dominated by actinides. Typically, this

is true at energies above 4 MeV at all cooling times and at energies above 3.5 MeV after 10 years. The major part of this higher range of the spectrum is contributed by ^{244}Cm after 90 days and at least 90% appears to be from ^{244}Cm during the range of 10 to 50 years cooling time.[23]

Because there is a significant uncertainty in the measured ^{244}Cm in spent fuel, there is a correspondingly large uncertainty in the higher energy groups of the gamma spectra. Fortunately, for spent fuel there is a reduction by many orders of magnitude in the source above 3.5 MeV. After weighing the importance of each energy group source strength upon the dose rate from typical shipping cask shield dimensions, the effective uncertainty in the gamma spectra tends to increase from that of decay heat power to the vicinity of 10 to 15% in the energy range 0.5 to 2.5 MeV, where the spectrum has a dominant effect upon the dose rates for most cases. The uncertainty determined from fission yield data and half-lives alone would not be this large. However, a significant part of the spectrum in this range is contributed by ^{134}Cs and ^{154}Eu, two fission products that are produced only from the neutron reaction with ^{133}Cs and ^{153}Eu rather than from the more commonly assumed process of direct fission yields and subsequent decays. The uncertainty in the computed cross sections for these reactions is expected to be greater than that of fission yield and decay data. Also, there is additional uncertainty applied to the shielding analysis. If there were no other sources of uncertainty or bias in the computation, the 10 to 15% spectra uncertainty discussed above leads to an uncertainty of 5 to 7.5% in the calculated gamma dose rates.

S2.3.4 NEUTRON SOURCE SPECTRA

The uncertainties associated with the neutron source strength are discussed in Sect. S2.2.7. The neutron emission is mainly from ^{242}Cm at shorter cooling times and from ^{244}Cm at longer times. The source computed from a given quantity of ^{244}Cm is more accurate due to less uncertainty in its spontaneous fission half-life. Probably the largest contribution to final neutron source strength uncertainties is from the inventory calculation. Although the (α,n) reactions produced a maximum of about 10% of the source, its importance is increased by the fact that it contributes almost all of the emission in the two highest energy groups of the SCALE 27-group neutron library. No reported uncertainties were noted in the data applied for calculating the neutron spectrum. Spectra measurements that include uncertainties have been reported[33] for ^{252}Cf and ^{242}Cm total neutron yields. A comparison with the data applied by SAS2 indicates that uncertainty for the data used in the lower neutron energy range is approximately 10% and for the higher energy range, which includes the (α,n) produced neutrons, the data uncertainty is probably in the vicinity of 20%.

At discharge, the neutron source is almost equally produced from ^{242}Cm and ^{244}Cm. The half-lives of ^{242}Cm and ^{244}Cm are about 163 days and 18 years, respectively. The measurements of absolute quantities of these isotopes in spent fuel were usually performed by determination of peak intensities with alpha counters. Because the energies of the peaks differ by only a few percent, and differences in measurements[34] of three dissolver runs were significant, it is difficult to adequately derive a very precise uncertainty in the computed inventory of the two isotopes. Thus, there remains some deficiency in the knowledge of the curium isotope uncertainties. However, applying reasonable estimates of uncertainties associated with the spectrum, the total uncertainty of the neutron spectrum is expected to lie in the range between 10 and 35%.

S2.3.5 SHIPPING CASK DOSE RATES

As discussed above, there has been no complete uncertainty analysis performed for the dose rates computed by SAS2. This uncertainty would depend upon uncertainties in the source spectra, the cross sections, and the approximations in the shielding analysis. Also, the uncertainty would tend to be problem-dependent. The presence of water in a shipping cask tends to reduce the neutron dose rate more than the gamma dose rate. In these cases (i.e., "wet" shipping casks) the gamma source may be considerably more significant on a relative basis. Thus, the total dose rate uncertainty from the "wet" cask depends substantially upon the gamma dose rate uncertainty.

Several types of errors or uncertainties could be introduced into the shielding calculation applying the primary gamma source. For discussion purposes, these errors are divided into the following five categories pertaining to gamma uncertainties: input data; point cross sections; collapsed cross sections; control parameters selected for the case; and approximations or assumptions inherent in the shipping cask problem. The following provides a simplified analysis of the gamma dose rate uncertainties. When "uncertainty" is used, it implies a magnitude of 1σ.

The major uncertainty in the input, for a given cask design, is usually that of the gamma source spectrum (Sects. S2.3.2 and S2.3.3). Uncertainties in the calculated spent fuel inventories (Sect. S2.3.1) applied for the fuel zone mixture should be of much less importance.

The sensitivity of the transmission fraction F of monoenergetic photons through a thickness x can be seen in the following simplified equations (i.e., with buildup for scattering ignored). Let Σ be the linear attenuation coefficient or total cross section, I_o and I be the incident and transmitted intensities, σ be standard deviation, and $\sigma_x = 0$. Then,

$$F = I/I_o = e^{-\Sigma x}, \tag{S2.3.1}$$

$$\sigma_F = \sigma_\Sigma \partial F/\partial \Sigma = -\sigma_\Sigma x e^{-\Sigma x}. \tag{S2.3.2}$$

The uncertainty in F is:

$$\sigma_F/F = -x\Sigma(\sigma_\Sigma/\Sigma) = \ln F(\sigma_\Sigma/\Sigma). \tag{S2.3.3}$$

This applies rigorously only to a single energy for I_o and I. For multienergy photons there are scattering transitions from higher energies to the lower energy of I. This would mean that for part of the path at the higher energy Σ would be somewhat less, but the path length increase from angular scattering may have a greater and opposite effect. A more rigorous treatment would be required to take these effects into account. However, Eq. (S2.3.3) does provide an estimate of the relationship between the uncertainties of the flux attenuation and cross sections. In the significant energy groups of a sample cask problem, the transmission fraction varied from 10^{-5} to 10^{-7}. Since $\ln(10^{-5}) = -11.5$ and $\ln(10^{-7}) = -16.1$, it follows, from Eq. (S2.3.3) that the uncertainty in the flux attenuation and, subsequently, the dose rate at the shipping cask surface, is about an order of magnitude greater than that of the cross sections.

The 18-group gamma libraries of the SCALE system were prepared using the SMUG code[35] and accurate ENDF/B point cross-section data such as that of Ref. 36. The evaluated uncertainty in the total photon point cross sections for heavy elements (e.g., uranium and lead) is in the range of 1 to 2%[20,37,38] for energies most significant to the problem (i.e., 0.4 to 3 MeV). Those pertaining to lighter elements are somewhat lower, but they have less effect upon most shipping cask analyses. Another source of error, possibly more important, is that a flat flux was assumed in the process for collapsing point data to cross sections for the energy group structure of the library. Also, the gamma line intensity of a source nuclide is converted to a group intensity in ORIGEN-S by applying the ratio of its energy to that of the midpoint of the group. The application of a photon energy group structure, which is very fine and properly distributed around the major line data, would indicate the magnitude of the uncertainty from collapsing gamma line data into broad energy groups.

The sizes of control parameters input to the case (e.g., mesh interval size) can significantly effect the quality of the results. Defaults of these parameters are input to sample case 2 in Sect. S2.6. Other values are applied in sample case 1 for the same problem, which decreases the computer time but also reduces the accuracy. The gamma dose rate at 2 m decreased by 27% in the computation in sample case 1. This illustrates the combined effect of the particular parameter changes.

The 1-D radial model in SAS2 assumes each component of the cask to be cylindrical in the radial direction and infinitely uniform in the axial direction. The infinite height of the cask is assumed for the radiation transport through the cask walls and calculation of the surface angular flux. However, in calculating

the flux and dose outside the shield, the XSDOSE module only integrates the surface angular flux over an axial height specified by the user as the cask height. This analysis procedure has been shown to provide favorable dose results along the axial centerline in comparison to analysis techniques that accurately model the radial and axial shape of the cask.[39-41] Another approximation is required from the fact that square cross-sectional areas of the assemblies are represented by circular zone geometries. Equal areas (i.e., equal densities) may be maintained in describing the problem, or the radius may be conservatively extended to the outer corner of the assemblies. The type of geometry conversion scheme applied in SAS2 for the fuel zone is decided by the user and should be evaluated if the nonconservative scheme (equal areas) is selected.

It is difficult to derive a good estimate of the uncertainty of the computed gamma dose rates. However, Eq. (S2.3.3) shows that the uncertainty in the cross-section data can be highly significant for the large attenuations that are usually encountered in spent fuel cases. The indication that the error depends upon Σx, in addition to $\sigma_{\Sigma\Sigma}$, shows that the final uncertainties tend to vary proportionately with the thickness of a given material. Thus, at least for some problems, the cross-section uncertainty may be the dominant source of error. Examples of the propagated uncertainty were calculated, assuming: the cross-section uncertainty after collapsing, is 1.5 to 3%; the cross-section bias is 0.5 to 1%; the 1σ of the source spectrum is 10 to 15%; other 1σ is 5 to 10%; -ln F is 12 to 15 for a uranium shield thickness of 10 cm; and the final dose rate is equally divided distributed into four energy groups (causing the 1σ of each group to be 5 to 7.5%). The computed gamma-dose-rate uncertainty, based upon Eq. (S2.3.3) and quadratic error propagation was in the range 17 to 39% [i.e., $12 \times 0.015 = 0.18$ and $0.5(0.18^2 + 0.1^2 + 0.05^2)^{1/2} + 12(0.005) = 0.166$, etc.]. A reduction from the 10-cm thickness would produce correspondingly lower uncertainties.

The uncertainty in the computed neutron dose rate is more difficult to estimate than the photon dose rate. There are much larger cross-section and source uncertainties for neutrons. Improved determinations of heavy-element inventory uncertainties and a neutron sensitivity analysis are required to evaluate this uncertainty.

In addition, a photon source is produced from (n,γ) reactions. It appears that for many shipping cask designs, the fraction of the dose rate from this source is relatively small, although certain aspects of a cask design may make the fraction significant. Several neutron-photon cross-section libraries are included in the SCALE package. The user may determine the contribution from these secondary photons by comparing the gamma dose rates of two cases that are identical in all input with the single exception that one applies the neutron-photon library and the other applies the library for only photon reactions.

S2.4 LOGICAL PROGRAM FLOW

This section presents the logical program flow and description of routines of the Shielding Analytical Sequence No. 2. Subroutine descriptions are combined into blocks, in separate subsections, according to their relationships in producing a common function, rather than using an alphabetical order by names. This procedure should enhance the clarity of the flow and structure of the program.

The SAS2 control module is basically a program that prepares or preprocesses data for other codes. All SCALE functional modules (other codes) may receive their code input data from a binary interface data set. Because these code interfaces are produced and updated later in the execution of the SAS2 case, the general approach in SAS2 is to produce a "master interface data set" containing each type of functional module case and then perform an updated copy of the proper data interface case as required in the logical flow of the program. It is helpful, or perhaps necessary, to read parts or all of Sects. S2.1 and S2.2 before reading this section. The program is divided into the following subroutine blocks: basic control and region allocation preparation routines; Material Information Processor and neutronics data preprocessor for the path A model (see Fig. S2.2.1); neutronics data preprocessor for the path B model (see Fig. S2.2.1); depletion analysis input and data preprocessor; master mixing table processor; shielding analysis input and data preprocessor; and recycle update processor. The chief controlling subroutine name is given in each block of routines. The routine which calls it is indicated (or, sometimes the multiple path of routines in the flow are listed). Major routines are shown, which are either directly or indirectly called. Other utility routines, common to various blocks, are listed. They are described either in Sect. S2.4.10 or in the SCALE section referenced in Sect. S2.4.11. A brief explanation of the function of each block of routines is also presented.

The final three subsections show the master and supplementary interface formats, briefly describe utility routines not given elsewhere, and present a cross reference to all routines in alphabetical order.

S2.4.1 BASIC CONTROL AND REGION ALLOCATION

Routine Name: SAS2

Calling Routine: This is the entry routine from the SCALE driver.

Routines Called: MAINS2, SAPREP, RECYC, ALOCAT, STSAS2, NEXPAS

Utility Routines: ENDNOW, CHARIN, ERROR, GETMS, OPNFIL, RESETM

Function: This block of subroutines (1) checks flags from the SCALE driver and returns a stop flag if error is in the last execution of a functional module [i.e., IC(7) = 0], and (2) saves and restores the array list from the driver, establishing a list of functional modules invoked by the driver in array AC. On the first pass, flow through MAINS2 and SAPREP prints the unit numbers, opens data sets either for the required file connection on a CRAY computer (or other machines) or for proper region allocation by ALOCAT on an IBM computer, and proceeds to perform data preprocessing in STSAS2. On later passes, these routines proceed to a type of update processor controlled by RECYC and NEXPAS. ENDNOW and CHARIN pertain to use of the halt and restart features of SAS2. GETMS and RESETM get and store arrays that interface with the SCALE driver.

S2.4.2 MATERIAL INPUT AND NEUTRONICS PATH A DATA PREPROCESSOR

Routine Name: STSAS2

Calling Routine: SAPREP via ALOCAT

Routines Called: NIXSUB, KNIGHT, NIXNEW, NITXSD, COPYNX, REDSAS, SETPRG, SETDRG, SHIELD

Utility Routines: BINRCF, BINRCX, FINDID, IDXCIT, UPDATE, GETLIB, WI, VOLJB, STOCHK, EPSIG, IDSET, INQOPN, LENWRT, MESAGE, and routines associated with KNIGHT (Sect. M7.3).

Function: This block of routines activates the KNIGHT Material Information Processor (for converting user input and Standard Composition Library data to arrays for preprocessor routines), the NIXNEW master mixing table processor, and the NITXSD data preprocessor (for processing data and writing code interface data sets for the BONAMI-S, NITAWL-II and XSDRNPM-S depletion analysis of path A). The KNIGHT routine block is described in other SCALE sections. COPYNX modifies the interfaces obtained from NITXSD for neutronics codes through calls to UPDATE, BINRCF, BINRCX and writes these interface files on the master interface data set, unit number MAS. REDSAS, SETPRG, and SETDRG are described in Sect. S2.4.3. See Sect. S2.4.4 for NIXNEW and NIXSUB and Sect. S2.4.6 for functions of SHIELD. STSAS2 performs the major control of flow during the first pass through SAS2 plus minor data and pointer management. It also writes the header and last records on MAS. Note that data processing for the path A model is done by NITXSD, whereas the path B model processing is produced by S2HDAT (see Sect. S2.4.5).

S2.4.3 DEPLETION ANALYSIS INPUT AND DATA PREPROCESSOR

Routine Names: REDSAS, SETPRG, SETDRG

Calling Routine: STSAS2

Routines Called: SETDCO, WRITRG, S2HDAT

Utility Routines: UPDATE, BINRCF, BINRCX, COPYNX, LENWRT, WRTBY1, WRFLUX, ERROR, SCALE Free-Form Reading Routines.

Function: This block of routines reads operating history data for the reactor fuel assembly and converts it to the interface case data required for COUPLE and ORIGEN-S. REDSAS applies the SCALE Free-Form Reading Routines in reading data, checks for errors, and prints the "Reactor History Data." SETDCO writes the interface for COUPLE. SETPRG sets pointers for ORIGEN-S arrays. SETDRG prepares data for each pass through ORIGEN-S during the depletion calculation (looping NCYC*NLIB/CYC times), and saves values of power and time of each pass on MAS (see Sects. S2.2.3 and S2.2.4). SETDRG calls WRITRG to write the case interface and then copies it onto MAS. (Later, the interface case is simply updated in each recycle pass.) Following the time-depletion loops, SETDRG and WRITRG repeat the process (IPASS=2) with power and mass converted to that of the assembly, as applied in the final case (Sect. S2.2.5). Note that concentrations during the time-dependent library production cases are in atoms/b-cm, which can be more easily updated on neutronics code interfaces. The power is converted similarly. Finally, the decay subcase is prepared (Sect. S2.2.5). The call from REDSAS to S2HDAT initiates the neutronics data preprocessor for the path B model (Sect. S2.4.5).

S2.4.4 MASTER MIXING TABLE PROCESSOR

Routine Name: NIXNEW

Calling Routine: STSAS2 via NIXSUB

Routines Called: NUCFLG, NEWMIX, NITIDS, NITEMP, NITDAT

Utility Routines: GETLIB, SHLIB, NUCFLG, STOCHK, WI

Function: There is a twofold purpose for reprocessing the mixing table produced by the Material Information Processor. First, several trace amounts of nuclides are added to the fresh fuel, so that cross sections are produced for all important nuclides (see Table S2.2.1). Second, since the mixing table from input contains path A and path B unit cell data and shipping cask data, NIXNEW separates the data for the separate problems. NIXNEW calls NUCFLG to check the SCALE library before adding new nuclides in the /FUELID/ list of Table S2.2.1. From the new size, MSNEW, of the depletion case mixing table, it sets pointers used by NITXSD. NIXNEW then: calls NEWMIX to expand the mixing table of the unit cell to include the trace nuclides; calls NITIDS to reorder the ID array for NITAWL-II when necessary; calls NITEMP to set temperature data for NITAWL-II; and, finally, calls NITDAT for adding resonance data for the trace nuclides applied by NITAWL-II.

S.2.4.5 NEUTRONICS PATH B DATA PREPROCESSOR

Routine Name: S2HDAT

Calling Routine: STSAS2 via REDSAS

Routines Called: RD1S2H, RD2S2H, SETGEO, MTAB2H, S2HBON, S2HNIT, S2HXSD, S2HOUT

Utility Routines: ERDX, GETLIB, INQOPN, LENWRT, SCALE Free-Form Reading Routines

Function: This block of routines controls the four main phases in data processing for the path B portion of the depletion model (i.e., the larger unit cell computation). First, user input data are read in calls to RD1S2H (for level-1 or level-2 input) and RD2S2H (for level-2 or level-3 input). Second, S2HDAT prepares most of the remaining parameters for the neutronics codes through calls to SETGEO and MTAB2H. The main purpose of SETGEO is to standardize geometry data of the unit cell from lower input levels (0 and 1) to that read with level-2. Most of the other data required by neutronics modules are prepared into a more organized form by MTAB2H. The dominant part of the process in MTAB2H is the construction of all mixing table arrays for the larger unit cell. This step involves the storing or calculating of data for arrays containing ID numbers, mixture numbers, atom densities, and temperatures of all nuclides in the depletion analysis.

The processing in MTAB2H includes various features that "smear" fuel zone densities, account for fuel combined with burnable poisons, store neutron poison nuclides at the start of the mixing array (to obtain depleted densities of these nuclides through a later call to DPOISB), compute approximate estimates of Dancoff factors through the call to SHELC (Sect. M7.3.8), set up NITAWL-II input data for resonance nuclides, and generate mesh intervals for XSDRNPM-S. The standard interval size for a burnable poison zone (with no fuel) is set near 0.05 cm. All fuel zones use a 0.2-cm interval, while all remaining zones use 0.08 cm. Intervals adjacent to zone boundaries are split into two intervals of equal size. These standard sizes are multiplied by the input factor FACMESH (see Table S2.5.1) when it is input.

The third control phase of S2HDAT produces the neutronics code input data interfaces, on unit No. 70, for the path B model. This control phase is performed by S2HBON, S2HNIT, and S2HXSD. Note that for level-3 input, the level-2 input preparation is simply overridden by any FIDAS-type array data input by level-3 rules (see Appendix A).

The fourth phase of S2HDAT is the printout of user input (non-FIDAS) through a call to S2HOUT.

S2.4.6 SHIELDING ANALYSIS INPUT AND DATA PREPROCESSOR

Routine Name: SHIELD

Calling Routine: STSAS2

Routines Called: SHDATA, SHRITE, SHRHO, SHDRY, CELLWT, SHMIX, SHBON, SHRES, SHNIWR, SHMESH, SHXSWR, WI, SCALE Free-Form Reading Routines

Utility Routines: STOCHK, DENH2O, UPDATE, NEWREC, SHLIB, WI, SHXI, EPSIG, GEPSIG, BINRCX, ERROR, GETLIB, INQOPN, LENWRT

Function: The objective of this subroutine block is to set up, using initial data, the cell-weighted case (optionally applied for the fuel cross sections in the final shielding analysis), and the final region geometry case applied to analyze the shipping cask. Then, the only changes required in the pass to SAS2 before these cases are executed are the final spent-fuel densities and neutron and gamma source data. In controlling the flow, SHIELD computes pointers derived mainly from mixing table sizes. SHIELD calls SHDATA to read and check the shipping cask input data, including the geometry, control parameters, etc. The data are printed and volume fractions are computed in SHRITE. SHRHO returns atom densities of the water from FUNCTION DENH2O for the input temperature and pressure in the cask, if DENFM = 0 and DRYFUEL = NO (see Table S2.5.1). Then, CELLWT makes the three code interfaces required for the shielding cell-weighted case by using the interfaces from the path A model depletion case and making the necessary changes in moderator nuclides, their densities, zone temperatures, and control parameters (e.g., for fixed source and cell-weighting). Moderator densities are either DENH and DENO, from DENH2O, or the input DENFM times the old reactor values. Allowance for sodium (e.g., from LMFBRs) is provided only by using DENFM. Update copies of an interface are performed with calls to UPDATE and NEWREC. CELLWT writes the interfaces for BONAMI-S, NITAWL-II and XSDRNPM-S in the next positions on the master interface data set.

SHIELD then calls routines to prepare the region geometry case. SHMIX prepares the mixing table from arrays of the master mixing table (see Sect. S2.4.4). The three neutronic codes can have lengths and ID numbers (identifiers) in their mixing tables that are different. The IDs of the SCALE library are used in array NB1 (4$ data) and duplicate IDs are modified in NBX (10$ data) of BONAMI-S. Then, XBX, the density array, is the same for BONAMI-S and XSDRNPM-S. Note that the size of NBX is the sum of the number of master library nuclides requested by NITAWL-II (MMT) plus the product of the number of cell-weighted nuclides (NWT) times the number of zones containing fuel. A counter, KOUNT, is incremented for BONAMI-S and XSDRNPM-S, whereas KOUNTN is used for NITAWL-II. Duplicate IDs are avoided by adding MS (number of compositions for path A unit cell) to the position value, or KOUNT. The first MMT positions for NITAWL-II (2$ data) are new nuclides of the cask, and the last MWT positions contain the same IDs as in the cell-weighted case, which gives the required order for library merging. An approximation is applied by using the fresh fuel densities in BONAMI-S. A single temperature of the cask is applied, in order to simplify input. Individual code parameters of the shielding case are selected as described in Sect. S2.2.8.

SHIELD calls SHRES to prepare resonance input data for NITAWL-II and calls SHMESH to produce the mesh intervals for XSDRNPM-S (Sect. S2.2.9). The cask shielding case data are written in the next positions on the master interface data set by: SHBON for BONAMI-S; SHNIWR for NITAWL-II; and SHXSWR for XSDRNPM-S. Data for XSDOSE are not written until a later pass in SAS2 (see Sect. S2.4.7).

S2.4.7 RECYCLE UPDATE PROCESSOR

Routine Name: NEXPAS

Calling Routine: RECYC via ALOCAT

Routines Called: PASNEW, CWTCYC, CASCYC, XSDOSE, FINXSD, NSOUR, SRCALC, DPOISB, DPOISN, DPOISX

Utility Routines: STOCHK, UPDATE, NEWREC, NEWDEN, CWTDEN, IDXCIT, INQOPN, MOVMAS, ENDNOW

Function: This subroutine block controls the flow during all passes into SAS2 after the first pass. The method used by SAS2 for managing problem data is to set up a typical interface case for all functional module cases during the first pass, to save the data on the master and supplementary interface data sets. Then, during later SAS2 passes, the interface data sets are updated as necessary using data produced by the execution of earlier cases. This substitution or updating process is the main function of routines called by NEXPAS. Also, prior to calling other routines, NEXPAS writes (in BCD) atom densities, source spectra and other data for each cycle on unit No. 72. During the passes pertaining to the production of time-dependent cross sections (see Sect. S2.2.4), the flow is directed to PASNEW. The paths taken for processing the path A or path B models of the depletion analysis (see Fig. S2.2.1) are determined by the condition of WHICHP equaling FIRST or SECOND, respectively. These control variables are set in MAINS2, which is called by the entry routine, SAS2. NEWDEN supplies or adjusts the nuclide densities produced by ORIGEN-S. Burnable poison nuclide densities are obtained or processed by calls to DPOISB, DPOISN, and DPOISX. New mixing-table densities are applied in producing interfaces for BONAMI-S, NITAWL-II, XSDRNPM-S and ORIGEN-S. In the processing for path A, the "full" densities produced by an ORIGEN-S depletion case are input to the neutronics codes. In the processing for path B, these densities are reduced properly or "smeared" over the cell, with the exception of those for burnable poisons (which must remain "full" densities, as input to the path B case). Boron in the moderator is treated as stated in Sect. S2.2.4. Proper unit numbers are changed for COUPLE and ORIGEN-S. The times and powers of the cycle are read from MAS in NEXPAS.

In the pass to SAS2 following the completion of the depletion analysis, NEXPAS calls CWTCYC for preprocessing the data from the optional shielding cell-weighted case. CWTCYC copies the BONAMI-S interface from MAS, since it is not changed. Then, the spent-fuel densities are returned from CWTDEN and used in writing the updated NITAWL-II interface. Similarly, the XSDRNPM-S interface is updated. Source data are read in FINXSD from the data sets produced by ORIGEN-S. The gamma source is converted from that of an assembly to source per cm^3. The neutron source is determined from NSOUR and SRCALC (Sects. S2.2.7 and S2.4.8). Then the XSDRNPM-S interface is completed in FINXSD.

The final pass into SAS2 calls CASCYC and subroutine XSDOSE from NEXPAS. CASCYC produces interfaces by copying them from MAS for BONAMI-S and NITAWL-II (since there is no new resonance treatment for the cell-weighted fuel nuclides), and obtains densities and sources similar to that for the cell-weighted case. The XSDRNPM-S interface is produced by CASCYC and FINXSD (with KASK=1, set to denote the shipping cask case). Finally, subroutine XSDOSE produces the interface for the XSDOSE module using default or input detector distances.

S2.4.8 FORMATS OF MASTER INTERFACE AND SUPPLEMENTARY INTERFACE DATA SETS

Scratch data sets are applied to communicate data from one pass to another in SAS2. These sets are called the master interface data set and the supplementary interface data set. Most of the information is in the form of the data interface to one of the functional modules. It is either exactly the data as applied, or it has the general structure so that new data (e.g., time-dependent atom densities) may be easily substituted. In addition to interface data, there are control parameters and variables in header records and the two last records. This subsection lists the type of each record, or set of records, to assist in reading or modifying the code.

A. Header Records on Master Interface Data Set:

1. The header record containing JPL and JP plus a list of parameters in the commons /SASCM/, /SASCM2/, /EXTRCM/ and /FRACIN/.

2. Powers and times applied by ORIGEN-S for each of the NSEG different time-dependent libraries produced. There are NSEG records, NSEG=NCYC*NLIB/CYC, from input data.

B. Sets of Master Interface Data (By Code, Case Type):

1. BONAMI-S, depletion unit-cell of path A model;

2. NITAWL-II, depletion unit-cell of path A model;

3. XSDRNPM-S, depletion unit-cell of path A model;

4. COUPLE, depletion library update;

5. ORIGEN-S, time-dependent depletion densities;

6. ORIGEN-S, final depletion and decay case;

7. BONAMI-S, cell-weight shield unit-cell;

8. NITAWL-II, cell-weight shield unit-cell;

9. XSDRNPM-S, cell-weight shield unit-cell;

10. BONAMI-S, region geometry shipping cask;

11. NITAWL-II, shipping cask library merge;

12. XSDRNPM-S, region geometry shipping cask.

C. Final Records on Master Interface Data Set:

1. dose rate detector distances from shipping cask surface; and

2. shielding library unit number, group sizes, fuel zone size, factor, and light-element data.

D. Sets of Supplementary Interface Data (By Code, Case Type):

1. BONAMI-S, depletion unit-cell of path B model;

2. NITAWL-II, depletion unit-cell of path B model; and

3. XSDRNPM-S, depletion unit-cell of path B model.

The three sets are repeated for each of the NSEG libraries, if MXREPEATS=0 (see Table S2.5.1).

S2.4.9 UTILITY ROUTINES

Utility routines applied by SAS2, which are not described above or in other SCALE sections, are briefly presented. The labeled common /FUELID/ is also included.

CHARIN – Reads characters for "Halt," "Restart," and other features from "=SAS2" card.

COPYNX – Copies code interface data, with minor updating, to MAS for BONAMI-S, NITAWL-II and XSDRNPM-S.

ENDNOW – Prints STOP 0 when "Halt" feature invoked, writing restart data on unit No. 55.

ERDX – Prints level-3 input error messages.

ERROR – Calls STOP and prints STOP 100, when an error occurs.

FINDID – Converts SCALE ID to ORIGEN-S ID and library type No.

/FUELID/ – This is a COMMON that is initialized in a BLOCK DATA routine. It contains the list of nuclides which SAS2 always inputs in trace quantities (1×10^{-20} atoms/b-cm) when not input by user. The nuclide list is ^{135}Xe, ^{133}Cs, ^{234}U, ^{235}U, ^{236}U, ^{238}U, ^{237}Np, ^{238}Pu, ^{239}Pu, ^{240}Pu, ^{241}Pu, ^{242}Pu, ^{241}Am, ^{242m}Am, ^{243}Am, ^{242}Cm, ^{243}Cm, ^{244}Cm, and the 1/v absorber. The 1/v absorber is used to calculate the THERM parameter applied in ORIGEN-S (Sects. F6.2.1 and F7.6.12, and Eqs. F6.2.7, F6.2.8, and F7.6.13).

GEPSIG – Computes $1/L_g$ in Eq. (S2.2.2) for mesh generator.

GETLIB – Converts input library name to appropriate output unit number (see Table M4.1.1 of Sect. M4).

IDSET – Reduces SCALE neutron cross-section library to include only the nuclides for the case, through a call to SHORTX (Sect. M7.3).

IDXCIT – Computes ID for excited-state nuclides in ORIGEN-S.

INQOPN – Opens a file via OPNFIL, when INQUIRE finds the file not opened.

LENWRT – Writes the array allocation size data in the -1$$ record on binary interfaces to functional modules, if needed.

MOVMAS – Reads to start of current cycle interface data on MAS2 for path B model PASNEW processing, if MXREPEATS=0 (see Table S2.5.1).

NEWREC – Writes and possibly edits one pair of code interface records.

SHLIB – Reads number of energy groups and nuclide ID numbers of a SCALE "master" library.

STOCHK – Compares total array size used with that allocated. If within 400 words, prints message. If full, calls ERROR to stop.

SHXI – Determines scattering power of nuclide for preprocessing of resonance data by subroutine SHRES.

UPDATE – Copies standard interface formatted data until the array identifier, IA, and data entry number, IBGN, are found. Only reads the record pair requested. Usually, the calling routine updates the record pair with NEWREC, BINRCX or BINRCF. When the output unit number is zero, the routine simply reads or skips to the proper record. The routine also returns after reading a negative identifier since this signals the end of a code interface. Thus, a complete code interface, excluding the single record of title for XSDRNPM-S, is skipped by requesting an identifier -1 (or -9 as usually sent by SAS2).

WI/WJ – Debug type edit of: name, array size, and array. WI is for floating-point data and WJ is for integers. Used in HALTXX case.

WRFLUX – Sets the "flux guess" array to 1 and writes the "flux guess" and "moments" array.

WRTBY1 – Writes pair of interface records for all nonzero parameters in data list, L, for array identifier, IA. This is similar to specifying all data with an Ai in FIDO (see Sect. M10), where i denotes the *ith* entry. This method allows the use of UPDATE more effectively.

S2.4.10 SUBROUTINE REFERENCE INDEX

The reference indices to subroutines written for SAS2 or directly called in the new SAS2 coding are given below. The functions of other subroutines (e.g., those applied by KNIGHT) are presented in Sects. M7.3.1 and M7.3.2. The conventions and applications of Free-Form Reading Routines are given in Sect. M3.

Name	Subsections (Described or Applied)
ALOCAT	M2.2.1, S2.4.1, S2.4.2, S2.4.7
AREAD	M2.2.3, M7.3, S2.4.3, S2.4.5, S2.4.6
BINRCF	M7.3, S2.4.2, S2.4.3
BINRCX	M7.3, S2.4.2, S2.4.3, S2.4.6
CASCYC	S2.4.7
CELLWT	S2.4.6
CHARIN	S2.4.1, S2.4.9
COPYNX	S2.4.3, S2.4.9
CWTCYC	S2.4.7
CWTDEN	S2.4.7
DENH2O	S2.4.6, Ref. 21
DPOISB	S2.4.5, S2.4.7
DPOISN	S2.4.7
DPOISX	S2.4.7
ENDNOW	S2.4.1, S2.4.7, S2.4.9
EPSIG	C4.3.3, M7.3, S2.4.2, S2.4.6
ERDX	S2.4.9
ERROR	S2.4.9, S2.4.1-S2.4.8
FINDID	S2.4.2, S2.4.9
FINXSD	S2.4.7
FREAD	M2.2.32, M3.3, S2.4.3, S2.4.5, S2.4.6

GEPSIG	S2.4.6, S2.4.9
GETLIB	S2.4.2, S2.4.4, S2.4.5, S2.4.6, S2.4.9
GETMS	C4.3.2, S2.4.1
IDSET	S2.4.1, S2.4.9
IDXCIT	S2.4.2, S2.4.5, S2.4.7, S2.4.9
INQOPN	S2.4.2, S2.4.5, S2.4.6, S2.4.7, S2.4.9
IREAD	M2.2.40, M3.3, S2.4.3, S2.4.5, S2.4.6
KNIGHT	M7.3, C4.3.3, S2.4.2
LENWRT	S2.4.3, S2.4.5, S2.4.6, S2.4.9
LREAD	M2.2.48, M3.3, S2.4.5
MAINS2	S2.4.1
MESAGE	M2.2.49, S2.4.2
MOVMAS	S2.4.7, S2.4.9
MTAB2H	S2.4.5
NEWDEN	S2.4.7
NEWMIX	S2.4.4
NEWREC	S2.4.5, S2.4.6, S2.4.7, S2.4.9
NEXPAS	S2.4.1, S2.4.7
NITDAT	S2.4.4
NITEMP	S2.4.4
NITIDS	S2.4.4
NITXSD	S2.4.2
NIXNEW	S2.4.2, S2.4.4
NIXSUB	S2.4.2, S2.4.4
NUCFLG	S2.4.4
OPNFIL	C4.3.2, S2.4.1, S2.4.9
PASNEW	S2.4.7
RD1S2H	S2.4.5
RD2S2H	S2.4.5
RECYC	S2.4.1, S2.4.7
REDSAS	S2.4.2, S2.4.3
RESETM	C4.3.2, S2.4.1
SAPREP	S2.4.1, S2.4.2
SAS2	S2.4.1
SCANON	M2.2.61, M3.3, S2.4.3
SETDCO	S2.4.3
SETDRG	S2.4.2, S2.4.3
SETGEO	S2.4.5
SETPRG	S2.4.2, S2.4.3
SHBON	S2.4.6
SHDATA	S2.4.6
SHDRY	S2.4.6
SHIELD	S2.4.2, S2.4.6
SHLIB	S2.4.4, S2.4.6, S2.4.9
SHMESH	S2.4.6
SHMIX	S2.4.6
SHNIWR	S2.4.6
SHORTX	M7.3, S2.4.9
SHRES	S2.4.6
SHRHO	S2.4.6
SHRITE	S2.4.6

SHXI	S2.4.6, S2.4.9
SHXSWR	S2.4.6
STOCHK	S2.4.2, S2.4.4, S2.4.6, S2.4.7, S2.4.9
STOP	M2.2.63, S2.4
STSAS2	S2.4.1, S2.4.2, S2.4.3, S2.4.4, S2.4.6
S2HBON	S2.4.5
S2HDAT	S2.4.2, S2.4.5
S2HNIT	S2.4.5
S2HOUT	S2.4.5
S2HXSD	S2.4.5
UPDATE	S2.4.2, S2.4.3, S2.4.6, S2.4.7, S2.4.9
VOLJB	M7.3, C4.3.3, S2.4.2
WI	S2.4.2, S2.4.4, S2.4.6, S2.4.9
WJ	S2.4.9
WRFLUX	S2.4.3, S2.4.9
WRITRG	S2.4.3
WRTBY1	S2.4.3, S2.4.9
XSDOSE	S2.4.7

S2.5 INPUT DATA DESCRIPTION

The user prepares SAS2 input by following the SAS2 input data requirements table in this section. Various free-form input features are reviewed to assist new users of SCALE control modules. A brief outline of all input data is given. The input description is presented by a summary-type format in a five-page input requirements table. However, prior to the table, a discussion on certain meanings and use of the table is presented. Following the table, data notes are presented for clarifying details of the description and denoting particular exceptions to the definitions. Finally, a "Halt" and "Restart" feature and other major supplemental options are described.

The user familiar with the SCALE-3 version of SAS2 may note the additions to input resulting from the change to the SAS2H model. In practice, the amount of the additional data depends largely upon the type of fuel assembly modeled. Usually either short or no input additions are required for PWR control rod assemblies. There may be significant input additions, however, for BWR or PWR burnable poison assemblies.

S2.5.1 REVIEW OF FREE-FORM INPUT FEATURES

All 80 columns of a card (or card-image record or line) may be used.

A data entry, numeric or alphanumeric, may be entered anywhere on the line, but without dividing the entry between two lines.

Numerical data must be followed immediately by a comma or one or more blanks.

Alphanumerical data must be followed by two blanks or an equal sign (=). Sometimes alphanumerical data may be followed by one blank in place of two (e.g., after entries for EL in Table S2.5.1) and within the data following the requirements of CSAS4. Even though some users may prefer to correctly apply one blank, the "two-blank rule" is the general convention of SAS2, and always produces correct results.

Floating-point data may be entered in various forms (e.g., the value 12340.0 may be entered as: 12340, 12340.0, 1.234+4, 1.234E+4, 1.234E4, 1.234E04, or with exponent indicator D replacing E). (Also 0.012 may be 12–3, 1.2–2, etc.)

Comment lines may be added to the input by using an apostrophe (') in column one and followed by a comment in the other 79 columns. These lines may appear anywhere (before or after any of the data entries in the input) except the positions just prior to a title line or a module activator line (e.g., =SAS2H).

Other features are presented in Sect. M3.

S2.5.2 OUTLINE OF INPUT DATA

I. Reactor Material and Lattice Data
   - A. Title, Library, and Lattice-Type
   - B. Material Compositions
     1. Fuel-Pin Cell
     2. Other Pin Cell or Guide Tube Cell
     3. Fuel Element Casing
     4. Channel Moderator
     5. Shipping Cask
   - C. Fuel-Assembly Unit-Cell Geometry

II. Reactor History Data and Larger Unit-Cell Geometry
   - A. Fuel-Assembly Parameters
   - B. Larger Unit-Cell Geometry
   - C. Power and Moderator History

III. Shipping-Cask System Data
   A. Library and Cask Parameters
   B. Shipping Cask Geometry
      1. Detector Positions (Optional)
      2. Zone Description
      3. Fuel-Assemblies/Fuel-Zone

S2.5.3 USE OF INPUT DATA REQUIREMENT TABLES

Before preparing input, the user should read Sects. S2.1 and S2.2. The input requirements are presented in Table S2.5.1. The left-hand column of the table gives the data block reference number, which is not an input entry. The next column of the table lists the variable name or keyword of the entry, and the remainder of each line defines the variable and gives useful comments. Sometimes the name is only for reference purposes and for denoting either integer (I, J, K, L, M, and N as first character) or floating-point data (unless specified in comments). Some of the variable names and keywords must be entered as part of the input data. These required entries are denoted by an asterisk. The variable names may be reduced to the first four left-hand characters plus the equal sign, if the user prefers that they be more concise than descriptive. If additional characters are added to the first four, a name may not exceed 12 characters before the "=." Variable names without an asterisk should not be entered.

The input description is divided into separate blocks of data, which are included between consecutive horizontal dashed lines. The first entry of a block of data must begin on a new line. Additional entries may be entered on the same line. When the block ends with the keyword END, the next entry must be on a new line. Except for the module activator (e.g., =SAS2H) and the title line, more than one line is permitted per block. Examples are sometimes shown after the block of data.

The general approach applied in SAS2 is to use the Material Information Processor of SCALE in reading all data through data block 6 (under I in the outline of Sect. S2.5.2). Except as noted in Table S2.5.1, any appropriate option listed in Table M7.4.3 and described in Sect. M7.4 is permitted in SAS2 also. For example, arbitrary materials could be included in the material data. These data blocks include all data for the initial case executed by the neutronics codes except for trace nuclides (see Table S2.2.1) which are added automatically by SAS2. Additionally, the Standard Composition block includes all material descriptions for the shipping cask except for the spent fuel compositions and cask coolant densities in the fuel zone. The multiple application of the Standard Composition block requires the fixed specifications of certain mixture numbers as shown (i.e., MX $\leq$ 3 for the fuel pin mixtures). Also, the volume used in computing the volume fractions, VF, of components in spent fuel zones should total the zone volume minus the total number of pins in the fuel zone (FUELBNDL*NPIN/ASSM) times the unit-cell volume. Any extra water in the assembly (e.g., lattice "holes") (see Sect. S2.3.1) should be part of the additional components in spent fuel zones (see Data Note A in Sect. S2.5.4).

Any data entry specified in the table is always required unless a condition for its omission or "optional" is stated in the comments. When the entry may be omitted, a default value is supplied by the code, usually the value is shown in parentheses at the end of the comments. The only exceptions to this method are the defaults computed by equations listed in Data Note B for INPLEVEL=0.

At the time of the present writing the 123-group SCALE library, which may be specified by LIB, contains incomplete data for application by SAS2. It is required that fluxes (MT=1099) be added for properly weighting the library during the energy collapse with XSDRNPM-S.

S2.5.4 IMPORTANT DATA NOTES

The user experienced in applying SAS2 or other SCALE control modules may find that Table S2.5.1 is sufficient for most cases. However, since some definitions or comments in the table could be subject to interpretation or may have an unusual exception, the following data notes are included.

Table S2.5.1 SAS2 input data requirements

Data block	Name or keyword	Definitions, comments, and examples
1	=SAS2*	(or =SAS2H as an alias name) Module activator, column 1. See Halt Feature and other PARM= parameters in Sect. S2.5.6
2	TITLE	An 80-character title. (Prints only 72 in XSDRNPM-S)
3	LIB	Name of SCALE library to be used in reactor analysis: HANSEN-ROACH; 27GROUPNDF4; 218GROUPNDF4; or 27BURNUPLIB (recommended). See Sect. M4 for more information on available libraries
	GE	Reactor lattice type. SAS2 always requires LATTICECELL Example: 27GROUPNDF4 LATTICECELL
4		(For more details, see Data Note A.)
	SC	Component name from Standard Composition Library (see Table M8.2.1). (For input of arbitrary materials, see Table M7.4.5.)
	MX	Mixture number of SC. MX≤3 if pin-cell; MX≥4 if cask or larger unit cell mixture
	DEN=*	Density of the standard composition (optional), g/cm^3
	VF	Density multiplier. Set to zero if using ADEN. May omit if END is next (1)
	ADEN	Atom density, atoms/barn-cm. Enter only if VF=0
	TEMP	Temperature, K, applied only if MX ≤ 3 or if larger unit cell mixture May omit if END is next (293)
	IZA	SCALE ZA number. Omit if VF=0. Use only for multiple isotope elements in Table M8.4.1
	WTP	Wt % for IZA. Repeat IZA-WTP pairs for 100% sum
	END*	End of this SC data. Repeat for all SC of case Examples: UO2 1 0.94 1000 92235 3.1 92238 96.9 END FE 4 0 4.2-3 END SS304 6 END
	END COMP*	Ends entire material data input. See Data Note A and Table M7.4.5 for more information
5	CPT	Type of rod-lattice: SQUAREPITCH or TRIANGPITCH only allowed in SAS2
	PITCH	Center-to-center spacing between fuel pins, cm
	FUELOD	Outside diameter of fuel in pin, cm
	MFUEL	Mixture number of fuel. Always enter 1 in SAS2
	MMOD	Moderator mixture number. Always 3 in SAS2
	CLADOD	Clad outside diameter, cm. There must be SC for clad
	MCLAD	Clad mixture number. Always 2 in SAS2
	CLADID	Clad inside diameter, cm. Omit this and next entry if no gap
	MGAP	Gap mixture number, if gap. Always 0 in SAS2
	END*	End of reactor-lattice. See Data Note A and Table M7.4.7 for more information

Table S2.5.1 (continued)

Data block	Name or keyword	Definitions, comments, and examples
	MORE DATA*	Optional data for XSDRNPM cases run during depletion analysis Entries may be in any order
	SZF=*	Spatial mesh factor. SZF: <1 for finer; >1 for coarser mesh (1)
	ISN=*	Order of angular quadrature (8)
	IIM=*	Maximum number of inner iterations (20)
6	ICM=*	Maximum number of outer iterations (25)
	EPS=*	Overall convergence criteria (0.0001)
	PTC=*	Scalar flux point convergence (0.0001)
	IUS=*	IUS=:1, upscatter scaling to speed convergence; 0, not scaled (0)
	END*	End of option. See Table M7.4.9 and accompanying description for additional options and more detailed information Example: MORE DATA ISN=16 SZF=0.9 END
		(The first six of the following may be in any order. See Data Note B for discussion.)
	NPIN/ASSM=*	Number of fuel-rods/assembly; control rods not included; burnable-poison fuel rods included
	FUELNGTH=*	Active length of fuel in rods, cm
	NCYCLES=*	Number of cycles exposed; commonly number of years (3)
	NLIB/CYC=*	Number of libraries made per cycle (1)
	LIGHTEL=*	Number of light elements in clad and assembly input in Data Block 10
	PRINTLEVEL=*	Print level (integer) requested. See Data Note C (4) (Omit the remainder of this block and Data Block 8, if INPLEVEL=0 or PARM=OLDSAS2.)
	INPLEVEL=*	Input level of data below (0)
7	NUMHOLES=*	Number of second type pins or "holes"/assembly Required only if INPLEVEL=1
	NUMINSTR=*	Number of instrument tubes/assembly (1). Required only if INPLEVEL=1
	MXTUBE=*	Mixture number of guide tube (2). Required only if INPLEVEL=1
	ORTUBE=*	Outside radius of guide tube, cm. Required only if INPLEVEL=1
	SRTUBE=*	Inside (small) radius of guide tube, cm. Required only if INPLEVEL=1
	ASMPITCH=*	Pitch between assemblies, cm. Required only if INPLEVEL=1
	NUMZTOTAL=*	Number of zones in describing larger cell. Required only if INPLEVEL=2 or 3
	MXREPEATS=*	=0/1; MIXES and RADIUS required: for each library made/only once (1). Required only if INPLEVEL=2 or 3
	MIXMOD=*	Mixture number of moderator (3). Required only if INPLEVEL=2 or 3
	FACMESH=*	Mesh size factor: Interval size = (default size)(FACMESH) is applied (1.0). Required if INPLEVEL=2 or 3
	END*	End of INPLEVEL scalar constants, required if INPLEVEL>0 See Appendix S2.A, which gives additional input, for INPLEVEL=3

Table S2.5.1 (continued)

Data block	Name or keyword	Definitions, comments, and examples
8 (Enter NCYCLES* NLIB/CYC times if MXREPEATS=0)		(Repeat the following, as pairs of data, NUMZTOTAL times.)
	MIXES	Mixture number of zone, inner zone first. Required if INPLEVEL = 2 or 3
	RADIUS	Outer radius of zone; ascending order, cm
9		Enter the following set for each cycle or NCYCLES times. Entries may be in any order, except for "END" See Data Note B
	POWER=*	Average specific power of assembly, megawatts
	BURN=*	Fuel irradiation period of reactor, days
	DOWN=*	Downtime, days, following BURN; except for last cycle where it is cooling time of spent fuel used in cask analysis
	BFRAC=*	Fraction of first-cycle boron density (from Data Block 4) for this cycle (1)
	H2OFRAC=*	Fraction of first-cycle H_2O density for this cycle. Note, "O" in H2OFRAC is a letter (1)
	TEMKCYC=*	Temperature of all nuclides this cycle, K. Defaults to Standard Composition value
	END*	Required if any entry omitted Example: POWER=15.2 BURN=330 DOWN=35.25 END
10 (Enter LIGHTEL times)		(Repeat the following LIGHTEL times, if LIGHTEL > 0)
	EL	Chemical symbol of element for which gamma source is to be included and (n,γ) Q-value/fission applied
	WTLITE	Effective weight/assembly, kg. See Data Note D Example: FE 6.2 CO 0.04 ZR 100

Table S2.5.1 (continued)

Data block	Name or keyword	Definitions, comments, and examples
11	ALIB	Name of SCALE library used for cask shielding analysis: 27N-18COUPLE; 22N-18COUPLE; or 18GROUPGAMMA, or those listed for LIB (The following entries may be in any order.)
	TEMPCASK=*	Cask temperature, used for all mixtures, K. Replaces TEMP in standard composition data for cask cases
	NUMZONES=*	Number of material zones in cask, i.e., number of radii, R
	DRYFUEL=*	Enter YES (if dry, i.e., no H_2O) to denote removal of fuel zone water derived from the moderator mixture, MX=3. Default of NO is for flooded cask. Follow with two or more blanks (NO)
	DETECTORS=*	Number (integer) of dose detector locations. Limit of 30. If zero, locations are 0, 1, 2, and 4 m from cask surface in midplane. If ≥0, ANSI standard dose conversion factors are used. If <0, other factors, possibly, are used (see Data Note F) (0)
	END	Required only if one of the above entries is omitted Example: 27N-18COUPLE TEMPCASK=300 NUMZONES=6 END
12		(DETECTORS number of entries. Omit, if DETECTORS=0)
(Enter DETECTORS times)	DTEC	Surface-to-detector distance, cm Example: 0 34.5 100 500
13 (Enter NUMZONES times)	MXZ	(Repeat pair of entries NUMZONES times. See Data Note E.) Zone mixture number; applies all SC of Data Block 4 where MX=MXZ
	R	Radius of zone, cm Example: 4 24.5 6 24.8 5 50.2 6 50.4 7 60.8 6 61
14 (Enter for each fuel zone)		(Repeat pair of entries for each fuel zone; limit of 5)
	ZONE=*	Zone number of fuel zone, or position of MXZ-R pair
	FUELBNDL=*	Number of spent fuel assemblies in zone. See Data Note E Example: ZONE=1 FUELBNDL=1 ZONE=3 FUELBNDL=5

Table S2.5.1 (continued)

Data block	Name or keyword	Definitions, comments, and examples
		(Enter, if required, or for changing defaults; in any order)
	PRESSURE=*	Cask water pressure, psia, for deriving densities. Either this or next entry required if DRYFUEL=NO (14.696)
	DENFM=*	Ratio of coolant density to that of the same moderator in reactor case. Always required in treating sodium (In entries below, x=C or x=S. The entry applies to XSDRNPM-S in the cell weight case if x=C, and for XSDRNPM-S in the shipping cask case if x=S)
15	SZFCASK=*	Mesh size factor: Interval size=(default size) × (SZFCASK) is applied (1.0)
	ISNx=*	Order of angular quadrature (8 for ISNC, 16 for ISNS)
	ICMx=*	Maximum number of outer iterations (25)
	EPSx=*	Overall convergence criteria (0.0001)
	PTCx=*	Scalar flux point convergence (0.0001)
	ICMx=*	Maximum number of outer iterations (25)
	ITMx=*	Maximum computer (CPU) time allowed in XSDRNPM-S, min. (defaults: 10, if x=C; 30, if x=S)
	END*	Required if all of the above entries are omitted Otherwise, it is optional. Starts after column one
16	END*	End of SAS2 module data. Starts in column one. A new SCALE case may follow

*Word, words or name (including =), which must be part of data entry. Requires only first four characters of names.

S2.5.4.1 Note A, Material and Lattice Input

Data Blocks 2–6 provide input to the Material Information Processor as described in Sect. M7.4. However, the input and description in Table S2.5.1 is significantly reduced from that shown in Table M7.4.3. The user should refer to Table M7.4.5 to augment Table S2.5.1 if an arbitrary material (one for which a standard composition is not available) is needed in the mixture specification. Also, the MORE DATA data block of Table S2.5.1 does not list all the optional parameters allowed by the Material Information Processor; however, it does list all the ones that are the most important to typical LWR designs. Finally, the restriction of SAS2 applicability to LATTICECELL geometries limits the necessary input description. The following information in this Data Note provides additional information to help the user better understand the Material Information Processor input as required by the SAS2 control module.

As in other control modules of the SCALE system (e.g., Sect. C4) material definitions are input as "standard composition specification data." Each mixture of a material zone includes all standard composition components, SC, having the same value of MX. All standard composition input names (e.g., UO2, U-235, H2O, or ZIRCALLOY), their theoretical densities, the master libraries on which they are included, and other significant data are available to the user in Table M8.2.1 (see The Standard Composition Library, Sect. M8). The code ignores nuclides that are not on the SCALE master library and alerts the user in a nonfatal warning message. When there is no entry for DEN, ADEN, or IZA and an arbitrary material is not being requested, the nuclide composition densities are derived from VF times the theoretical density included in the standard composition library. Pairs of IZA and WTP are entered only when the desired isotopic distribution is different from the natural isotopic distribution of Table M8.4.1. Note the sum of all WTP input must equal 100%. The theoretical density in the Standard Composition Library (see Table M8.2.1) may be replaced by input of DEN= value, entered between MX and VF. Then the material density used is DEN*VF.

In order to apply the total material description to both the depletion calculation of the reactor and the shipping cask shielding analysis, it is necessary to restrict mixtures 1–3 ($MX \leq 3$) to the assembly pin-cell depletion cases. Specifically, the user should apply MX=1 for the fuel mixture, MX=2 for the pin-clad, and MX=3 for the moderator mixture. Since all nuclides that are generated during the irradiation period and have significant effects upon the problem should be included in the neutronic analysis portion of SAS2 (to ensure the current spectrum calculation), the code automatically introduces the most important nuclides in trace amounts (10^{-20} atoms/b-cm) to the fuel mixture MX=1 if they are not already input by the user. These automatically supplied nuclides must be on the master library and in the list for /FUELID/ (see Sect. S2.4.9 and Table S2.2.1). Other nuclides may be input by the user by entering SC (e.g., TH-232) and also MX=1, VF=0, and ADEN=1-20.

Other mixture numbers ($MX \geq 4$) apply to either the larger unit cell of the SAS2H model or the multiregion geometry shipping cask case. The user may refer to Fig. S2.2.2 and Data Note B for details of how the mixture numbers of the larger unit cell are applied in the complete cell description. This more complex geometry represents the fuel assembly coupled with the spider assembly containing either guide tubes, burnable poison pins, or rods of some other type. Also, channel moderator (between assemblies) and the casing or housing enclosing the assembly in some designs, require mixture numbers. In particular, mixtures (other than 2, 3, or 500) specified by MXTUBE, MIXMOD, or MIXES, in Data Blocks 7–8 require standard composition specifications for the mixture.

Since part of the light elements (e.g., clad elements or alloys) are not depleted by SAS2 during the library production of the burnup analysis, the following special selection conditions are used to determine which light-element nuclides are acceptable for depletion in ORIGEN-S during the library production portion of SAS2.

1. The light-element nuclide must be input as a standard-composition (SC) isotope, instead of an element or an alloy. WTP entries change elements appropriately to isotopes. Refer to Table M8.2.1 in Sect. M8 to determine if a standard composition is a SC isotope. It must represent a single nuclide whose numeric ID is not a multiple of 1000.

2. The nuclide density must be at least 10^{-10} atoms/b-cm.

3. The mixture number, MX, partly controls its selection. Only the fuel-zone (MX=1) and the clad-zone (MX=2) nuclides, except for ^{1}H and ^{16}O, are depleted in mixtures of the fuel-pin case. This excludes nuclides in the moderator (i.e., MX=3). In the larger unit cell case, in addition to the fuel-zone nuclides, any other light-element nuclides for which $Z<84$ (where Z is the atomic number) and $4 \leq MX \leq 10$ are acceptable for depletion.

4. When a nuclide appears more than once in nonfuel zones of the larger unit cell, the one with the largest acceptable mixture number is used.

5. When a nuclide is acceptable to both the larger unit cell and the fuel pin cell, the one with the larger mass per assembly calculated by the code is used.

The light elements selected by the above criteria are included in the ORIGEN-S case of each pass, and the depleted number densities are used in the neutronics codes to update the cross-section libraries. The effect that other light elements have on the ORIGEN-S input power-to-flux conversion is considered by including the light elements input in Data Block 10 (and not selected by the above criteria). If a light-element nuclide is being depleted in accordance with the above criteria and it is not included in the data associated with Data Block 10, the densities input for the neutronics codes are converted to the weight per assembly for use in the final assembly depletion computation by ORIGEN-S. Also, if the mixture in which the nuclide is being depleted in the library passes is not the only material containing the nuclide, the correct total quantity of the nuclide may be depleted in the final ORIGEN-S case by including it in Data Block 10. (Also, see Data Note D on light elements of fuel assembly.)

The above rules prevent neutron depletion from being computed for moderator (MX=3) boron which is changed by input and/or linear interpolation (see Sect. S2.2.4). The moderator boron input in the standard composition specification should be the average (midpoint) boron for the first irradiation cycle. Over a cycle irradiation time (input as BURN entry in Data Block 9), a linear interpolation (assuming 1.9 times the average initially and 0.1 times the average at the end) is used to determine the appropriate boron level (at the midtime between libraries) if multiple libraries per cycle are requested (NLIB/CYC of Data Block 7). Average moderator boron levels for later cycles are set by entering BFRAC in Data Block 9. This entry value is used in each cycle to multiply the first-cycle boron level to obtain the correct average boron.

As stated above, mixtures denoted by $MX \geq 4$ pertain to either the larger unit cell or materials to be used in the shipping cask analysis. Three of the materials in the shipping cask are not input as standard composition data of Data Block 4. They are (1) the spent fuel material, which is computed and applied by the code; (2) the clad, which is derived from the code for each fuel zone; and (3) the shipping cask coolant (or part of the coolant, at least, as explained below), which is derived from other input data. These three materials are part of that contained in a cask fuel zone (see Data Note E).

For each shipping cask fuel zone, a unique mixture number must be available to identify the extra material to be added to the zone for the shielding analysis. The extra material mixture identified for a fuel zone is combined with the spent fuel mixture and then the total mixture (spent fuel plus extra material) is identified in the code with the unique "extra material" mixture number input by the user. For K fuel zones, the extra material mixture numbers must be MX=3+k, k=1, K. Nonfuel zones then must have mixture numbers MX>3+K. If no extra material is desired for a fuel zone, the user should supply a dummy mixture with VF=0 and ADEN=1-20 to be used in the MXZ entry of Data Block 13 for the fuel zone.

Extra material to be included in a shipping cask fuel zone is determined with the same methods as used for other materials. Its zone-averaged atom density may be entered in ADEN, or, if an element or compound is at full theoretical density, its volume fraction in the zone may be entered in VF. Otherwise, VF = (fraction of the zone volume) * (fraction of theoretical density). Usually, for the wet cask, extra water

(water in the cask cavity but not included in the pin cell description) must be added by using the following rule. Compute the extra water volume from:

$$V_{water} = \text{(the zone volume)} - \text{(other extra material volume)} - \text{(FUELBNDL*NPIN/ASSM*PITCH}^2\text{*FUELNGTH)}, \quad \text{(S2.5.1)}$$

where the last line is the total volume of all the pin cells in the cask as computed by the input provided in Data Blocks 7 and 14. Using V_{water}, the volume fraction VF may be derived.

The code uses the material and geometry input data for the fuel pin cell, the final spent fuel inventory, the number of pins per assembly (NPIN/ASSM entry of Data Block 7), the number of assemblies per cask (sum of FUELBNDL entries in Data Block 14), and the fuel length (FUELNGTH entry of Data Block 7) to calculate the appropriate material number densities for the cask fuel zones. Note that setting DRYFUEL=YES removes that part of the shipping cask coolant (specifically H_2O compositions) in the fuel zone derived from the input moderator mixture MX=3 (a necessity to ensure a "dry" cask).

Certain limitations of SAS2 are required for LMFBR cases. The LMFBR ORIGEN-S library must be input to SAS2 on unit No. 21. Since sodium is the reactor moderator, either sodium must be the shipping cask coolant or a dry cask case must be applied. Changing to water is not an available feature in the present SAS2 code.

Data describing the gap between fuel and clad may be omitted in the reactor-lattice data. The differences in results between the use of hot or cold dimensions usually is not significant, if total fuel per assembly is the same.

Water densities at various pressures and temperatures may be interpolated from Tables S2.5.2 and S2.5.3, which were computed by the DENH2O routine borrowed from the LEOPARD-II code.[21] These data may be used in deriving VF for the reactor moderator or DENFM for the shipping cask coolant.

S2.5.4.2 Note B, Assembly, Larger Unit Cell, and Cycle Parameters

This data note discusses the input in Data Blocks 7–9.

The number of fuel rods/assembly, NPIN/ASSM, for a square-lattice of the reactor, is usually smaller than the square of the number of rods per row, (i.e., there are guides and control rods in the assembly). The actual number of pins in an assembly should be input.

The time for each reactor cycle (entries of Data Block 9) may correspond to (1) the time between reactor refueling (traditionally one year), (2) shorter times, at which the history changes (due to power steps or shutdowns), or (3) the complete irradiation time of the assembly. The latter option is used to only approximately represent the average history and requires the least computer time. The user determines NCYCLES, the total number of cycles. NLIB/CYC is the number of equally spaced libraries produced per cycle irradiation time, BURN. The total number of libraries produced for the final depletion calculation equals NCYCLES*NLIB/CYC. For each cycle, the average moderator boron concentration can be set using the multiplier BFRAC of Data Block 9. The value of BFRAC is multiplied by the boron number density in the moderator (MX=3) to obtain the average boron for a cycle. If NLIB/CYC>1, then the boron concentration for the midtime between libraries is obtained using the average boron concentration and a linear interpolation (assuming 1.9 and 0.1 times the average boron is present at the start and completion of the cycle, respectively). If the actual boron curve over the cycle time cannot be reasonably approximated by this linear interpolation, then the number of cycles should be increased and NLIB/CYC set equal to one. The boron change over the reactor history can then be approximated using the BFRAC entry. Note that if H2OFRAC and BFRAC are equal, the boronconcentration remains constant. Where important shutdowns or power magnitudes change within the refueling cycle, it may be logical to increase the number of cycles.

Table S2.5.2 Density of subcooled water (g/cm^3) at various temperatures and pressures

Temperature (°C)	Temperature (°F)	Pressure, psia								
		3000	2500	2000	1500	1000	800	600	400	200
10.0	50	1.0084	1.0069	1.0055	1.0040	1.0025	1.0019	0.0013	1.0007	1.0000
37.8	100	0.0018	0.0004	0.9989	0.9975	0.9960	0.9954	0.9948	0.9942	0.9936
65.6	150	0.9893	0.9878	0.9864	0.9849	0.9834	0.9828	0.9822	0.9815	0.9809
93.3	200	0.9725	0.9709	0.9694	0.9679	0.9663	0.9656	0.9650	0.9644	0.9637
121.0	250	0.9522	0.9505	0.9489	0.9472	0.9455	0.9449	0.9442	0.9435	0.9428
148.9	300	0.9289	0.9271	0.9252	0.9234	0.9215	0.9208	0.9200	0.9192	0.9185
176.7	350	0.9026	0.9006	0.8985	0.8964	0.8943	0.8934	0.8925	0.8916	
204.4	400	0.8733	0.8709	0.8685	0.8660	0.8634	0.8624	0.8613	0.8603	
232.2	450	0.8405	0.8375	0.8345	0.8314	0.8281	0.8268	0.8255		
260.0	500	0.8029	0.7992	0.7952	0.7911	0.7869	0.7851			
265.6	510	0.7947	0.7907	0.7866	0.7822	0.7776				
271.1	520	0.7862	0.7820	0.7776	0.7729	0.7680				
276.7	530	0.7775	0.7729	0.7682	0.7632	0.7579				
282.2	540	0.7683	0.7635	0.7584	0.7530	0.7472				
287.8	550	0.7589	0.7537	0.7482	0.7423					
293.3	560	0.7490	0.7434	0.7374	0.7310					
298.9	570	0.7386	0.7326	0.7261	0.7190					
304.4	580	0.7278	0.7212	0.7141	0.7062					
310.0	590	0.7164	0.7092	0.7012	0.6923					
315.6	600	0.7043	0.6963	0.6874						
321.1	610	0.6915	0.6825	0.6724						
326.7	620	0.6777	0.6676	0.6558						
332.2	630	0.6629	0.6512	0.6370						
337.8	640	0.6467	0.6329							
343.3	650	0.6288	0.6119							
348.9	660	0.6086	0.5866							
354.4	670	0.5850								
360.0	680	0.5559								

Table S2.5.3 Water densities (g/cm^3) in low range of temperatures and pressures

		(Computed by the DENH2O routine) Pressure, psia				
Temperature (°C)	Temperature (°F)	≤25	50	100	150	200
10.0	50	0.9995	0.9996	0.9997	0.9999	1.0000
23.9	75	0.9972	0.9973	0.9974	0.9976	0.9977
37.8	100	0.9930	0.9931	0.9933	0.9934	0.9936
51.7	125	0.9874	0.9874	0.9876	0.9877	0.9879
65.6	150	0.9804	0.9805	0.9806	0.9808	0.9809
79.4	175	0.9723	0.9724	0.9725	0.9727	0.9728
93.3	200	0.9632	0.9632	0.9634	0.9636	0.9637
107.2	225	0.9531	0.9532	0.9534	0.9535	0.9537
121.0	250		0.9423	0.9425	0.9426	0.9428
135.0	275		0.9305	0.9307	0.9309	0.9311
148.9	300			0.9181	0.9183	0.9185
162.8	325			0.9046	0.9049	0.9051
176.7	350				0.8905	0.8908
190.6	375					0.8755
	ρ-sat (T-sat, °F)	0.9467 (115.6)	0.9276 (138.3)	0.9035 (163.9)	0.8858 (181.1)	0.8717 (193.9)

In addition to the standard type fuel pin, a second type of rod or guide tube may be included in the SAS2 assembly model description. Unless "PARM=OLDSAS2" is denoted on the module activator card (see Sect. S2.5.6), a larger-unit-cell description is required in the input. Two examples of the larger unit cell are shown in Fig. S2.2.2. The cell geometry starts with the INPLEVEL entry of Data Block 7. The four input level requirements are discussed below.

Level 0 Data Block 7 requires no additional input data. A PWR control rod assembly is developed from the fuel pin cell and number of fuel pins input plus an assumed guide tube size. Default data are given below. If the INPLEVEL entry is omitted (giving level 0 input by default), the END entry must be excluded and Data Block 8 is skipped. Even though the input data can be identical to that if PARM=OLDSAS2 is specified, the older version assumes an infinite lattice of fuel pin cells and does not include the effect of water holes and guide tubes.

Level 1 This input level uses the same assembly design model (i.e., Fig. S2.2.2(a) with fuel pins and an empty guide tube) as that in level 0, except that the guide tube and assembly pitch data may be specified.

Level 2 This input level is needed for all other types of PWR and BWR assemblies and allows the larger unit cell model to be specified.

Level 3 Input for this level is explained in Appendix S2.A. INPLEVEL=3 is a more complex method of providing user-supplied data to each functional module and allows more complex models to be evaluated. However, the adding of changing of one or two parameters from that set in level 2 input, usually is not difficult.

All the following defaults are applied in level 0 input and also in other input levels when required and not overridden:

MXTUBE = 2;
MIXMOD = 3;

$$\text{NUMHOLES} = (\sqrt{\text{NPIN/ASSM}}|_{\text{trunc}} + 1)^2 - (\text{NPIN/ASSM}) - 1;$$

NUMINSTR = 1;

$$\text{ASMPITCH} = (\sqrt{\text{NPIN/ASSM}}|_{\text{trunc}} + 1)(\text{PITCH});$$

ORTUBE = (0.5)(PITCH) - 0.05;
SRTUBE = ORTUBE - 0.045085.

All the above variable names are defined in Data Block 7 (except PITCH, which is found in Data Block 5) of Table S2.5.1. The equation for NUMHOLES assumes one instrument tube and NPIN/ASSM $\geq (N-1)^2$ for an N×N assembly lattice. These conditions may not always be correct, and, if not, the user may apply corrected data in level 1 input. The equation for ASMPITCH assumes the same conditions and no additional channel space. Although ORTUBE is arbitrary, the thickness of the guide tube is the average of that found in a 15×15 and a 17×17 fuel assembly. The mixtures used for the clad and moderator are the same as those used in the fuel pin cell calculation. The mixture number of the fuel zone is always set internally by SAS2 to 500. The mixture 500 composition is computed internally by the code using cell-averaged or homogenized densities of the fuel-pin-cell case.

Six of the seven default values of level 0 input may be changed in level 1 input. The other parameter, MIXMOD, can be only changed by level 2 input. Note that changing MXTUBE to another mixture number requires a standard composition (with SC, etc.) for the mixture.

Level 2 input is more detailed and requires an explicit geometry description of the entire larger unit cell, as depicted in Fig. S2.2.2(b). The "second" type of pin, different than the fuel pin, is at the center of the cell. The moderator surrounding it has an outer radius which should be equal to the maximum radius of the fuel pin cell (producing an area of PITCH^2). Then the fuel zone should be next, with an outer radius that conserves the fuel/moderator volume ratio and a mixture number always set to 500. Finally, zones such as a fuel element casing or channel moderator may be given outside the fuel zone. Note that a different moderator composition from that of the fuel could be used. Often there is no change in the moderator components, but their density is different. This density change can be input by adding standard composition data using new densities with a different mixture number.

There are cases in which the coupled assembly is changed during reloading to a different type, such as from a burnable poison assembly in one cycle to a control rod assembly in the next cycle. A different set of mixture numbers and radii can be input for each library produced by setting MXREPEATS=0. The MIXES and RADIUS data must be repeated NCYCLES* NLIB/CYC times, if MXREPEATS=0. If a nuclide is produced essentially from one of the nuclides being removed as part of an unloaded mixture, the product nuclide is also unloaded (as may be necessary in the evaluation) only by including it with a density $\geq 10^{-10}$ atoms/b-cm as part of the same mixture.

All burnable poison assemblies (for either BWR or PWR fuel) require level 2 input data. Note that the neutron poison element may be contained either within a fuel pin or within a rod containing only light elements. When fuel and burnable poison are in the same pin, the standard composition specification data for the fuel and burnable poison element or isotopes should have the same mixture number and the fuel composition cannot be changed from that of the standard fuel pin in the assembly. Since the SAS2 method

does not deplete more than one set of fuel densities in these cases, the code sets the fuel composition to be uniform throughout the fuel and burnable poison region. Even though constant fuel density and enrichment are assumed, the effects from the flux changes due to the neutron poison, as well as that from zones outside of the fuel zone, are weighted into the final cross sections.

The models utilized by SAS2, either in path A or path B, always assume a constant material composition and power in the axial direction of the fuel assembly. Even though only a part of the assembly designs have axial variations in fuel and burnable poison compositions, there are axial changes in moderator densities and power in all assemblies. The approximation used to determine the average water density may have a significant effect upon the results.

The axial moderator density of the PWR assembly, in general, changes considerably less than that for the BWR. Thus, a frequent practice in using SAS2 for PWR assemblies is to derive the average density from Table S2.5.2, using the water pressure and the average core temperatures. Of course, accurate values of axial water densities and powers could be used to derive a power-weighted value as a better effective density. However, in PWR cases, there probably would not be a highly significant change in the results from this method because the density change is not extremely large.

A much greater axial change occurs in the moderator density in fuel assemblies for the BWR than those for the PWR. Consequently, it has been shown that a significantly improved approximation of the effective water density in the BWR is an important requirement in achieving more nearly the same accuracy in isotopic results for the BWR as that obtained for the PWR. In general, the BWR assembly is contained within a casing, which separates the water into the fuel zone moderator and the channel moderator. There are different methods of obtaining "effective" moderator densities. Acceptable values of effective moderator density may be known from previous analyses. If moderator density and relative power are known as a function of axial zone, a power-weighted density may be applied. When the data are available at various fuel burnups, the densities may be changed in SAS2 for each cycle used. Where only the moderator densities are given, BONAMI-S, NITAWL-II, and XSDRNPM-S may be applied to unit-pin-cell (cylindrical) and slab models to estimate the axial power distribution. In one possible method, only the power for fresh fuel, as derived by these neutronics codes, may be applied. In an extension of this method, preliminary depletion calculations may be used to change the fuel composition and the computed power as a function of burnup or cycle. Also, simple applications of axial densities would be to use either the average density or the volume-weighted density.

Other considerations in making the BWR model may be very significant. Using the same procedure as that described for the PWR plus axial power-weighted moderator densities tends to overmoderate the system and subsequently underestimate the resonance region cross sections. The decreases in computed cross-section values appear to have a major influence on elements heavier than uranium. The following considerations may help reduce the overmoderation bias:

1. Determine the effective axial moderator density from volume weighting instead of power weighting, which is usually significantly larger.

2. Frequently, it is assumed that the density of the water in the channel is that of the inlet or the average of the first node (about 20% of height) of the axial dimension. It may be estimated that this density is constant because there is a very low transfer of heat through the moderator having large void fractions inside the channel tube. However, any density decrease plus the channel water displacement resulting from the average axial position of the control rods may be simulated by reducing the channel moderator density. Even though the reduction may be only estimated, a reasonable decrease (about 10%) may avoid part of the overmoderation bias.

3. Add boron (or ^{10}B) to the channel moderator composition in order to simulate the boron in the cruciform rod and make the average k-effective during the burnup approach unity. It may require one or two trial cases to derive an estimate of the boron density.

4. Do not represent the assembly with larger unit cells containing only one gadolinia-bearing rod per cell. Instead, model one gadolinia-bearing rod at the center, surround with a fuel zone equivalent to all of the remaining rods of the assembly, add the channel tube and moderator, and then insert within the fuel zone a thin ring containing the remainder of the gadolinium of the assembly. Conserve the gadolinium mass by applying the proper volume and density. The volume is determined from the density and mass. The gadolinium density throughout the model is required to remain constant (applying the same mixture number as that of the central gadolinium zone) in order to permit the single density depletion limit by SAS2 to be correct in both zones. Also, place the gadolinium ring at a position so that the fuel zone area external to the center of the ring is equal to the area of the fuel pins surrounding the gadolinium pins in the assembly. This method of splitting the assembly in the model of the larger unit cell avoids a significant bias in the moderation of the system and tends to outweigh the somewhat local influence of the gadolinium, which rapidly becomes depleted during part of the first operational cycle.

As can be surmised from the previous discussion, development of a BWR assembly model that gives accurate results is not a straightforward task. The user should be careful in the selection of a final model for his application. References 32 and 41 provide good examples of BWR models developed for SAS2H. In particular, Ref. 41 is interesting because three separate SAS2H cases were used to represent, respectively, the top, middle, and bottom regions of the fuel assembly. Use of three cases allowed the changing axial moderator density to be considered more accurately.

S2.5.4.3 Note C, Control of Print Level

The quantity of printed output is determined in SAS2 from the value entered for PRINTLEVEL in Data Block 7. The range of integers between "1" and "10," inclusive, produce substantially different quantities of print. Information such as problem definitions, various monitor data, and certain computed results are printed without a user option. Other data, which the user may apply for analyzing quality or other purposes, are allowed to be optional. The entry of PRINTLEVEL=L (where L is an integer in the range 1 to 10, inclusive) will produce all tables triggered by the value of L. Lower L-values usually produce the most important tables. For $L \geq 7$, the quantity of output is extremely large; so unless particular data from the option are needed, the user is recommended to input $L \leq 6$. PRINTLEVEL values of 4, 5, and 6 are most frequently applied. The default is L=4.

Table S2.5.4 is presented to describe the L-values required for optional tables. A type of table produced by a functional module may have different L-values for different types of cases executed by the code. These case differences are listed on lines below the table name. When there is no difference for all cases, a single L-value is given. The print cutoffs in D under ORIGEN-S apply to the preceding table output described in A, B, and C, and pertain to tables printed for the specified "units." The note "Not Used" means that another type of computation of the data, printed elsewhere, is performed for the application by SAS2.

The print produced by the neutronics modules for the larger unit cell case is not directly specified in Table S2.5.4. However, the print controls for XSDRNPM-S in executing these cases (the large cell of the SAS2H model) are precisely the same as for the second and later pin-cell depletion cases. The prints produced by higher print levels in BONAMI-S and NITAWL-II for the pin-cell cases are not produced by any print level for the larger unit cell cases. There would tend to be less interest in these prints. (Often there are no nuclides processed with resonances for these cases.) If the prints are absolutely necessary, they may be requested in the level-3 input for the case.

Table S2.5.4 Print produced by PRINTLEVEL=L
(Default: PRINTLEVEL=4)

Tables printed, if L meets required L-value (apply to all cases, unless specified)	Required L-value
BONAMI:	
A. Shielded Cross Sections	
1. No edit in first pin-cell case	--
2. All other cases	L≥6
B. Bondarenko Factors	
1. No edit of first pin-cell case	--
2. All other cases	L≥7
NITAWL-II:	
A. Reaction Cross Sections	
1. No edit of first pin-cell case	--
2. Other pin-cell depletion cases	L=10
3. Cell-weighted shield case	L≥9
4. Region geometry shield case	L≥9
B. P_0 Transfer Cross Sections	
1. Region geometry shield case	L=10
2. No edit of other cases	--
XSDRNPM-S:	
A. 1-D Mixture Cross Sections	L≥8
B. P_3 Mixture Cross Sections	L=10
C. Scalar Group-Interval Fluxes	
1. First pin-cell depletion case	L≥5
2. Other pin-cell depletion cases	L≥4
3. Cell-weighted shield case	L≥5
4. Region geometry shield case	L≥1
D. Angular Fluxes	
1. Region geometry shield case	L=10
2. No edits of other cases	--
E. Fine-Group Balance Tables	
1. Region geometry shield case	L≥1
2. All other cases	L≥2
F. Broad-Group Balance Tables	
1. All pin-cell depletion cases	L≥8
2. Not collapsed in shield cases	--
G. Weighted 1-D Cross Sections	
1. None in region geometry shield case	--
2. All other cases	L≥7
H. Weighted P_0 Transfer Cross Sections	
1. None in region geometry shield case	--
2. All other cases	L=10
I. Zone Dose Rate Activities	
1. Region geometry shield case	L≥1
2. None for other cases	--
J. Interval Dose Rate Activities	
1. Region geometry shield case	L≥1
2. None for other cases	--

Tables printed, if L meets required L-value (apply to all cases, unless specified)	Required L-value
ORIGEN-S:	
A. Light Element Concentrations	
1. Exposure, if depleted, g-atoms	L≥1
(Note: Below are decay case table units.)	
2. Nuclides listed, grams	L≥5
3. Elements listed, curies	4≤L≤6;L=10
4. Nuclides listed, curies	L≥7
5. Elements listed, watts	4≤L≤6;L=10
6. Nuclides listed, watts	L≥7
7. Elements listed, γ-watts	L=4;L=10
8. Nuclides listed, γ-watts	L≥5
9. Nuclides listed, m^3 air for guide	L≥9
10. Nuclides listed, m^3 water for guide	L≥9
B. Actinide Concentrations	
1. Exposure cases, nuclides, g-atoms	L≥1
(Note: Below are decay case table units.)	
2. Elements listed, g-atoms	L≥1
3. Nuclides listed, g-atoms	L≥1
4. Elements listed, grams	L≥3
5. Nuclides listed, grams	L≥3
6. Elements listed, curies	4≤L≤5;L=10
7. Nuclides listed, curies	L≥6
8. Elements listed, watts	4≤L≤6;L=10
9. Nuclides listed, watts	L≥7
10. Elements listed, γ-watts	L=4;L=10
11. Nuclides listed, γ-watts	L≥5
12. Nuclides listed, m^3 air for guide	L≥9
13. Nuclides listed, m^3 water for guide	L≥9
C. Fission Product Concentrations	
1. Exposure cases, nuclides, g-atoms	L=10
(Note: Below are decay case table units.)	
2. Elements listed, g-atoms	L≥9
3. Nuclides listed, g-atoms	L≥9
4. Elements listed, grams	L≥4
5. Nuclides listed, grams	L≥4
6. Elements listed, curies	4≤L≤5;L=10
7. Nuclides listed, curies	L≥6
8. Elements listed, watts	4≤L≤6;L=10
9. Nuclides listed, watts	L≥7
10. Elements listed, γ-watts	L≥5
11. Nuclides listed, γ-watts	L≥4
12. Nuclides listed, m^3 air for guide	L≥9
13. Nuclides listed, m^3 water for guide	L≥9

Table S2.5.4 (continued)

Tables printed, if L meets required L-value (apply to all cases, unless specified)	Required L-value
D. Nuclide Concentration Print-Deletion-Cutoffs (Cutoff tested at fifth time step.)	
1. Exposure: 1E-8 atoms/b-cm or g-atoms of element	L≥1
2. Decay cases: g-atoms, grams, curies	
a. 1E-6	L=4
b. 7E-7	L=5
c. 5E-7	L=6
d. 1E-7	L≥7
3. Decay cases for all other units	
a. 1E-8	L≥4
b. 7E-9	L=5
c. 5E-9	L=6
d. 1E-9	L≥7
E. Time-Dependent Cooled Photon Spectra (not used)	L≥4
F. ORIGEN-S Cooled Neutron Source Used	L≥4
G. Cooled Fuel Assembly γ-Spectrum Used	L≥1
H. Neutron Absorption and k_∞, Final Case	
1. Neutron production, absorption and k_∞	L≥5
2. Fission product absorption fraction	L≥6
3. Absorption fractions of all nuclides	L≥7
XSDOSE:	
A. Dose Rates at DTEC in Midplane	L≥1
B. Dose Rates at DTEC in Planes FUELENGTH/4 and FUELENGTH/2 from Midplane	L≥7
SAS2:	
Special edit of code interfaces, as written, and later, as updated. "Debug" type of arrays and scalers	L≥7
printed. Some are printed also by using HALTXX.	L≥1
Since triggers are L=10 or L<0, apply absolute value of L in the above tests.	L≥1 L=10,L≤0

*The spectrum is identical. The print may be desired in the first case pass when the case is halted after that pass.

S2.5.4.4 Note D, Light Elements of Fuel Assembly

It is not required to input the light elements of the fuel assembly other than the input of clad, guide tubes, and burnable poisons as standard compositions (SC) in the execution of SAS2. Also, the default, LIGHTEL=0, may be applied. However, there are cases in which a significant improvement in the computed dose rates and isotopic quantities may result from specifying LIGHTEL>0 in Data Block 7 and listing the light elements in Data Block 10.

The improvement in results for LIGHTEL>0 is caused by two features. First, the energy computed from Q-values of neutron reactions with the atoms of the light elements are applied in converting power to flux in ORIGEN-S. Secondly, the gamma source spectrum computed by ORIGEN-S includes all photons emitted from the activation products of light elements in addition to that of actinides and fission products.

The weights of elements entered in this part of the input do not affect densities in the neutronics analysis, which uses only the standard compositions (SC) entered in the unit-cell material description.

The quantity input for each light element should be the weight, in kilograms, of that element in all of the clad and structural material [e.g., spacers, contained along the active fuel length (FUELENGTH) of the assembly]. The material is assumed by SAS2 to be uniform in the axial dimension. A user may also wish to calculate activation products of light elements in the end fittings and plenum regions of the assembly by using the input of Data Block 10. However, since these light elements are not in the fuel region, their input quantity needs to be reduced to correspond to the estimated change in the absolute magnitude of the neutron flux and shifts in the neutron spectrum. References 23, 42, and 43 discuss the reduction (or scaling factors) needed for different assembly regions and different light elements.

When data are available, the user may include almost all elements of the clad and structural materials in order to be complete. However, many elements have only a minor effect upon the results and could be omitted. The importance of a nuclide in the conversion of power to flux may be derived by comparing the product of its absorption reaction Q-value times its reaction rate per assembly with the product of 200 MeV times the fission reaction rate per assembly of the major fissile isotopes. A simplified formula was derived as a first-order measure of F, the percentage increase in the energy per fission from the inclusion of a given nuclide. A Q-value of 5 MeV was assumed, since the reaction energy Q-value of most nuclides is in the vicinity of this value or smaller. A 3.3 wt % ^{235}U PWR fuel assembly was applied. Then,

$$F \doteq 0.1\, M\sigma_a/A\ , \qquad \text{(S2.5.2)}$$

where

A = atomic mass of the nuclide,

σ_a = nuclide (ORIGEN-S) absorption cross section, b,

M = nuclide mass/assembly, kg.

For example, if $A = 50$, $\sigma_a = 3$ b, and $M = 50$ kg, then $F = 0.3\%$. The formula given by Eq. (S2.5.2) should be applied only as a guide for determining the importance of including an element as input and should not be considered to be exact.

The gamma source produced from light elements is usually more important to the final dose rates than the percentage increase in energy per fission from light elements. Material of high-cobalt content and spent fuel that is cooled for several years or more are conditions where light-element activation products need to be considered. In a case applying a 90-day cooling time, about 1% of the gamma source of the spent fuel assembly is from cobalt. Other elements producing at least half the source strength of cobalt are zirconium and niobium. It was determined that the cobalt produced 1.5% of the total dose rate, by comparing the sample case with results computed in a similar case without including cobalt in the input. Another comparison was made between cases, where the decay time was changed to a 5-year cooling time. The contribution from cobalt was 28% of the gamma dose rate and 17% of the total dose rate. A case applying a 10-year cooling time indicated a higher fraction of the gamma dose rate from cobalt and about the same fraction of the total dose rate from cobalt. (Of course, these fractions may be cask-design dependent.) In essence, these cases illustrate the large significance that cobalt content can have in the final results. The user may be able to obtain good estimates of the cobalt content of materials or, possibly, use a safety factor commensurate to the intended application of the results. Furthermore, the user may decide to omit cobalt and other light elements from the input, upon consideration of their importance.

S2.5.4.5 Note E, Zone Description of Cask

The zone description of the shipping cask is somewhat similar to geometry information input to other codes (e.g., XSDRNPM). A single mixture number identifies all the components in the material definition data that are uniformly "mixed" in a single material zone. In order to prepare data, the user may depict the cross-sectional area of the shipping cask as a number of concentric circles. The radius of each circle represents the boundary between different materials. The innermost nonfuel zone would be identified by mixture number 4+K, where K is the number of fuel zones (see Data Note A), the mixture of the next nonfuel zone by 5+K, and incrementing each mixture number by 1. When a nonfuel zone contains a material identical to that in a previous nonfuel zone, an identical mixture number may be used. Each pair of a mixture number, MXZ, and a corresponding outer radius bounding the mixture, R, are repeated in the input for NUMZONES number of times. The radii must be in ascending order. The zone number, which is not input, is identified by the position of the pair MXZ= and R (i.e., the first pair represents zone number 1 or the most central zone, etc.).

Fuel elements may be contained either in one or more zones, depending upon the cask design. The fuel zone number and number of assemblies in the zone are entered for every fuel zone, as described in the input table. SAS2 limits the number of fuel zones allowed to five. The densities of "extra" material in the fuel zone, which is not in the fuel assembly, must be computed from proper consideration of fuel zone radii (see below). Data Note A discusses the need to define a unique mixture number of "extra" material for each fuel zone. The spent fuel isotopics are added to this "extra" material mixture to create the fuel zone mixture which is identified by the "extra" mixture number input by the user.

Since the SAS2 1-D radial calculation requires the definition of zones as concentric cylinders, the square geometry of assemblies must be approximated. Even though the method applied is a user decision, two examples are presented in the following. Consider that a square array of four fuel elements are at the center of the cask. (A special convention should be used to represent the cross-sectional area of an assembly in order to be consistent with the SAS2 conversion of unit-cell densities to zone-averaged densities. An assembly having an N×N square lattice and a pitch, P, is depicted by a square having sides equal to N*P.) In the first example compute the area of the square that circumscribes the four fuel elements, as depicted by the SAS2 convention. Then, compute the radius of the circle that has an equal area. This is the radius applied as that of the fuel zone. This method conserves volume and maintains equal zone-averaged densities between the square and circular representations of the zone. The square geometry tends to cause the dose rate on the cask surface at the midplane to be a variable; the maximum values are at the intersections with the extended diagonals of the square, and the minimum values are at midpoints along the arc between adjacent maximum points. The volume conservation method is expected to produce dose rates that are near the average of the variable values. In the second example, the inner zone radius is taken to be the distance from the center to the comer of the square circumscribing the four fuel elements. This method would tend to produce a dose rate greater than that from the first method. More than one fuel zone may be applied if there are a larger number of fuel assemblies and significant space and/or shielding material (i.e., a basket wall) between them.

S2.5.4.6 Note F, Optional Flux-to-Dose-Rate Factors

The flux-to-dose-rate factors applied, as the default, in SAS2 are multigroup values derived from those in the ANSI Standard. It is recommended that these be applied by the user, because they were the choice of evaluators and applying others can result in a degree of confusion. However, since a user may want to apply other dose conversion factors, the option was made available by entering a negative value for DETECTORS. Then, for all sets available on the SCALE library, ALIB, the dose conversion factors identified by any of the following MT numbers will be applied: 9001, 9002, 9026, 9027, 9028, 9029, 9501, 9502, 9503, and 9504. An edit of the SCALE library shows which of the MT numbers are on the library (the identifier is ID=900). Also, XSDOSE prints the identification title of all dose conversion factors requested and applies those available on the SCALE library. The identification title of the above dose conversion factors is listed in Table S1.4.8.

S2.5.5 INPUT/OUTPUT UNIT REQUIREMENTS

A job control procedure for IBM systems is included as a file on the SCALE tape received by users. The statements in this section assume the use of this job control procedure. Otherwise, the job control language (JCL) should include the data set definitions for the proper libraries and all scratch data sets, with parameter modifications as indicated. Some of the data set definition parameters are problem-dependent. For example, larger-group libraries may require increases in the SPACE parameters of some IBM data sets.

Applying 27-Group Libraries

Table S2.5.5 presents a list of I/O requirements for most problems that apply the 27 neutron-group SCALE library in the depletion cases and the 27n-18γ-group SCALE library in the shield cases. All the data sets for units listed in the table are scratch data sets, unless the "restart" feature is being applied. Other data sets (permanent) which are accessed by SAS2 are the ORIGEN-S Binary Working Library on unit 21; the Master Photon Data Base on unit 26; and SCALE cross-section libraries selected from units 81-88, inclusive.

Note that the space used on a unit may be problem-dependent. The required allocation with the IBM SPACE parameter is dependent upon track size and the tracks per cylinder. The space allocation specified in Table S2.5.5 and the SCALE procedure (where there is no override) is intended to be adequate when the units are either 3330 or 3350 unit types. However, there is no guarantee that these allocations will provide the required space for all problems encountered. When there is inadequate space (i.e., a B37 message code on mainframe IBM systems), increase the space substantially and resubmit the case.

In addition to the I/O requirements of Table S2.5.5, other scratch data sets and three permanent data sets are required. Because all of these data sets are in the procedure, they will automatically be allocated on the IBM system for any SAS2 case. An input ORIGEN-S binary library, which determines the nuclides available to the ORIGEN-S cases, is on unit No. 21. The specific applications of all of the scratch data sets used by the various functional modules are not presented in this section. Except for the space allocation requirements given in this section, the additional information is not usually needed in using SAS2 with the SCALE job control procedure for IBM systems.

Applying Larger-Group Libraries

SCALE libraries with group structures as large as 218 groups have been applied in the depletion cases by SAS2. Numerous space allocation increases were required. Important size parameters were ISN=8 (default) and SZF=0.87, producing 22 mesh intervals (more than default). The space sizes were adjusted to that required by a 218-group structure library and application of 3350 type units. The space allocations, after adjustment, are as follows:

```
Unit 1, SPACE=(TRK,(2000,40))
Unit 4, SPACE=(TRK,(500,40))
Unit 8, SPACE=(CYL,(6,1))
Unit 9, SPACE=(CYL,(13,1))
Unit 12, SPACE=(TRK,(1500,30))
Unit 16, SPACE=(TRK,(80,20))
Unit 18, SPACE=(TRK,(1500,20))
Unit 19, SPACE=(TRK,(50,20))
```

Table S2.5.5 I/0 requirements for mainframe IBM system

(Unit numbers and parameters listed are either essential or recommended for problems using 27-group libraries. When these are not listed, the override is usually not necessary. The order of units through unit 90, inclusively, is the same as the SCALE IBM procedure and may not be changed.)

Unit No.	SPACE[a] TRK,(I,J)	RECFM	LRECL	BLKSIZE	BUFL	Purpose
1		VBS	X	9440	10232	Scratch (Master Library for NITAWL-11)
4		VBS	X	9440	10232	Scratch (Working Library from NITAWL-11)
12		VBS	X	9440	10232	Scratch
13		FA		133	150	ORIGEN-S FIDO edit
14		VBS	X	9440	10232	XSDRNPM path B flux
15		VBS	X	9440	10232	COUPLE output library
16	200,80					XSDRNPM angular fluxes
17		VBS	X	9440	10232	Scratch
18		VBS	X	9440	10232	Scratch
19		VBS	X	9440	10232	Scratch
90	10,8					Master Interface (Sect. S2.4.8)
33[b]	30,5	VBS	X	9440	10232	ORIGEN-S multi-burnup binary library
70	10.8	VBS	X	9440	10232	Supplementary Interface (Sect. S2.4.8)
71[c]	10,5	VBS	X	9440	10232	ORIGEN-S concentrations
72[d]	10,5	FB	80	6400		BCD, SAS2 concentrations
74	2,2	FB	80	800		ORIGEN-S, n,γ-spectra
53	90,5	FBS	X	3664	4088	XSDRNPM path A model flux
55[e]	2,1	FBS	X	3664	4088	Driver halt data

[a]Applies to either 3330 or 3350 unit types in IBM-type computers. If blank, use mainframe procedure.
[b]For further description and format, see Sects. F6.5.1, F7.6.3, M6.1.2, and M6.7.2.
[c]For the exact format, see subroutine SCALEN in ORIGEN-S code.
[d]Format presented in Appendix S2.B.
[e]Required to be included only for halt, restart, or "skipshipdata" features.

The allocations should be properly corrected for other unit types.

S2.5.6 HALT, RESTART, AND OTHER FEATURES

The "Halt," "Restart," "Keep," and other features are available to reduce the computational cost and allow intermediate computations by other SCALE modules within a single submission of a job. Various parametric studies and projects requiring only intermediate results may be performed with savings exceeding one-half of the cost of the standard complete-type executions. A very short "data check" case may be submitted. Also, cases may be restarted with certain types of data modifications or after an early termination of a prior case, if proper data sets are saved.

The above features are applied through information input on the module activator line (i.e., the line containing "=SAS2"). The SCALE driver permits character data input following the entry of PARM=, with "P" entered in column 11. Then the keywords must be entered following the "=" with no blank spaces permitted in the list. The keywords may be separated by commas if the entire list is enclosed in parentheses or apostrophes. An example is shown below for each feature and their combinations.

The keywords requested using PARM are printed in the output. Do not be surprised to see other keywords listed. Sometimes these extra keywords are added to the PARM list automatically in the IBM job control procedure being used, in order for SCALE to work with various local operating systems. Also, the CRAY log listing may have spaces after every four characters.

Halt Feature:

=SAS2 PARM=HALTii

The "Halt" feature causes the SAS2 case to terminate following the path B calculation of a specified pass through SAS2 and the functional modules invoked by the SCALE driver and the subsequent return from SAS2. Refer to subsections S2.2.4 and S2.2.8 for definitions of "pass." The two characters "ii" specify the number of the last pass to be completed. For example: HALT02 halts SAS2 after the "PASS 2" library is produced; HALT'00 halts it after making the "PASS 0" library; and HALTXX halts it after all preprocessing of data interfaces, making the master interface data sets (on units 70 and 90), and before invoking functional modules. Let J=NCYCLES*NLIB/CYC (see Table S2.5.1), where J is the number of ORIGEN-S libraries produced by the case. If ii=J, the SAS2 case halts after the final ORIGEN-S case and, if ii=J+1, it halts after the cell-weighted fixed source case. Note that ii must be two characters, requiring a zero to precede if ii$\leq$9. Typically, the input for an entire case must be entered, even when not applied before the halt. However, if the SKIPSHIPDATA feature is used, the shipping cask data can be omitted.

One of the objectives of using a "Halt" case is to restart the case later. When the restart feature is used, as explained below, the case begins where the HALTii case terminated with one exception. A HALTXX case may not be restarted at the point of termination. Instead of restarting the HALTXX case, rerun the complete case. Only a small fraction of the case time is used in the part preceding the HALTXX termination. However, when a case has been halted after pass ii, some of the data on units 70 and 90 may be respecified with a HALTXX case before restarting the first case from the point after pass ii.

When a "Restart" case is to be submitted later, the proper data sets must be saved. Always save data on unit 55, since it contains data returned to the SCALE driver for a proper restart. Save data on units 70 and 90 either in the first halt case or a subsequent HALTXX case, which prepares input data modifications to functional module cases that have not been invoked before the halt. Save the "flux data" on units 14 and 53 and atom-density data on unit 72, if ii<J. Also, save all ORIGEN-S libraries produced before the halt, if ii<J or whenever they are to be applied in a later ORIGEN-S case. Save data on unit 74, if ii$\geq$J. Data on unit 71 are required for all "Restart" cases. The concentrations on unit 71 are those at discharge, in the first pair of records, and those after the SAS2 case cooling time (DOWN on last "cycle" card) in the second pair, when ii$\geq$J. When 1 < ii < J, the concentrations in the first two positions on the data set, are those at the midpoint and starting times of the ORIGEN-S library produced by the next pass. The gamma spectrum computed at DOWN is on unit 74. Thus, an ORIGEN-S case may be executed to produce modified data on units 71 and 74. Two examples are (1) the discharged concentrations may be cooled for a different time with updated values written on 74 and 71 (position 2); and (2) elements or nuclides may be added to or removed from the concentrations (e.g., cobalt) before computing the spectrum to be applied by SAS2.

When there is no intention to restart SAS2 or execute another code applying the SAS2 data sets, it is unnecessary to save any of the data sets. However, if SAS2 halts the case when a code execution was unsuccessful (when specifying a halt case), data are written on unit 55 as though it were a halt after the last successful pass. This type of termination can be caused from exceeding the requested lines, I/O counts, or CPU time. A restart may be applied only if the proper data sets were saved.

Restart Feature:

=SAS2 PARM=RESTARTS

The restart feature may be applied only after a successful halt (other than a HALTXX) of a SAS2 case. This rule implies that all proper data sets have been saved, as explained above. The new case simply starts where the halt case terminated. The case continues until completed, if all module executions are successful. **All PARMs input in the previous SAS2 case, except the HALT which is optioned, are required in the new case.**

The only data required after the module activation card are a title line and an END line. Applying the same data (i.e., all input after the module activation card) used in the halt case, however, does not cause the case to fail. The title card in the first halt case is used throughout the depletion case, and the title card of the restart case is used in the shipping cask case. Also, see comments on "Restart, Halt, and Keep."

One of the primary purposes of the restart feature is to continue processing the data specified by the user input (Sect. 2.5.3). New user input, other than the title line, is ignored in the restart case. The user input to the initial SAS2 case is processed and stored in the master interface data set on units 70 and 90. Thus, the restart case may be executed to complete the original SAS2 case.

However, the restart feature may be applied for other purposes. Several data sets are produced by SAS2 and applied later in the flow of the execution. During the intermission between a halt case and a restart case, the user may remake one or more of the data sets for an appropriate change in the problem. An example of this is shown in sample case 3, where ORIGEN-S is executed for a different cooling time before the last restart case is invoked.

Also, there is an entirely different type of application of the restart feature, in which the user input to the initial SAS2 case may be modified (e.g., restart a case with a new cask geometry specification. Since user input to the restart case is ignored, the following procedure is required. A new case, applying PARM=HALTXX and the complete user input containing desired modifications, should be submitted. Then, this new case writes a new master interface data sets on units 70 and 90. Finally, a subsequent restart case will apply the different data, as specified on the interfaces. Only appropriate changes (i.e., data that apply to the restart case) should be specified.

Restart and Halt:

```
=SAS2    PARM=RESTARTSHALTii
```

A restart and a new halt may be applied with this PARM option. The case starts where the old halt case terminated and halts after "PASSii" is completed. A subsequent restart case starts after "PASSii." Only the title and END lines are required.

Restart, Halt, and Keep:

```
=SAS2    PARM=RESTARTSHALTiiKEEP
```

This PARM specification executes the same passes as the preceding feature; however, the user plans to make a subsequent case start where this case started, so the data written on unit 55 are not changed. Note that any data sets that are rewritten during the executed passes, except for that on unit 55, may need to be copied elsewhere before execution of this case. Then, they can be remade before the subsequent case. Only the title and END lines are required.

Skipping Cask Cell-Weight Case in Cask Analysis:

```
=SAS2    PARM=SKIPCELLWT
```

This feature skips almost all of the cell-weighted case in the shipping cask analysis. Dose results change insignificantly when this option is used for a cask in which the fuel zones are dry. This option can save considerable execution time in the shielding analysis.

Executing SCALE-3 Version of SAS2:

=SAS2 PARM=OLDSAS2

This feature solves the complete problem in the method using the SAS2 method of SCALE-3. The model is an infinite lattice of the fuel-pin-cell representation of the path A model. The only exception is that the ORIGEN-S cross sections are cell-weighted (as in SAS2H) instead of region-weighted (as in SCALE-3).

Changing to Region-Weighted Cross Sections:

=SAS2 PARM='OLDSAS2,NOCELLWT

This feature executes the older version of SAS2 (from SCALE-3) producing region-weighted cross sections, as in SCALE-3. Apostrophes or parentheses allow use of a comma between keywords.

Skipping Shipping Cask Data, if Halting:

=SAS2 PARM=(HALT03,SKIPSHIPDATA)

This feature can be used only when the case is halted prior to the cask analysis (e.g., at reactor discharge). The shipping cask data, which previously were required even when not used because of the HALTii, do not have to be included (starting with ALIB of Data Block 11 in Table S2.5.1). If a restart is to be used later for the cask analysis, this feature may not be used. Use of this option without setting the halt feature will force a halt for ii=J.

Changing SAS2 Core Allocation:

=SAS2 PARM=SIZE=

This feature changes the word size allocated to arrays in SAS2 from 200,000 to value of xxxxxxx.

Check in Material Information Processor

=SAS2 PARM=CHECK

This feature checks all standard composition specification data and the fuel-pin-cell geometry, writing error messages and stops before running case. HALTXX does this and edits more data.

S2.5.7 PRECAUTION IN USING NON-SCALE LIBRARIES (ZA NUMBERS, MU)

The cross-section library to be used by SAS2 is specified by LIB in data block 3 of the input requirements listed in Table S2.5.1. There are four libraries that are appropriate for SAS2, which are identified by the following input entries:

1. HANSEN-ROACH
2. 27GROUPENDF4
3. 27BURNUPLIB
4. 218GROUPNDF4

The SCALE library specified by "123GROUPGMTH" may not be used by SAS2 without proper preprocessing.

In addition to the cross-section data, SAS2 requires each set of data for a nuclide to contain a proper SCALE identifier, a ZA number, and flux data (given in the MT 1099 data). All SCALE neutron cross-section libraries, unless otherwise specified, are considered to contain the proper data to be used by SAS2 for any of the nuclides on the library. It should be noted that any material which is an alloy or element, and, thus, not identified as an isotope by the identifier and ZA number, cannot be depleted by SAS2. Although such materials may not be depleted or generated by the code, they may be input (e.g., as clad) and used with a constant density in the flux calculation of the neutronics treatment.

Cross-section libraries have been produced and used by SCALE modules that are not under the configuration control of the SCALE system. The user is advised to take certain precautions before using any of these libraries with SAS2. The identifiers should follow the proper SCALE procedure of being the ZZAAA number for any ground-state isotope or ZZ601 for an excited-state isotope. These identifiers are required to use any of the SCALE neutronics control modules (e.g., CSAS4 or CSASN). Before applying the library to SAS2 cases, the user should also determine (possibly using editing codes) that the nuclides have proper ZA numbers in the directory records and flux data in the MT 1099 data. Users producing non-SCALE cross-section libraries that have potential use with SAS2 should use procedures that supply the data required by SAS2.

S2.6 SAMPLE CASES

The input to four sample cases and examples of some of the printed output are included in this subsection. The first three cases are variations of the same problem for a PWR fuel assembly. The fourth case is an example for a BWR fuel assembly. The first case contains a selection of relatively large-interval-size parameters in order to have a test case using less computer time than the more typical cases. The printout shown applies to the first case only. However, the computed dose rates for all cases are tabulated for comparison checks with the results from other sample cases performed by the user, or in the fourth case, for comparisons with measurements.

S2.6.1 SAMPLE CASE 1 DESCRIPTION

The description for sample case 1, which is basically the same for the first three cases, is presented in full for the first case only. Then, only changes in data will be given for sample cases 2 and 3.

General Description of Problem

A shipping cask is designed with a stainless steel basket, a B_4C neutron poison for criticality control, a depleted uranium shield for absorbing photons, and a water shield for reducing the neutron dose. The cask is to contain PWR fuel assemblies having a 33-MWd/kgU burnup. The assemblies had been coupled with control rods while within the reactor.

The data assumed to be given are presented first. It is followed with calculated data required for the input. Then, mixing tables are constructed, and the final sample case 1 input is listed.

Given Assembly-Description Data

UO_2 fuel rods on 17 × 17 square lattice
Number of fuel rods per assembly = 264
Number of absorber rods per control rod assembly = 24
Active fuel length = 365.76 cm (144 in.)
Fuel mass = 461.4 kg U per assembly
Content of U, wt %: ^{234}U = 0.028, ^{235}U = 3.2, ^{236}U = 0.015, ^{238}U = 96.757
Zircaloy guide tubes and clad for fuel rods
Average temperatures, K: fuel, 811; clad, 620; H_2O, 570
Average water-moderator pressure = 1.55×10^7 pascals (2250 psia)
Average moderator temperature, degrees F = 567
Average moderator boron content = 550 ppm (by weight)
Rod pitch = 0.496 in. = 1.25984 cm
Fuel rod clad OD = 0.374 in. = 0.94996 cm
Fuel rod clad ID = 0.329 in. = 0.83566 cm
Guide tube outside radius = 0.241 in. = 0.61214 cm
Guide tube inside radius = 0.225 in. = 0.57150 cm

Effective light-element mass, kg/assembly:

C	= 0.05999	N	= 0.03377	O	= 62.14	Al	= 0.04569
Si	= 0.06586	P	= 0.1422	Ti	= 0.04983	Cr	= 2.340
Mn	= 0.1096	Fe	= 4.599	Co	= 0.03344	Ni	= 4.402
Zr	= 100.8	Nb	= 0.3275	Mo	= 0.1816	Sn	= 1.652

Light elements in end fittings and plenum are included with effective weights as obtained with scaling factors from Ref. 42. The user may round off input values to 2 or 3 significant figures.

Given Power and Cooling History of Assemblies

Burnup = 33 GWd/tU = 33 MWd/kgU
Specific power = 37.5 kW/kgU = 17.3025 MW/assembly
Cycles in (simplified) first sample case = 1
Cycle time = burnup/power = 33,000/37.5 = 880 d
Spent fuel cooling period = 5 years = 1826.25

Given Shipping-Cask Description Data

Type of fuel coolant: none, dry fuel
Temperature of cask (assumed), K = 325
Pressure = 1.032×10^5 pascals (14.969 psia) (not used in dry fuel case)
Number of zones = 9
Materials by zone radii (densities given later in the mixing table):

1; 12.75 cm; 1 fuel assembly, SS304, N
2; 21.72 cm; B_4C, SS304
3; 38.05 cm; 6 fuel assemblies, SS304, N
4; 47.63 cm; Void
5; 48.90 cm; SS304
6; 57.40 cm; U-metal at 0.27 wt % ^{235}U
7; 61.35 cm; SS304
8; 72.78 cm; water
9; 73.22 cm; SS304

Given SAS2 Parameter Selections (Not Defaults)

Reactor-fuel-depletion-case library: 27(n) groups
Shielding-analysis-case library: 27(n)-18(g) groups
Number of libraries produced/cycle = 1
Input level (SAS2H data) option = 1
Print level option = 5
Fuel-pin-case mesh size factor (coarser mesh) = 1.2
Larger-unit-cell interval size increase factor = 1.4
Shield case interval size increase factor = 2.0
Shield region-geometry cask case convergences = 10^{-3}
Order of angular quadrature of cask case = 8
Skip cask cell-weight case, or PARM='SKIPCELLWT'
Trace of ^{59}Co in reactor coolant to update its cross section (included in the moderator because its flux is felt to better represent the flux in the structural regions where the ^{59}Co is primarily located)
Default dose detector locations: 0, 1, 2, and 4 m from surface

Calculation of Volume Fraction (VF) for UO_2 Fuel

First, compute atomic weights of U and UO_2 as A_u and A_T, respectively.

$^{234}N = 0.00028\ \rho_u\ N_o/234.041 =$ $0.00120 \times 10^{-3}\ \rho_u\ N_o$
$^{235}N = 0.03200\ \rho_u\ N_o/235.044 =$ $0.13614 \times 10^{-3}\ \rho_u\ N_o$
$^{236}N = 0.00015\ \rho_u\ N_o/236.046 =$ $0.00064 \times 10^{-3}\ \rho_u\ N_o$
$^{238}N = 0.96757\ \rho_u\ N_o/238.051 =$ $4.06455 \times 10^{-3}\ \rho_u\ N_o$
$N_u =$ $4.20253 \times 10^{-3}\ \rho_u\ N_o$
$A_u = \rho_u\ N_o/N_u = 1/4.20253 \times 10^{-3} =$ 237.952
$A_O =$ 31.999
$A_T =$ 269.951

Then, compute mass, volume, and density of UO_2:

$M_{UO_2} = M_u\ A_T/A_u = (461.4)(269.951)/(237.952) = 523.448$ kg
$V_{Fuel\ assm.} = 264\ \pi\ (0.83566/2)^2(365.76) = 5.29602 \times 10^4$ cm^3
$\rho_{UO_2} = 5.23448 \times 10^5/5.29602 \times 10^4 = 9.8838$ g/cm^3
ρ(theor., UO_2) = 10.96/cm^3 (Table M8.2.1)
$VF_{fuel} = 9.8838/10.96 = 0.9018$, for UO_2 (MX=1)

Calculation of Density (DEN) for Reactor Moderator

T, degrees F = 567
P, psia = 2250
ρ_{H_2O} (or DEN) = 0.733 g/cm^3 (Table S2.5.2, interpolated)

Comments on Calculations of VF and DEN

Note that parts of the above calculations were made to illustrate the details of a more complete procedure in deriving input data. The lengthy atomic weight computation is not needed if the UO_2 weight and volume of an assembly are given or if either the UO_2 density or volume fraction is given. In practice, simply setting the atomic weight of uranium to equal 238 (in the 2 to 5 wt % ^{235}U range) is correct for a three-place accuracy of VF. (Note on accuracy: The fractional changes in isotopic inventories usually computed are approximately the same or less than the fractional change in the H/U atomic ratio of the case. Thus, three-place accuracy should be sufficient.)

A volume fraction (VF) could have been used in place of density (DEN) for H_2O. The boron content of 550 parts per million in the moderator was input for this case as an arbitrary material, permitting a direct method of entering the 550 and avoiding the necessity of the user converting from ppm to atom/b-cm for either the elemental boron or ^{10}B and ^{11}B. The description and examples of arbitrary materials are given in Sects. M7.4, M7.5, and C4.4.4.

Preparation of Mixing Tables

Next, derive the input "mixing tables" (discussed in Sect. S2.2.3 and Data Note A of Sect. S2.5.4). All the data required for the mixing table of the fuel-pin cell, shown in Table S2.6.1, are either given or calculated. The data for the shipping cask mixing table in Table S2.6.2 have been similarly derived. This is the same shipping cask applied in sample cases for SAS1 in Sect. S1. Figure S2.6.1 shows the geometric model of the shipping cask. SAS2 computes only the radial detector dose rates, whereas SAS1 can compute both radial and axial detector dose rates. Results for a problem evaluated by SAS1 and SAS2 in the radial direction are nearly identical, if similar parameters are used.

Table S2.6.1 Fuel-pin-cell mixing table of sample cases 1 to 3

MX	Component	Wt %	Density	VF	Atoms/b-cm	T,K	Type
1	UO_2			0.9018		811	Fuel
	^{234}U	0.028					
	^{235}U	3.200					
	^{236}U	0.015					
	^{238}U	96.757					
2	Zircaloy			1.0		620	Clad
3	H_2O		0.733	1.0		570	Mod.
	Boron	100.0	0.733	550.0E-6			
	^{59}Co			0.0	1.0E-20		

Table S2.6.2 Shipping cask mixing table of sample cases 1 to 3

MX	Component	Wt %	Density	VF	Atoms/b-cm	Type
4,5	SS304			2.1375E-2		Fuel zones
	N		1.22E-3	0.5530		2 atm. pres.
6	SS304			2.1712E-2		Neutron poison
6	B_4C			7.7066E-2		
7	N			0.0	1.0E-20	Void
8	SS304			1.0		Cask body
9	U-metal			1.0		Photon shield
	^{235}U	0.27				
	^{238}U	99.73				
12	H_2O			0.9440		Neutron shield

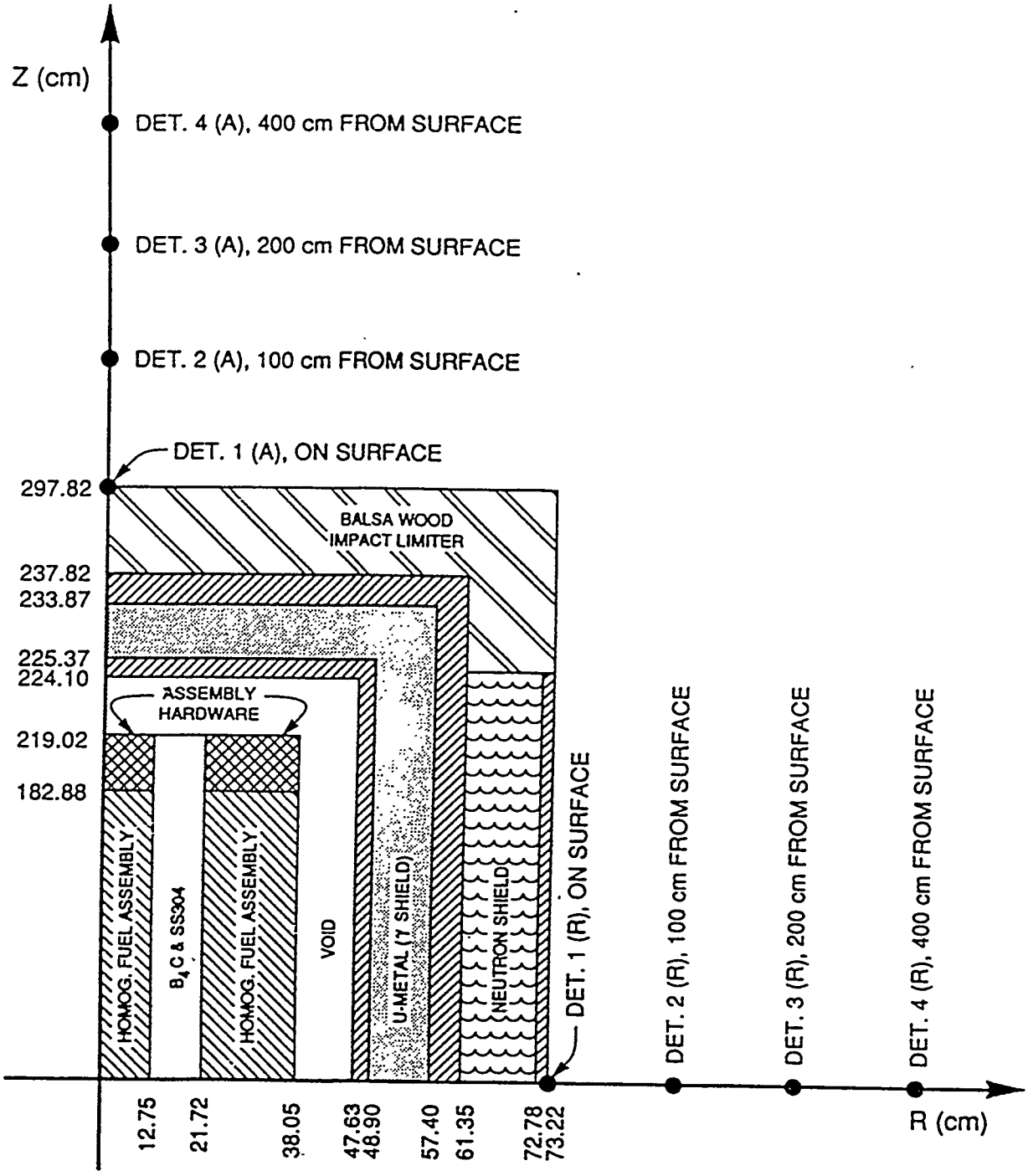


Figure S2.6.1 Model of shipping cask for PWR fuel assemblies

S2.6.2 SAMPLE CASE 1 INPUT

```
=SAS2H     PARM='SKIPCELLWT'
SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK
27GROUPNDF4     LATTICECELL
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  THIS PART OF INPUT:  MIXTURES OF FUEL-PIN-UNIT-CELL
'
UO2 1 0.9018 811 92234 0.028 92235 3.2 92236 0.015 92238 96.757 END
'  ....ABOVE METHOD USES WT %'S OF URANIUM ISOTOPES
ZIRCALLOY 2  1              620 END
H2O       3 DEN=0.733 1   570 END
ARBM-BORMOD  0.733 1 1 0 0 5000 100 3 550.0E-6  570  END
'  ....ABOVE IS 550 PPM BORON IN MODERATOR
CO-59     3  1-20           570 END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  MIXTURES OF SHIPPING CASK:
'
SS304        4                2.1375-2  END
N            4 DEN=1.22-3     0.553     END
SS304        5                2.1375-2  END
N            5 DEN=1.22-3     0.553     END
SS304        6                2.1712-2  END
B4C          6                7.7066-2  END
N            7                1-20      END
SS304        8                          END
U(.27)METAL  9                          END
H2O         12                0.944     END
END COMP
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  FUEL-PIN-CELL GEOMETRY:
'
SQUAREPITCH  1.25984 0.83566 1 3 0.94996 2  END
MORE DATA  SZF=1.2  END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  ASSEMBLY AND CYCLE PARAMETERS:
'
NPIN/ASSM=264 FUELNGTH=365.76 NCYCLES=1 NLIB/CYC=1
PRINTLEVEL=5
LIGHTEL=16  INPLEVEL=1
NUMINS= 1  ORTUBE= 0.61214  SRTUBE=0.5715 FACMESH=1.4  END
'  ....ABOVE IS LARGER-UNIT-CELL GEOMETRY ADDITIONS
POWER=17.3025  BURN=880  DOWN=1826.25 END
 C    0.05999  N    0.03377  O   62.14     AL  0.04569
 SI   0.06586  P    0.1422   TI  0.04983  CR  2.340
 MN   0.1096   FE   4.599    CO  0.03344  NI  4.402
 ZR 100.8      NB   0.3275   MO  0.1816   SN  1.652
'  ....ABOVE DATA ARE LIGHT ELEMENTS (KG) PER ASSEMBLY
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  ZONE DESCRIPTION OF CASK:
'
27N-18COUPLE  TEMPCASK(K)=325 NUMZONES=9 DETECT=0 DRYFUEL=YES  END
4 12.75  6 21.72  5 38.05  7 47.63  8 48.90

9 57.40  8 61.35 12 72.78  8 73.22
ZONE=1  FUELBNDL=1  ZONE=3  FUELBNDL=6
  SZFCASK=2  ISNS=8  EPSS=1-3  PTCS=1-3 END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
END
```

[Job execution requirements are given for both IBM and CRAY computers. For the IBM mainframe: 30,000 I/O, 8 min (CPU), and 16,000 lines. For CRAY X-MP: 4.5 min (CPU), and 14,000 lines.

Output and Computed Dose Rates

See Sect. S2.6.9 for a description of some of the printed output from sample case 1. Computed dose rates for the first three sample cases, which are similar problems, are listed in Table S2.6.3. These dose rates represent the values calculated on the IBM mainframe at ORNL at the completion of the code development effort. Use of different computers or subsequent updates to SCALE data libraries may cause results somewhat different from those reported in Table S2.6.3.

Table S2.6.3 Dose rates computed in similar cases

Sample case	Cooling time, y	Dose rates (mrem/h) at 2 m	
		Gamma ray	Neutron
1	5	3.51	1.36
2	5	4.79	1.52
3A	5	4.61	1.53
3B	10	1.87	1.28

S2.6.3 SAMPLE CASE 2 DESCRIPTION

Sample case 2 illustrates the effect of applying some of the default parameters in place of those used in sample case 1. The input data for the two cases are identical, except for the following changes in sample case 2:

1. Apply the default mesh interval sizes in the fuel-pin cell geometry.

2. Apply the default size guide tubes, which are automatically supplied by changing the input level 1 to the default input level 0, for the larger unit cell data.

3. Apply the default mesh interval sizes in the larger unit cell geometry. Because only defaults are applied to the larger unit cell, the input for the case reverts to that of the SCALE-3 version of SAS2. However, the code still applies for the improved SAS2H procedures.

S2.6.4 SAMPLE CASE 2 INPUT

```
=SAS2H     PARM='SKIPCELLWT'
SAS2 SAMPLE CASE 2: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK
27GROUPNDF4     LATTICECELL
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  THIS PART OF INPUT:  MIXTURES OF FUEL-PIN-UNIT-CELL
'
UO2 1 0.9018 811 92234 0.028 92235 3.2 92236 0.015 92238 96.757 END
'  ....ABOVE METHOD USES WT %'S OF URANIUM ISOTOPES
ZIRCALLOY 2  1              620 END
H2O       3 DEN=0.733 1   570 END
ARBM-BORMOD  0.733 1 1 0 0 5000 100 3 550.0E-6  570  END
'  ....ABOVE IS 550 PPM BORON IN MODERATOR
CO-59     3  1-20          570 END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  MIXTURES OF SHIPPING CASK:
'
SS304        4                2.1375-2  END
N            4 DEN=1.22-3     0.553     END
SS304        5                2.1375-2  END
N            5 DEN=1.22-3     0.553     END
SS304        6                2.1712-2  END
B4C          6                7.7066-2  END
N            7                1-20      END
SS304        8                          END
U(.27)METAL  9                          END
H2O         12                0.944     END
END COMP
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  FUEL-PIN-CELL GEOMETRY:
'
SQUAREPITCH  1.25984 0.83566 1 3 0.94996 2  END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  ASSEMBLY AND CYCLE PARAMETERS:
'
NPIN/ASSM=264 FUELNGTH=365.76 NCYCLES=1 NLIB/CYC=1
PRINTLEVEL=5
LIGHTEL=16
'  ....ABOVE SHOWS NO LARGER-UNIT-CELL GEOMETRY ADDITIONS, DEFAULTS USED
POWER=17.3025  BURN=880  DOWN=1826.25 END
 C    0.05999  N    0.03377  O   62.14     AL  0.04569
 SI   0.06586  P    0.1422   TI  0.04983  CR  2.340
 MN   0.1096   FE   4.599    CO  0.03344  NI  4.402
 ZR 100.8      NB   0.3275   MO  0.1816   SN  1.652
'  ....ABOVE DATA ARE LIGHT ELEMENTS (KG) PER ASSEMBLY
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'  ZONE DESCRIPTION OF CASK:
'
27N-18COUPLE  TEMPCASK(K)=325 NUMZONES=9 DETECT=0 DRYFUEL=YES  END
4 12.75  6 21.72  5 38.05  7 47.63  8 48.90
9 57.40  8 61.35 12 72.78  8 73.22
ZONE=1  FUELBNDL=1  ZONE=3  FUELBNDL=6

 END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
END
```

[Job execution requirements on the IBM mainframe, recommended: 32,000 I/O, 13 min (CPU), and 16,000 lines. IBM (3033)/CRAY X-MP CPU time ratio is in 2.5 to 3.5 range.]

4. Apply the defaults for the angular quadrature (i.e., 16), the problem convergences (i.e., 10^{-4}), and the mesh interval sizes in the shipping cask case.

5. Make proper title line.

No printout is listed here for this sample case. However, the computed dose rates at 2 m from the cask surface are listed in Table S2.6.3. The influence from the different input parameters to sample cases 1 and 2 (e.g., the mesh intervals) may be noted by comparison with the corresponding dose rates.

S2.6.5 SAMPLE CASE 3 DESCRIPTION

Sample case 3 provides examples of two major changes from sample case 2. It illustrates the use of the "halt" and "restart" features of SAS2. Also, a more detailed reactor history is applied.

Consider a project in which the user is requested to compute dose rates as a function of cooling time of the spent fuel. Even though only two different cooling times are used in this example, more could be included. The sample case shows the method of computing multiple cases within the submission of only one job. The calculation of the reactor discharge concentrations is not repeated, which saves computer time. This feature is particularly significant in this case, because the case produces three libraries.

The given data for this case are the same as that given for sample case 2, except for the following changes:

Given SAS2 Parameters Selected

Number of cycles in case = 3
Print level option = 4

Given Power and Cooling History of Assemblies

Cycle 1:
  Reactor power = 18.3025 MW/assembly
  Irradiation period = 290 d
  Shutdown period = 30 d

Cycle 2:
  Reactor power = 17.3025 MW/assembly
  Irradiation period = 300 d
  Shutdown period = 60 d
  Fraction of first-cycle boron density = 0.95

Cycle 3:
  Reactor power = 16.3025 MW/assembly
  Irradiation period = 290 d
  Fraction of first-cycle boron density = 0.92

Spent fuel cooling periods:
  A. 5 y
  B. 10 y

Although there is no printout listed here for this sample case, the dose rates at 2 m from the cask surface are given in Table S2.6.3.

S2.6.6 SAMPLE CASE 3 INPUT

```
=SAS2H    PARM='HALT03,SKIPCELLWT'
SAS2 SAMPLE CASE 3: 33 MWD/KGU, 17*17 PIN, PWR, 3 CYC, DRY-FUEL CASK
27GROUPNDF4    LATTICECELL
UO2 1 0.9018 811 92234 0.028 92235 3.2 92236 0.015 92238 96.757 END
ZIRCALLOY 2  1          620 END
H2O       3 DEN=0.733 1  570 END
ARBM-BORMOD  0.733 1 1 0 0 5000 100 3 550.0E-6  570  END
CO-59     3  1-20       570 END
SS304       4            2.1375-2  END
N           4 DEN=1.22-3  0.553     END
SS304       5            2.1375-2  END
N           5 DEN=1.22-3  0.553     END
SS304       6            2.1712-2  END
B4C         6            7.7066-2  END
N           7            1-20      END
SS304       8                      END
U(.27)METAL 9                      END
H2O        12            0.944     END
END COMP
SQUAREPITCH  1.25984 0.83566 1 3 0.94996 2  END
NPIN/ASSM=264 FUELNGTH=365.76 NCYCLES=3 NLIB/CYC=1
PRINTLEVEL=4
LIGHTEL=16
POWER=18.3025  BURN=290  DOWN=30 END
POWER=17.3025  BURN=300  DOWN=60  BFRAC=0.95 END
POWER=16.3025  BURN=290  DOWN=1826.25  BFRAC=0.92 END
 C    0.05999  N    0.03377  O  62.14     AL  0.04569
 SI   0.06586  P    0.1422   TI  0.04983  CR  2.340
 MN   0.1096   FE  4.599    CO  0.03344  NI  4.402
 ZR 100.8      NB  0.3275   MO  0.1816   SN  1.652
27N-18COUPLE  TEMPCASK(K)=325 NUMZONES=9 DETECT=0 DRYFUEL=YES  END
4 12.75  6 21.72  5 38.05  7 47.63  8 48.90
9 57.40  8 61.35 12 72.78  8 73.22
ZONE=1  FUELBNDL=1  ZONE=3  FUELBNDL=6
END
END
=SAS2H    PARM='RESTARTS,SKIPCELLWT'
SAS2 SAMPLE CASE 3A: 33 MWD/KGU, 17*17 PIN, PWR, 3 CYC, DRY-FUEL CASK
END
=ORIGENS
0$$ A8 26 A11 -71 E 1T
 SAMPLE CASE 3B
3$$ 21 0 1 -88 A33 -88 4** A4 1-35 2T
35$$ 0 4T
56$$ A14 5 1 74 E 5T
 SAMPLE CASE 3B
60**  0.3 5I1 7 8.5 10
65$$  1 8Z 1 2Z 1 8Z 2Q21  61** F1-3
81$$ 2 0 26 1 E 82$$ A10 2
6T
 SAMPLE CASE 3B
56$$ 2Z A10 10 E 6T
56$$ F0 T
END
=SAS2H    PARM='RESTARTS,SKIPCELLWT'
SAS2 SAMPLE CASE 3B: 33 MWD/KGU, 17*17 PIN, PWR, 3 CYC, DRY-FUEL CASK
END
```

[Job execution requirements on the IBM mainframe, recommended: 72,000 I/O, 16 min (CPU), and 30,000 lines. IBM(3033)/CRAY X-MP CPU time ratio is in 2.5 to 3.5 range.]

S2.6.7 SAMPLE CASE 4 DESCRIPTION

Sample case 4 is an example pertaining to an analysis of an actual storage cask designed to contain 52 BWR spent fuel assemblies. Gamma and neutron dose rates have been measured[44,45] at various positions on the surface of the cask. Note: the assembly design and reactor moderator density data[45] used in this case are different than that for the assemblies in the measurements because the readily available data[44,45] did not include some of the required assembly specifications. The operating history and burnup of the assembly nearest the detector locations ARE applied in the calculations. Also, the case applies a somewhat different cask model, which is more complete (e.g., for part of the basket material) than that used in the reported[44,45] calculations. Although this case is not intended to be as complete as a more detailed analysis, it should at least give an estimate of the comparison of a SAS2 thick shield calculation with dose rates that are actually measured.

Given Case Assembly-Description Data

Generally, the assembly and moderator specifications used in this case are those of Ref. 46. The 189-kg U assembly and fuel rod data are listed in Table S2.6.4. The weighted average ^{235}U enrichment is 2.40 wt % ^{235}U and other uranium isotopic contents are 0.021 wt % ^{234}U, 0.011 wt % ^{236}U, and 97.568 wt % ^{238}U.

The SAS2H model for the assembly locates a gadolinium poison rod at the center of the larger unit cell. Four gadolinium poison rods (type 5 rods listed in Table S2.6.4) are located in the assembly, as shown in Fig. S2.6.2. Thus, one fourth of the channel casing material and channel moderator should be placed in the two zones outside of the fuel zone of the larger unit cell. The axially fission-weighted water density of 0.4817 for the fuel-pin-unit-cell case is derived from a reflected slab case computed by XSDRNPM-S using the moderator zone densities of Table S2.6.5 (see discussion in Data Note B in Sect. S2.5.4) and case 3 (Fig. S2.A.3) in S2.A. Except for gadolinium and cobalt, light-element masses per assembly shown in the SAS2H input (Sect. S2.6.8) are derived by a method consistent with that used in other SAS2 cases in Refs. 23 and 47 and Sect. M6.7 by similarly applying data from Tables 3.7, 4.3, and 4.4 of Ref. 42. Gadolinium content is computed from data in Table S2.6.4. The ^{59}Co contents in Ref. 42 are one-half the maximum handbook values for the various materials. However, for this case, it is assumed that the ^{59}Co content is zero (for materials influencing the side dose rate). Note that in the few cases in the past (known to the authors) where the cobalt content was measured, the measured amount was sufficiently less than that of the handbook value. Thus, it was felt that this assumption on the ^{59}Co content would produce less bias than that generated from using the higher assumption. (However, a zero ^{59}Co assumption may not be good when it is required to maintain conservatism.) The mixing table densities for the fuel-pin-cell input and the larger-unit-cell input are listed in Tables S2.6.6 and S2.6.7, respectively.

Given Operating Power and Cooling History of Assembly

The BWR assembly CZ209 located at 26.5° from the reference point and at an outer position in the basket, was analyzed for the radiation sources. It is assumed that the assembly cooled for 2.6 y after discharge and has the operating history (Table 4.3 of Ref. 44 and Table 4.1 of Ref. 45) given in Table S2.6.8.

Table S2.6.4 BWR assembly description for sample case 4

Assembly general data:	
Lattice, designer	8 × 8, General Electric
Type	Burnable poison
Water density, vol-av, g-cm^{-3}	0.392
Water temperature, av K	558
Number of poison rods	4
Number of holes	1
Channel material	Zircaloy-4
Channel water density, av, g-cm^{-3}	0.743
Fuel rod data:	
Pellet diameter, in.	0.4160
Gap (diametrical), in.	0.0090
Rod OD, in.	0.493
Fuel rod pitch, in.	0.640
Pellet stack density, % TD	94
Clad material	Zircaloy-2
Active fuel length, in.	148
Plenum (fuel rod) length, in.	10
Fuel temperature, K	840
Clad temperature, K	620
Type 1: 31 rods, wt % ^{235}U	2.64
Type 2: 16 rods, wt % ^{235}U	2.30
Type 3: 8 rods, wt % ^{235}U	2.12
Type 4: 4 rods, wt % ^{235}U	1.65
Type 5: 4 rods, wt % ^{235}U	2.30, with 2.0 wt % Gd_2O_3

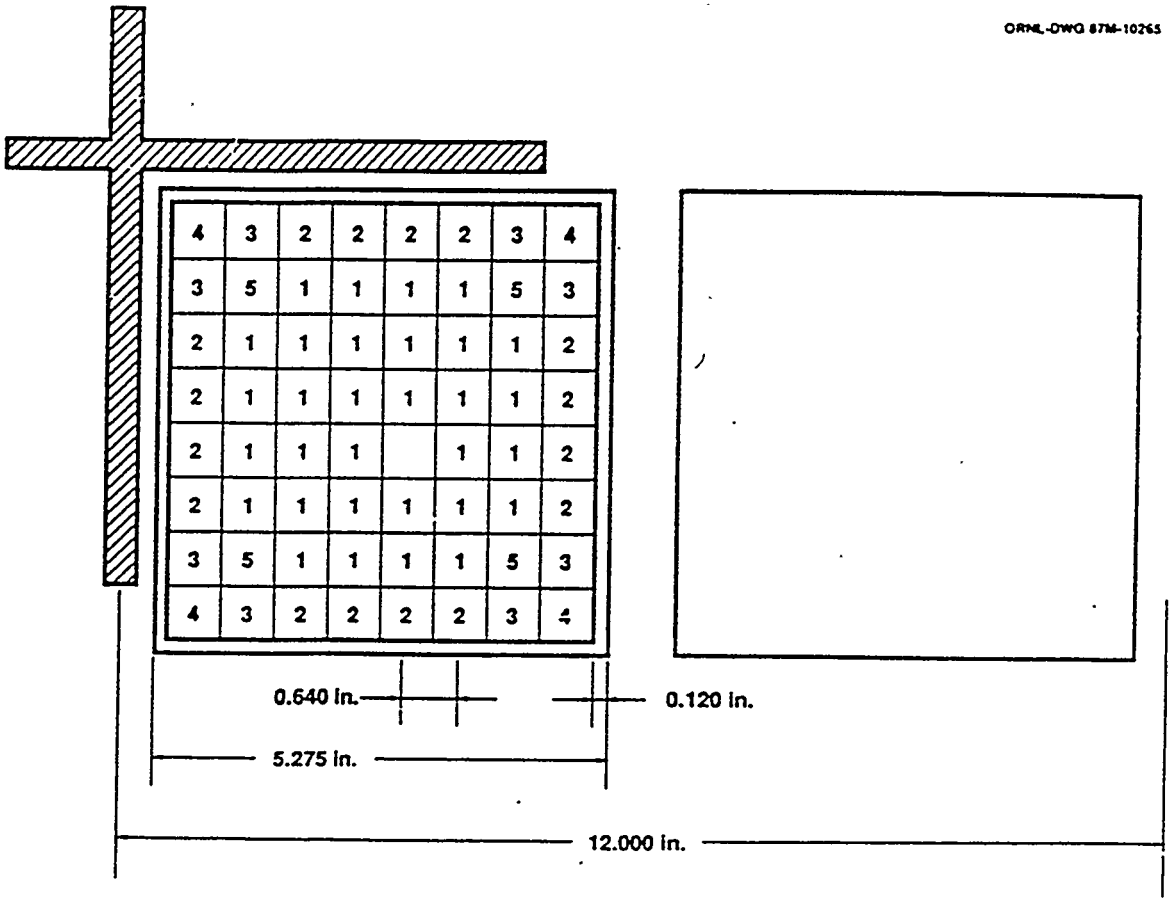


Figure S2.6.2 BWR assembly schematic for sample case 4

Table S2.6.5 Axial water densities of BWR for sample case 4

Top of node (Z, in.)	Density at Z ($g\text{-}cm^{-3}$)	Average density in node ($g\text{-}cm^{-3}$)	Average water temperature (K)
30.83	0.692	0.743	552
43.17	0.569	0.600	558
55.50	0.472	0.494	558
67.83	0.400	0.417	558
80.17	0.347	0.360	558
98.67	0.293	0.309	558
123.33	0.250	0.264	558
148.00	0.228	0.234	558

Table S2.6.6 Fuel-pin-cell mixing table for sample case 4

MX	Component	Wt %	Density[a]	VF	T,K	Type
1	UO_2		9.87	1.0	840	Fuel
	^{234}U	0.021				
	^{235}U	2.400				
	^{236}U	0.011				
	^{238}U	97.568				
2	Zircaloy			1.0	620	Clad
3	H_2O			0.4817	558	Mod.

[a]Input as DEN.

Table S2.6.7 Larger-unit-cell mixing table for sample case 4

MX	Component	Wt %	Density[a]	VF	T,K	Radius, cm
9	UO_2		9.87	1.0	840	0.53975
	Gd_2O_3		9.87	0.02		
	^{154}Gd	2.18				
	^{155}Gd	14.80				
	^{156}Gd	20.47				
	^{157}Gd	15.65				
	^{158}Gd	24.84				
	^{160}Gd	21.86				
	O	150.00[b]				
2	Zircaloy			1.0	620	0.62611
3	H_2O			0.4817	558	0.91715
500	(Smeared fuel calculated by SAS2)					3.6398
10	Zircaloy			1.0	588	3.8103
11	H_2O	0.743			552	4.3261

[a]Input as DEN (arbitrary material described in Sect. C4.4).
[b]Equivalent oxygen, considering total gadolinium = 100.

Table S2.6.8 BWR assembly operating history for sample case 4

Cycle	Accumulated time, d	Time difference, d	Burnup, GWd/MTU	Cycle burnup, GWd/assm.	Power, MW/assm.
1	807	807	10.651	2.013	2.494
	866	59	10.651	0	0
2	1367	501	21.430	2.037	4.066
	2166	799	21.430	0	0
3	2878	712	25.383	0.747	1.049

Given SAS2 Parameter Selections

Reactor-fuel-depletion-case library: 27(n) groups
Shielding-analysis-case library: 27(n)-18(g) groups
Number of libraries produced/cycle = 1
Input level (SAS2H data) option = 2
Print level option = 4
Skip cask cell-weight case, or PARM='SKIPCELLWT'
Detector locations (at midplane, only): 0, 2.54, 100, and 200 cm from cask
Defaults for all mesh sizes, angular quadratures, time, and convergences

Given Storage-Cask-Description Data

Type of fuel zone coolant: none, dry fuel
Temperature of cask, K = 380
Number of zones = 9
Materials by zone radii (densities given in Table S2.6.9):
1; 75.32 cm; 52 fuel assemblies, SS304, boral, Cu, zircaloy
2; 75.70 cm; zircaloy
3; 75.93 cm; boral
4; 76.57 cm; Cu
5; 79.29 cm; SS304
6; 90.09 cm; Pb
7; 95.17 cm; SS304
8; 110.41 cm; ethylene glycol water solution
9; 111.05 cm; SS304

Table S2.6.9 Storage cask mixing table for sample case 4

MX	Component	ATPM[a]	Density[b]	VF	Type (part)
4	SS304			0.1624	(Fuel zone, with
	Cu			3.832E-2	part of basket and
	B_4C		2.034E-2		casing)
	Al		2.486E-2		
	Zircaloy			3.97E-2	
12	Zircaloy				Casing
13	B_4C		2.156	0.35	Boral
	B	4			
	C	1			
	Al	100		0.65	
14	Cu			1.0	Basket
5	SS304			1.0	Shield clad
6	Pb			1.0	Gamma shield
7	H_2O soln.			1.0	Neutron shield
	C		0.212		(Water and
	O		0.732		ethylene glycol)
	H		0.109		

[a]Atoms of this element per molecule of arbitrary material (Sect. C4.4).
[b]Input as DEN (Sect. C4.4).

Measured Data

A profile of measured gamma dose rates was obtained along the axial elevation of the cask surface. An average of the gamma dose rates measured at 26.5° from a reference point was derived by height-segment weighting of the averages of consecutive dose rates determined between 60- and 420-cm elevations (the active fuel region). The thermoluminescent dosimeters (TLDs) used to obtain the profile of dose rates may require a calibration to the gamma spectrum because the TLDs do not measure energy spectra. However, by applying photon spectra determined by other instrumentation, it was concluded that a TLD recalibration was not necessary. The average gamma dose rate derived by height-segment weighting is 12.5 mrem/h. The gamma dose at the cask midplane (peak) is 14.4 mrem/h.

The determination of the average neutron dose rate to be used for comparisons is somewhat less direct. Neutron measurements at 26.5° using track etch dosimeters (TEDs) are applied, following the same method used for photons, with one exception. At the elevation of 223 cm, the 26.5° dose rate value appears questionable because it is about twice the size of the average of the other four measurements over the 0 to 45° range at the same elevation. Also, this large measurement is 1.8 to 4.1 times any of the other values measured at the same angle and at heights corresponding to the lower half of the fuel location. Rather than completely discarding the questionable value, the large value plus the other four values at 223-cm elevation are averaged to obtain the neutron dose rate at that height. Then, the height-segment weighted neutron dose rate, before calibration, is 2.66 mrem/h. Three different types of neutron spectra measuring instruments and flux-to-dose rate conversion factors were used for calibration of the TEDs. The final average neutron dose rate, after applying the average calibration factor, is 1.24 mrem/h. The midplane (peak) neutron dose rate is 1.77 mrem/h after calibration.

Comparison of Calculated and Measured Doses

Table S2.6.10 compares the measured doses with the calculated doses obtained from the SAS2H sequence. The calculated doses are low compared with the measured neutron dose and high compared with the measured gamma dose. The differences between measured and SAS2H-computed values may result from several reasons.

Table S2.6.10 Computed dose rates and measurements for case 4,[a] in mrem/h

Radiation type	SAS2H[b]	Average dose measurement[c]	Midplane dose measurement
Gamma dose rate	19.0	12.5	14.4
Neutron dose rate	1.02	1.24	1.77

[a]Located at 26.5° on cask surface.
[b]Computed with different BWR assembly design.
[c]Height-segment weighted average at side of cask (after calibration).

1. The SAS2H analysis used a different BWR assembly design.

2. Uncertainty in the spent fuel depletion model.

3. The SAS2H analysis assumed the cask to be fully loaded with assemblies having the characteristics of the one assembly nearest the detector location.

4. The SAS2H model homogenizes the fuel over the entire cask cavity.

5. General limitations of a 1-D computational model.

6. Uncertainty in the cross-section data.

Gamma and neutron sources were calculated by ORIGEN2 in the computations reported in Refs. 44 and 45 and may be compared with those of sample case 4. Although different group structures limit the comparisons, the gamma source above 1 MeV computed by ORIGEN2 was 12% greater than that calculated by SAS2H/ORIGEN-S. The total neutron source derived by ORIGEN2 was 43% greater than that determined by SAS2H/ORIGEN-S. This neutron source difference is consistent with that of a comparison study[48] in which the neutron source, for BWR fuel after five years decay, computed by ORIGEN2 was 29% greater than that calculated by SAS2H/ORIGEN-S.

A more extensive calculational comparison (using multidimensional models, etc.) with the measured data is needed to better quantify the sources of discrepancy with the measured data. An independent effort is being made to study these sources of discrepancy.

S2.6.8 SAMPLE CASE 4 INPUT

```
=SAS2      PARM='SKIPCELLWT'
SAS2 SAMPLE CASE 4: 25 MWD/KGU, 8*8 PIN, BWR, 3 CYC, DRY FUEL CASK
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   MIXTURES OF FUEL-PIN-UNIT-CELL:
'
27BURNUPLIB     LATTICECELL
UO2  1 DEN=9.87  1  840  92234  0.021 92235 2.4 92236 0.011
                    92238 97.568  END
ZIRCALLOY  2 1  620    END
H2O  3 DEN=0.5039  1  558 END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   MIXTURES OF SHIPPING CASK:
'
SS304      4  0.1624 END
CU         4  3.832-2 END
B4C        4  DEN=2.034-2 1 END
AL         4  DEN=2.486-2 1 END
ZIRCALLOY  4  3.97-2  END
'                ....ABOVE IS AVERAGE SS, CU & BORAL FUEL BASKET
'                    AND CHANNEL DENSITIES OF FUEL ZONE....
ZIRCALLOY  12  END
'                ...ABOVE IS ZIRC. IN ASSEMBLY CHANNEL
ARBM-B4C      2.156  2 1 1 0   5000 4   6012 1   13  0.35 END
ARBM-AL       2.156  1 0 0 0  13027 100          13  0.65 END
'                ....ABOVE IS BORAL IN OUTER SIDE OF TUBE
CU         14  END
'               ....ABOVE IS THE CU IN OUTSIDE OF BASKET
SS304      5  1 END
'               ....ABOVE IS STAINLESS STEEL CLAD, 3 PLACES IN CASK
PB         6  END
'               ....ABOVE IS THE LEAD FOR GAMMA SHIELD
C          7  DEN=0.212  1 END
O          7  DEN=0.732  1 END
H          7  DEN=0.109  1 END
'                ....ABOVE IS ETHYLENE GLYCOL/H2O FOR NEUTRON SHIELD
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   MIXTURES OF LARGER-UNIT-CELL:
'
UO2  9 DEN=9.87  1  840  92234  0.021 92235 2.4 92236 0.011
                    92238 97.568  END
ARBM-GDBURN  9.87   7 0 1 1
          64154  2.18  64155 14.80  64156 20.47
          64157 15.65  64158 24.84  64160 21.86
           8016 150.0  9   0.02  840  END
```

```
'                 ....ABOVE IS 2 WT % GADOLINIUM (AS GD2-OX3) IN THE
'                     BURNABLE POISON PINS OF BWR ASSEMBLY....
ZIRCALLOY  10  1  588 END
'                 ....ABOVE IS ZIRCALLOY CASING AROUND ASSEMBLY
H2O        11 0.743  552 END
'                 ....ABOVE IS CHANNEL MODERATOR AT HIGHER DENSITY
END COMP
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'      FUEL-PIN-CELL GEOMETRY:
'
SQUAREPITCH   1.6256 1.0795  1 3  1.25222  2  END
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'    ASSEMBLY AND CYCLE PARAMETERS:
'
NPIN/ASSM=63  FUELNGTH=376  NCYCLES=3  NLIB/CYC=1
PRINTLEVEL=4  LIGHTEL=15  INPLEVEL=2  NUMZONES=6   END
9 0.53975 2 0.62611 3 0.91715 500 3.6398 10 3.8103 11 4.3261
'           ..THESE MIXTURES & RADII PLACE GADOLINIUM PIN AT CENTER
'             OF 1/4 OF ASSEMBLY FUEL, CASING & CHANNEL MOD.
POWER=2.49    BURN=807  DOWN= 59  END
POWER=4.07    BURN=501  DOWN=799  END
POWER=1.05    BURN=712  DOWN=950  END
       C   0.03222 N   0.01534  O 28.86      AL 0.008748
       SI  0.01796 P   0.008133 TI 0.01070   CR 0.4274
       MN  0.03348 FE  1.197    NI 0.4139    CU 0.00231
       ZR 93.93    NB  0.003161 SN 1.535
'
' - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - - -
'
'   ZONE DESCRIPTION AND OTHER PARAMETERS OF CASK:
'
27N-18COUPLE   TEMPCASK(K)=380 DETECTORS=4 NUMZONES=9 DRYFUEL=YES END
0  2.54  100  200
4 75.32  12 75.70  13 75.93  14 76.57  5 79.29
6 90.09  5 95.17  7 110.41  5 111.05
ZONE=1  FUELBNDL=52
  END
END
```

[Job execution requirements on the IBM mainframe recommended: 52,000 I/O, 20 min (CPU), 28,000 lines. IBM(3033)/CRAY X-MP CPU time is in 2.5 to 3.5 range.]

S2.6.9 SAMPLE OUTPUT DESCRIPTION

Samples of 16 pages from the printed output of sample case 1 are shown in Figs. S2.6.3 through S2.6.21, inclusively. The output list of parameters, composition data, and geometry (unit cell) of the problem are described in Sect. C4.6. The remaining input processor lists are shown in Figs. S2.6.3, S2.6.4, and S2.6.5. These figures are followed with a few of the tables printed during the depletion calculation passes and the final ORIGEN-S decay case. The computed gamma and neutron spectra are shown in Figs. S2.6.14 and S2.6.15, respectively. Other figures show some of the shielding analysis data and results, which includes mixing tables and computed dose rates at the 1-m detector. Even though none of the output from sample cases 2 and 3 are shown, the dose rates computed at the 1-m detector are listed in Table S2.6.3. Note that the output of all of these cases represent that obtained with the initial release version of SCALE 4.0 and is provided here primarily to illustrate the format of the output. Updates to the codes or data libraries may cause the output provided by the code distribution center to differ slightly from that provided in this section.

```
**** REACTOR HISTORY DATA ****

NPIN/ASSM=       264
FUELNGTH=  3.658E+02
NCYCLES=           1
NLIB/CYC=          1
LIGHTEL=          16
PRINTLEVEL=        5

                                                    .....AVERAGE DENSITY.....
CYCLE   POWER(MW)  BURN, DAYS  DOWN, DAYS  RELATIVE TO THAT IN CYCLE 1
                                                 BORON       WATER
  1     1.730E+01   8.800E+02   1.826E+03     1.000E+00   1.000E+00

LIGHT ELEMENTS    KG/ASSEMBLY

      C               0.060
      N               0.034
      O              62.140
      AL              0.046
      SI              0.066
      P               0.142
      TI              0.050
      CR              2.340
      MN              0.110
      FE              4.599
      CO              0.033
      NI              4.402
      ZR            100.800
      NB              0.327
      MO              0.182
      SN              1.652
```

Figure S2.6.3 Input processor list of reactor history and light-element data

```
**** LARGER CELL DATA (USING SAS2H) ****

INPLEVEL=          1
NUMHOLES=         24
NUMINSTR=          1
MXTUBE=            2
SRTUBE=    5.715E-01
ORTUBE=    6.121E-01
NUMZONES=          4
MIXMODER=          3
MXREPEATS=         1
FACMESH=   1.400E+00

**** LARGER CELL GEOMETRY

ZONE   XSDRNPM MIXTURE   RADIUS (CM)

  1          3           5.7150E-01
  2          2           6.1214E-01
  3          3           7.1079E-01
  4          1           2.4367E+00
```

Figure S2.6.4 Input processor list of larger unit cell options and geometry

```
**** SHIPPING CASK PARAMETERS ****

LIB          27N-18COUPLE LIBRARY (ON UNIT NO. 88)
MXX                     9 MIXTURES, PLUS SPENT FUEL
NUMZONES                9 MATERIAL ZONES
NFUELZONES              2 ZONES CONTAINING FUEL
DETECTORS               4 RADIAL DISTANCES TO DOSE DETECTORS
TEMPCASK(K)  3.2500E+02 TEMPERATURE OF FUEL IN CASK
PRESSURE     1.4969E+01 WATER PRESSURE IN FUEL ZONES
SZFCASK      2.0000E+00 FACTOR TIMES DEFAULT SPATIAL INTERVAL SIZE

**** PARAMETERS INPUT TO OVERRIDE DEFAULTS ****

ISNS                    8 CASK ORDER OF ANGULAR QUADRATURE
EPSS           1.000E-03 CASK OVERALL PROBLEM CONVERGENCE
PTCS           1.000E-03 CASK SCALAR FLUX CONVERGENCE

**** CASK GEOMETRY - MATERIAL DESCRIPTION ****

  ZONE    RADIUS    MIXTURE NUMBER     NUMBER OF    FRACTION OF    FUEL ZONE
          (CM)      INPUT  XSDRNPM     ASSEMBLIES   ZONE VOLUME    CONDITION

    1     12.750    FUEL     1            1          0.82047        DRY
    1     12.750       4     1            -          -              -
    2     21.720       6     3            -          -              -
    3     38.050    FUEL     2            6          0.81991        DRY
    3     38.050       5     2            -          -              -
    4     47.630       7     4            -          -              -
    5     48.900       8     5            -          -              -
    6     57.400       9     6            -          -              -
    7     61.350       8     5            -          -              -
    8     72.780      12     9            -          -              -
    9     73.220       8     5            -          -              -

**** DETECTOR DISTANCES TO CASK SURFACE, CM ****

                    0.000
                  100.000
                  200.000
                  400.000

**** SHIELD MESH INTERVALS ****

   4 MESH INTERVALS IN ZONE  1
   2 MESH INTERVALS IN ZONE  2
   5 MESH INTERVALS IN ZONE  3
   2 MESH INTERVALS IN ZONE  4
   2 MESH INTERVALS IN ZONE  5
  22 MESH INTERVALS IN ZONE  6
   2 MESH INTERVALS IN ZONE  7
   9 MESH INTERVALS IN ZONE  8
   2 MESH INTERVALS IN ZONE  9

... END OF INPUT DATA PROCESSING ...
```

Figure S2.6.5 Input processor list of shipping cask data

AT 0 D, SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL

GENERAL PROBLEM DESCRIPTION DATA BLOCK

GENERAL PROBLEM DATA

IGE	1/2/3 = PLANE/CYLINDER/SPHERE	2	ISN	QUADRATURE ORDER	8
IZM	NUMBER OF ZONES	3	ISCT	ORDER OF SCATTERING	3
IM	NUMBER OF SPACIAL INTERVALS	14	IEVT	0/1/2/3/4/5/6=Q/K/ALPHA/C/Z/R/H	1
IBL	0/1/2/3 = VACUUM/REFL/PER/WHITE	1	IIM	INNER ITERATION MAXIMUM	20
IBR	RIGHT BOUNDARY CONDITION	3	ICM	OUTER ITERATION MAXIMUM	25
MXX	NUMBER OF MIXTURES	3	ICLC	-1/0/N--FLAT RES/SN/OPT	0
MS	MIXING TABLE LENGTH	23	ITH	0/1 = FORWARD/ADJOINT	0
IGM	NUMBER OF ENERGY GROUPS	27	IFLU	NOT USED(ALWAYS WGTD)	0
NNG	NUMBER OF NEUTRON GROUPS	27	IPRT	-2/-1/0/N=MIXTURE XSEC PRINT	-2
NGG	NUMBER OF GAMMA GROUPS	0	ID1	0/1/2/3=NO/PRT ND/PCH N/BOTH	53
IFTG	NUMBER OF FIRST THERMAL GROUP	15	IPBT	-1/0/1=NONE/FINE/ALL BAL. PRT	0

SPECIAL OPTIONS

IFG	0/1 = NONE/WEIGHTING CALCULATION	1	IPN	0/1/2 DIFF. COEF. PARAM	0
IQM	VOLUMETRIC SOURCES (0/N=NO/YES)	0	IDFM	0/1 = NONE/DENSITY FACTORS 38*	0
IPM	BOUNDARY SOURCES (0/N=NO/YES)	0	IAZ	0/N = NONE/N ACTIVITIES BY ZONE	0
IFN	0/1/2 = INPUT 33*/34*/USE LAST	53	IAI	0/1=NONE/ACTIVITIES BY INTERVAL	0
ITMX	MAXIMUM TIME (MINUTES)	10	IFCT	0/1=NO/YES UPSCATTER SCALING	0
IDT1	0/1/2/3=NO/XSECT/SRCE/FLUX--OUT	0	IPVT	0/1/2=NO/K/ALPHA PARAMETRIC SRCH	0
ISX	BROAD GROUP FLUXES	0	ISEN	OUTER ITERATION ACCELERATION	0
IBLN	ACTIVITY DATA UNIT	0	NBND	BAND REBALN PARAMETER	0
JBKL	0/1/2 BUCKLING GEOMETRY	0			

WEIGHTING DATA (IFG=1)

ICON	-1/0/1=CELL/ZONE/REGION WEIGHT	-1	IHTF	TOTAL XSECT PSN IN BRD GP TABLES	3
IGMF	NUMBER OF BROAD GROUPS	27	NDSF	PSN G-G OR FILE NUMBER	4
ITP	0/10/20/30/40 0/C/E/AC/A	0	NUSF	TABLE LENGTH OR MAX ORDER	4
IPP	-2/-1/0/N=WGTED XSECT PRINT	-2	MSCM	EXTRA 1-D X-SECT POSITIONS	0
IAP	-1/N ANISN XSECT PRINT	-1			

FLOATING POINT PARAMETERS

EPS	OVERALL CONVERGENCE	1.00000E-04	DY	CYL/PLA HT FOR BUCKLING	0.00000E+00
PTC	POINT CONVERGENCE	1.00000E-04	DZ	PLANE DEPTH FOR BUCKLING	0.00000E+00
XNF	NORMALIZATION FACTOR	1.00000E+00	VSC	VOID STREAMING CORRECTION	0.00000E+00
EV	EIGENVALUE GUESS	0.00000E+00	PV	IPVT=1/2--K/ALPHA	1.00000E+00
EVM	EIGENVALUE MODIFIER	0.00000E+00	EQL	EV CHANGE EPS FOR SEARCH	1.00000E-03
BF	BUCKLING FACTOR=1.420892	1.42089E+00	XNPM	NEW PARAM MOD FOR SEARCH	7.50000E-01

THIS CASE WILL REQUIRE 2367 LOCATIONS FOR MIXING
THIS CASE HAS BEEN ALLOCATED 200000 LOCATIONS

Figure S2.6.6 XSDRNPM Path A of PASS 0 problem definition page

AT 0 D, SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL

13Q ARRAY HAS 23 ENTRIES.

14Q ARRAY HAS 23 ENTRIES.

15Q ARRAY HAS 23 ENTRIES.

DATA BLOCK 2 (MIXING TABLE, ETC.)

	NUCLIDES ON TAPE	CCCC IDENTIFICATION
1	999	
2	1001	
3	5010	
4	5011	
5	8016	
6	6	
7	27059	
8	40302	
9	54135	
10	55133	
11	92234	
12	92235	
13	92236	
14	92238	
15	93237	
16	94238	
17	94239	
18	94240	
19	94241	
20	94242	
21	95241	
22	95243	
23	96244	

MIXTURE	MIXING TABLE COMPONENT	ATOM DENSITY
1	92234	6.27704E-06
1	92235	7.14316E-04
1	92236	3.33414E-06
1	92238	2.13256E-02
1	8016	4.40991E-02
3	6	2.45085E-02
2	40302	4.25156E-02
3	1001	4.90170E-02
3	5010	4.43773E-06
3	5011	1.80159E-05
3	27059	9.09453E-22
1	54135	1.00000E-20
1	55133	1.00000E-20
1	93237	1.00000E-20
1	94238	1.00000E-20
1	94239	1.00000E-20
1	94240	1.00000E-20
1	94241	1.00000E-20
1	94242	1.00000E-20
1	95241	1.00000E-20
1	95243	1.00000E-20
1	96244	1.00000E-20
1	999	1.00000E-20

ELAPSED TIME 0.02 MIN.

15527 LOCATIONS WILL BE USED

35Q ARRAY HAS 15 ENTRIES.

36Q ARRAY HAS 14 ENTRIES.

39Q ARRAY HAS 3 ENTRIES.

40Q ARRAY HAS 3 ENTRIES.

47Q ARRAY HAS 27 ENTRIES.

51Q ARRAY HAS 27 ENTRIES.

Figure S2.6.7 XSDRNPM mixing table data of Path A of PASS 0

```
LOGICAL ASSIGNMENTS

MASTER LIBRARY   12
WORKING LIBRARY  17
SCRATCH FILE     18
NEW LIBRARY       1

P R O B L E M   D E S C R I P T I O N

IGR--GEOMETRY (0/1/2/3--INF MED/SLAB/CYL/SPHERE                    2

IZM--NUMBER OF ZONES OR MATERIAL REGIONS                           4

MS--MIXING TABLE LENGTH                                           29

IBL--SHIELDED CROSS SECTION EDIT OPTION (0/1--NO/YES)              0

IBR--BONDARENKO FACTOR EDIT OPTION (0/1--NO/YES)                   0

ISSOPT--DANCOFF FACTOR OPTION                                      0

CONVERGENCE CRITERION    1.00000E-03

GEOMETRY CORRECTION FACTOR FOR WIGNER RATIONAL APPROXIMATION  1.350E+00

       3Q ARRAY HAS     29 ENTRIES.

       4Q ARRAY HAS     29 ENTRIES.

       5Q ARRAY HAS     29 ENTRIES.

       6Q ARRAY HAS      4 ENTRIES.

       7Q ARRAY HAS      4 ENTRIES.

       8Q ARRAY HAS      4 ENTRIES.

       9Q ARRAY HAS      4 ENTRIES.

      10Q ARRAY HAS     29 ENTRIES.

      11Q ARRAY HAS      4 ENTRIES.

M I X I N G   T A B L E

ENTRY   MIXTURE   ISOTOPE   NUMBER DENSITY   NEW IDENTIFIER
    1         3      8016    2.45085E-02              201
    2         3      1001    4.90170E-02              202
    3         3      5010    4.43773E-06              203
    4         3      5011    1.80159E-05              204
    5         3     27059    9.09453E-22              205
    6         2     40302    4.25156E-02              206
    7         1     92234    2.16907E-06           200007
    8         1     92235    2.46836E-04           200008
    9         1     92236    1.15213E-06           200009
   10         1     92238    7.36919E-03           200010
   11         1      8016    1.52387E-02           200011
   12         1      8016    1.35642E-02           200012
   13         1     40302    4.29381E-03           200013
   14         1      1001    2.71285E-02           200014
   15         1      5010    2.45606E-06           200015
   16         1      5011    9.97090E-06           200016
   17         1     27059    5.03337E-22           200017
   18         1     54135    3.45556E-21           200018
   19         1     55133    3.45556E-21           200019
   20         1     93237    3.45556E-21           200020
   21         1     94238    3.45556E-21           200021
   22         1     94239    3.45556E-21           200022
   23         1     94240    3.45556E-21           200023
   24         1     94241    3.45556E-21           200024
   25         1     94242    3.45556E-21           200025
   26         1     95241    3.45556E-21           200026
   27         1     95243    3.45556E-21           200027
   28         1     96244    3.45556E-21           200028
   29         1       999    3.45556E-21           200029
```

Figure S2.6.8 BONAMI mixing table data of Path B of PASS 0

```
                    AT 0 D, SECOND PART OF SAS2H PASS TO MAKE LIBRARY

   13Q ARRAY HAS      29 ENTRIES.

   14Q ARRAY HAS      29 ENTRIES.

   15Q ARRAY HAS      29 ENTRIES.

                    DATA BLOCK 2 (MIXING TABLE, ETC.)
```

	NUCLIDES ON TAPE	CCCC IDENTIFICATION	MIXTURE	MIXING TABLE COMPONENT	ATOM DENSITY
1	202		3	201	2.45085E-02
2	203		3	202	4.90170E-02
3	204		3	203	4.43773E-06
4	201		3	204	1.80159E-05
5	205		3	205	9.09453E-22
6	206		2	206	4.25156E-02
7	999		1	92234	2.16907E-06
8	1001		1	92235	2.46836E-04
9	5010		1	92236	1.15213E-06
10	5011		1	92238	7.36919E-03
11	8016		1	8016	1.52387E-02
12	6		1	6	1.35642E-02
13	27059		1	40302	4.29381E-03
14	40302		1	1001	2.71285E-02
15	54135		1	5010	2.45606E-06
16	55133		1	5011	9.97090E-06
17	92234		1	27059	5.03337E-22
18	92235		1	54135	3.45556E-21
19	92236		1	55133	3.45556E-21
20	92238		1	93237	3.45556E-21
21	93237		1	94238	3.45556E-21
22	94238		1	94239	3.45556E-21
23	94239		1	94240	3.45556E-21
24	94240		1	94241	3.45556E-21
25	94241		1	94242	3.45556E-21
26	94242		1	95241	3.45556E-21
27	95241		1	95243	3.45556E-21
28	95243		1	96244	3.45556E-21
29	96244		1	999	3.45556E-21

```
ELAPSED TIME    0.03 MIN.

 19963 LOCATIONS WILL BE USED

    35Q ARRAY HAS      22 ENTRIES.

    36Q ARRAY HAS      21 ENTRIES.

    39Q ARRAY HAS       4 ENTRIES.

    40Q ARRAY HAS       4 ENTRIES.

    47Q ARRAY HAS      27 ENTRIES.

    51Q ARRAY HAS      27 ENTRIES.
```

Figure S2.6.9 XSDRNPM mixing table data of Path B of PASS 0

SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK
POWER= 1.968E-04MW, BURNUP=8.6574E-02MWD, FLUX= 4.03E+13N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAM ATOMS
BASIS = CONVERTED TO ATOMS/(BARN-CM)

	CHARGE	110.0 D	220.0 D	330.0 D	440.0 D
HE 4	0.00E+00	2.59E-10	1.53E-09	6.43E-09	2.10E-08
U232	0.00E+00	1.55E-13	3.50E-13	6.23E-13	1.00E-12
U233	0.00E+00	1.32E-11	2.29E-11	2.99E-11	3.49E-11
U234	6.28E-06	5.94E-06	5.62E-06	5.30E-06	5.00E-06
U235	7.14E-04	6.11E-04	5.22E-04	4.44E-04	3.76E-04
U236	3.33E-06	2.19E-05	3.74E-05	5.05E-05	6.16E-05
U237	0.00E+00	7.52E-08	1.07E-07	1.36E-07	1.65E-07
U238	2.13E-02	2.13E-02	2.12E-02	2.12E-02	2.11E-02
U239	0.00E+00	1.12E-08	1.12E-08	1.15E-08	1.18E-08
U240	0.00E+00	5.99E-39	9.56E-36	7.01E-34	1.47E-32
NP236	0.00E+00	9.65E-13	4.92E-12	1.31E-11	2.68E-11
NP237	0.00E+00	5.65E-07	1.49E-06	2.66E-06	4.04E-06
NP238	0.00E+00	1.42E-09	3.75E-09	6.89E-09	1.08E-08
NP239	0.00E+00	1.61E-06	1.61E-06	1.65E-06	1.70E-06
NP240M	0.00E+00	5.24E-41	8.36E-38	6.13E-36	1.29E-34
NP240	0.00E+00	5.59E-11	5.60E-11	5.89E-11	6.28E-11
PU236	0.00E+00	1.36E-16	6.03E-16	1.58E-15	3.37E-15
PU238	0.00E+00	2.18E-08	1.10E-07	2.88E-07	5.79E-07
PU239	0.00E+00	3.98E-05	6.49E-05	8.02E-05	8.95E-05
PU240	0.00E+00	3.18E-06	8.96E-06	1.45E-05	1.89E-05
PU241	0.00E+00	7.12E-07	3.87E-06	9.15E-06	1.54E-05
PU242	0.00E+00	2.12E-08	2.43E-07	9.22E-07	2.22E-06
PU243	0.00E+00	5.21E-12	5.99E-11	2.33E-10	5.82E-10
PU244	0.00E+00	3.08E-28	4.91E-25	3.60E-23	7.57E-22
PU245	0.00E+00	5.56E-34	8.89E-31	6.69E-29	1.45E-27
AM241	0.00E+00	2.57E-09	2.78E-08	9.71E-08	2.13E-07
AM242M	0.00E+00	2.39E-11	4.25E-10	1.90E-09	4.86E-09
AM242	0.00E+00	6.66E-12	7.21E-11	2.59E-10	5.88E-10
AM243	0.00E+00	4.03E-10	9.52E-09	5.65E-08	1.90E-07
AM244	0.00E+00	2.69E-13	6.36E-12	3.87E-11	1.34E-10
AM245	0.00E+00	4.10E-32	6.21E-29	4.43E-27	9.12E-26
CM242	0.00E+00	1.24E-10	2.62E-09	1.37E-08	4.04E-08
CM243	0.00E+00	4.38E-13	1.84E-11	1.46E-10	5.79E-10
CM244	0.00E+00	8.44E-12	4.11E-10	3.81E-09	1.79E-08
CM245	0.00E+00	4.56E-14	4.25E-12	5.70E-11	3.45E-10
CM246	0.00E+00	5.26E-16	1.01E-13	2.11E-12	1.78E-11
CM247	0.00E+00	8.27E-19	3.18E-16	1.01E-14	1.15E-13
CM248	0.00E+00	5.82E-21	4.58E-18	2.23E-16	3.52E-15
CM249	0.00E+00	6.77E-26	5.34E-23	2.67E-21	4.36E-20
CM250	0.00E+00	3.47E-30	5.56E-27	4.29E-25	9.62E-24
TOTALS	2.20E-02	2.20E-02	2.19E-02	2.18E-02	2.17E-02
FLUX		3.94E+13	3.95E+13	4.05E+13	4.19E+13

.RESULTS ON LOGICAL UNIT NO. 71, POSITION 1, FOR TIME STEP 4, SUBCASE 1. (RUN POSITION 1, CASE POSITION 1)
TITLE: SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK

.RESULTS ON LOGICAL UNIT NO. 71, POSITION 2, FOR TIME STEP 4, SUBCASE 1. (RUN POSITION 1, CASE POSITION 1)
TITLE: SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK

.RESULTS ON LOGICAL UNIT NO. 71, POSITION 3, FOR TIME STEP 0, SUBCASE 1. (RUN POSITION 1, CASE POSITION 1)
TITLE: SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK

.RESULTS ON LOGICAL UNIT NO. 71, POSITION 4, FOR TIME STEP 1, SUBCASE 1. (RUN POSITION 1, CASE POSITION 1)
TITLE: SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK

.TERMINATED LOGICAL UNIT NO. 71 WITH ZERO FLAG RECORD.

Figure S2.6.10. Part of ORIGEN-S actinide table of PASS 0

13Q ARRAY HAS 23 ENTRIES.

14Q ARRAY HAS 23 ENTRIES.

15Q ARRAY HAS 23 ENTRIES.

DATA BLOCK 2 (MIXING TABLE, ETC.)

	NUCLIDES ON TAPE	CCCC IDENTIFICATION	MIXTURE	MIXING TABLE COMPONENT	ATOM DENSITY
1	999		1	92234	5.00071E-06
2	1001		1	92235	3.75615E-04
3	5010		1	92236	6.15666E-05
4	5011		1	92238	2.10890E-02
5	8016		1	8016	4.40991E-02
6	6		3	6	2.45085E-02
7	27059		2	40302	4.25156E-02
8	40302		3	1001	4.90170E-02
9	54135		3	5010	4.43773E-06
10	55133		3	5011	1.80159E-05
11	92234		3	27059	9.09453E-22
12	92235		1	54135	8.13150E-09
13	92236		1	55133	2.42690E-05
14	92238		1	93237	4.03981E-06
15	93237		1	94238	5.78545E-07
16	94238		1	94239	8.95361E-05
17	94239		1	94240	1.89466E-05
18	94240		1	94241	1.54014E-05
19	94241		1	94242	2.22333E-06
20	94242		1	95241	2.13450E-07
21	95241		1	95243	1.89540E-07
22	95243		1	96244	1.78878E-08
23	96244		1	999	1.00000E-20

ELAPSED TIME 0.02 MIN.

15527 LOCATIONS WILL BE USED

35Q ARRAY HAS 15 ENTRIES.

36Q ARRAY HAS 14 ENTRIES.

39Q ARRAY HAS 3 ENTRIES.

40Q ARRAY HAS 3 ENTRIES.

47Q ARRAY HAS 27 ENTRIES.

51Q ARRAY HAS 27 ENTRIES.

Figure S2.6.11 Mixing table data of Path A of PASS 1

SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK ACTINIDES
POWER= 17.30MW, BURNUP= 15226.MWD, FLUX= 4.14E+13N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAM ATOMS
BASIS = SINGLE REACTOR ASSEMBLY

	CHARGE	220.0 D	440.0 D	660.0 D	880.0 D
HE 4	0.00E+00	1.32E-04	1.52E-03	8.27E-03	2.66E-02
PB206	0.00E+00	1.70E-19	4.56E-18	2.85E-17	9.92E-17
PB207	0.00E+00	2.80E-15	3.49E-14	1.53E-13	4.28E-13
PB208	0.00E+00	6.20E-12	5.37E-11	2.04E-10	5.52E-10
PB209	0.00E+00	2.15E-18	1.01E-17	2.90E-17	6.62E-17
PB210	0.00E+00	1.97E-16	1.44E-15	4.44E-15	9.57E-15
PB211	0.00E+00	2.00E-18	1.18E-17	3.27E-17	6.58E-17
PB212	0.00E+00	5.59E-14	2.53E-13	6.77E-13	1.42E-12
PB214	0.00E+00	7.19E-20	2.55E-19	5.05E-19	7.89E-19
TH227	0.00E+00	1.47E-15	8.68E-15	2.41E-14	4.85E-14
TH228	0.00E+00	8.81E-11	3.99E-10	1.06E-09	2.23E-09
TH229	0.00E+00	4.78E-12	2.32E-11	6.85E-11	1.67E-10
TH230	0.00E+00	7.83E-07	1.29E-06	1.58E-06	1.69E-06
TH231	0.00E+00	1.58E-09	2.50E-09	3.20E-09	3.64E-09
TH232	0.00E+00	3.41E-08	1.13E-07	2.22E-07	3.49E-07
TH233	0.00E+00	8.05E-14	2.75E-13	5.80E-13	9.83E-13
TH234	0.00E+00	2.75E-08	2.74E-08	2.72E-08	2.70E-08
PA231	0.00E+00	1.27E-07	3.76E-07	6.85E-07	9.95E-07
PA232	0.00E+00	2.13E-10	6.49E-10	1.27E-09	1.99E-09
PA233	0.00E+00	3.69E-09	1.09E-08	2.00E-08	3.00E-08
PA234M	0.00E+00	9.30E-13	9.31E-13	9.32E-13	9.35E-13
PA234	0.00E+00	1.31E-12	2.95E-12	5.31E-12	8.25E-12
U232	0.00E+00	3.54E-08	9.74E-08	2.03E-07	3.54E-07
U233	0.00E+00	2.36E-06	3.54E-06	4.03E-06	4.08E-06
U234	5.52E-01	4.90E-01	4.34E-01	3.81E-01	3.31E-01
U235	6.28E+01	4.57E+01	3.30E+01	2.32E+01	1.59E+01
U236	2.93E-01	3.38E+00	5.54E+00	7.04E+00	8.01E+00
U237	0.00E+00	9.56E-03	1.40E-02	1.81E-02	2.17E-02
U238	1.88E+03	1.86E+03	1.85E+03	1.84E+03	1.83E+03
U239	0.00E+00	1.06E-03	1.08E-03	1.15E-03	1.24E-03
U240	0.00E+00	8.24E-31	1.24E-27	8.93E-26	1.84E-24
NP236	0.00E+00	5.40E-07	2.82E-06	7.73E-06	1.60E-05
NP237	0.00E+00	1.37E-01	3.57E-01	6.24E-01	9.10E-01
NP238	0.00E+00	3.60E-04	9.66E-04	1.82E-03	2.86E-03
NP239	0.00E+00	1.52E-01	1.55E-01	1.66E-01	1.78E-01
NP240M	0.00E+00	7.21E-33	1.08E-29	7.81E-28	1.61E-26
NP240	0.00E+00	5.62E-06	5.90E-06	6.79E-06	7.84E-06
PU236	0.00E+00	6.92E-11	3.75E-10	1.19E-09	2.91E-09
PU238	0.00E+00	1.06E-02	5.33E-02	1.41E-01	2.80E-01
PU239	0.00E+00	6.31E+00	8.87E+00	9.85E+00	1.02E+01
PU240	0.00E+00	9.04E-01	2.14E+00	3.00E+00	3.46E+00
PU241	0.00E+00	2.57E-01	1.12E+00	2.16E+00	2.98E+00
PU242	0.00E+00	1.52E-02	1.46E-01	4.73E-01	9.72E-01
PU243	0.00E+00	4.01E-06	3.97E-05	1.38E-04	3.06E-04
PU244	0.00E+00	4.24E-20	6.36E-17	4.59E-15	9.48E-14
PU245	0.00E+00	7.60E-26	1.17E-22	9.11E-21	2.03E-19
AM241	0.00E+00	1.83E-03	1.53E-02	4.12E-02	6.95E-02
AM242M	0.00E+00	2.65E-05	3.26E-04	1.04E-03	1.91E-03
AM242	0.00E+00	4.54E-06	3.92E-05	1.13E-04	2.06E-04
AM243	0.00E+00	6.29E-04	1.28E-02	6.67E-02	1.95E-01

Figure S2.6.12 Part of final case actinide depletion table

SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK ACTINIDES
DECAY, FOLLOWING REACTOR IRRADIATION IDENTIFIED BY: POWER= 17.30MW, BURNUP= 15226.MWD,
FLUX= 4.14E+13N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAMS
BASIS =SINGLE REACTOR ASSEMBLY

	INITIAL	304.4 D	608.7 D	913.1 D	1217.5 D	1521.9 D	1826.2 D
HE 4	1.06E-01	1.94E-01	2.31E-01	2.54E-01	2.74E-01	2.92E-01	3.11E-01
PB208	1.15E-07	3.16E-07	6.19E-07	9.95E-07	1.43E-06	1.90E-06	2.39E-06
TH228	5.08E-07	9.35E-07	1.25E-06	1.47E-06	1.64E-06	1.75E-06	1.84E-06
TH230	3.88E-04	5.69E-04	7.50E-04	9.33E-04	1.12E-03	1.30E-03	1.49E-03
TH232	8.10E-05	1.27E-04	1.73E-04	2.19E-04	2.64E-04	3.10E-04	3.56E-04
TH234	6.32E-06	6.32E-06	6.32E-06	6.32E-06	6.32E-06	6.32E-06	6.32E-06
PA231	2.30E-04	2.34E-04	2.37E-04	2.40E-04	2.43E-04	2.46E-04	2.49E-04
PA233	6.98E-06	7.50E-06	7.50E-06	7.51E-06	7.51E-06	7.52E-06	7.52E-06
U232	8.20E-05	8.19E-05	8.14E-05	8.08E-05	8.02E-05	7.97E-05	7.91E-05
U233	9.51E-04	1.02E-03	1.08E-03	1.15E-03	1.22E-03	1.28E-03	1.35E-03
U234	7.74E+01	7.79E+01	7.84E+01	7.88E+01	7.93E+01	7.97E+01	8.02E+01
U235	3.73E+03	3.73E+03	3.73E+03	3.73E+03	3.73E+03	3.73E+03	3.73E+03
U236	1.89E+03	1.89E+03	1.89E+03	1.89E+03	1.89E+03	1.89E+03	1.89E+03
U237	5.14E+00	2.14E-05	2.06E-05	1.98E-05	1.90E-05	1.83E-05	1.76E-05
U238	4.35E+05	4.35E+05	4.35E+05	4.35E+05	4.35E+05	4.35E+05	4.35E+05
NP236	3.78E-03	3.78E-03	3.78E-03	3.78E-03	3.78E-03	3.78E-03	3.78E-03
NP237	2.16E+02	2.21E+02	2.21E+02	2.21E+02	2.21E+02	2.21E+02	2.21E+02
NP239	4.24E+01	4.08E-05	4.08E-05	4.08E-05	4.08E-05	4.08E-05	4.07E-05
PU238	6.65E+01	7.10E+01	7.17E+01	7.16E+01	7.12E+01	7.07E+01	7.03E+01
PU239	2.43E+03	2.48E+03	2.48E+03	2.48E+03	2.48E+03	2.48E+03	2.48E+03
PU240	8.30E+02	8.30E+02	8.30E+02	8.30E+02	8.31E+02	8.31E+02	8.31E+02
PU241	7.19E+02	6.91E+02	6.64E+02	6.39E+02	6.14E+02	5.91E+02	5.68E+02
PU242	2.35E+02	2.35E+02	2.35E+02	2.35E+02	2.35E+02	2.35E+02	2.35E+02
AM241	1.68E+01	4.44E+01	7.10E+01	9.65E+01	1.21E+02	1.44E+02	1.67E+02
AM242M	4.62E-01	4.60E-01	4.59E-01	4.57E-01	4.55E-01	4.53E-01	4.52E-01
AM242	4.99E-02	5.51E-06	5.49E-06	5.47E-06	5.45E-06	5.43E-06	5.40E-06
AM243	4.74E+01	4.74E+01	4.74E+01	4.74E+01	4.74E+01	4.74E+01	4.74E+01
CM242	5.92E+00	1.64E+00	4.50E-01	1.24E-01	3.49E-02	1.04E-02	3.64E-03
CM243	1.73E-01	1.70E-01	1.66E-01	1.63E-01	1.60E-01	1.56E-01	1.53E-01
CM244	1.12E+01	1.08E+01	1.05E+01	1.02E+01	9.85E+00	9.54E+00	9.24E+00
CM245	4.04E-01	4.04E-01	4.04E-01	4.04E-01	4.04E-01	4.04E-01	4.04E-01
CM246	4.97E-02	4.97E-02	4.97E-02	4.97E-02	4.97E-02	4.97E-02	4.97E-02
CM247	7.18E-04	7.18E-04	7.18E-04	7.18E-04	7.18E-04	7.18E-04	7.18E-04
CM248	5.38E-05	5.38E-05	5.38E-05	5.38E-05	5.38E-05	5.39E-05	5.39E-05
CF249	7.32E-08	4.09E-07	5.82E-07	6.71E-07	7.16E-07	7.39E-07	7.50E-07
TOTAL	4.45E+05	4.45E+05	4.45E+05	4.45E+05	4.45E+05	4.45E+05	4.45E+05

Figure S2.6.13 Final decay case actinide table

GAMMA SOURCE SPECTRUM FOR GAMMA LINES (SAS2)

1826.25 DAY TIME OF THE REQUESTED NUCLIDES

ENERGY INTERVAL IN MEV		PHOTONS / SECOND	MEV / SECOND
1.0000E-02 TO	5.0000E-02	1.2005E+15	3.6015E+13
5.0000E-02 TO	1.0000E-01	3.4004E+14	2.5503E+13
1.0000E-01 TO	2.0000E-01	3.0362E+14	4.5542E+13
2.0000E-01 TO	3.0000E-01	8.2766E+13	2.0691E+13
3.0000E-01 TO	4.0000E-01	5.5248E+13	1.9337E+13
4.0000E-01 TO	6.0000E-01	5.8008E+14	2.9004E+14
6.0000E-01 TO	8.0000E-01	1.8675E+15	1.3072E+15
8.0000E-01 TO	1.0000E+00	2.6463E+14	2.3817E+14
1.0000E+00 TO	1.3300E+00	2.4123E+14	2.8103E+14
1.3300E+00 TO	1.6600E+00	5.9442E+13	8.8866E+13
1.6600E+00 TO	2.0000E+00	9.3632E+11	1.7135E+12
2.0000E+00 TO	2.5000E+00	2.4573E+12	5.5289E+12
2.5000E+00 TO	3.0000E+00	6.8574E+10	1.8858E+11
3.0000E+00 TO	4.0000E+00	8.5008E+09	2.9753E+10
4.0000E+00 TO	5.0000E+00	3.6366E+06	1.6365E+07
5.0000E+00 TO	6.5000E+00	1.4593E+06	8.3908E+06
6.5000E+00 TO	8.0000E+00	2.8622E+05	2.0751E+06
8.0000E+00 TO	1.0000E+01	6.0764E+04	5.4688E+05
TOTALS		4.9985E+15	2.3599E+15

TOTAL ENERGY FROM NUCLIDES WITH SPECTRUM DATA = 2.3598E+15

TOTAL ENERGY FROM NUCLIDES WITH NO SPECTRUM DATA = 4.1513E+10

Figure S2.6.14 ORIGEN-S gamma source spectrum

TOTAL (ALPHA-N PLUS SPON. FISSION) NEUTRON SOURCE SPECTRUM AS A FUNCTION OF TIME
(USING REACTION SPECTRA FOR URANIUM DIOXIDE)

SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK
NEUTRON SPECTRA, NEUTRONS/SEC/BASIS
BASIS = SINGLE REACTOR ASSEMBLY

	BOUNDARIES, MEV		INITIAL	304.4 D	608.8 D	913.1 D	1217.5 D	1521.9 D	1826.2 D
1	6.43E+00	- 2.00E+01	4.733E+06	2.982E+06	2.443E+06	2.245E+06	2.142E+06	2.066E+06	2.000E+06
2	3.00E+00	- 6.43E+00	6.389E+07	3.673E+07	2.860E+07	2.579E+07	2.448E+07	2.360E+07	2.285E+07
3	1.85E+00	- 3.00E+00	6.939E+07	4.025E+07	3.156E+07	2.859E+07	2.721E+07	2.628E+07	2.549E+07
4	1.40E+00	- 1.85E+00	3.418E+07	2.131E+07	1.738E+07	1.596E+07	1.524E+07	1.472E+07	1.427E+07
5	9.00E-01	- 1.40E+00	4.512E+07	2.852E+07	2.342E+07	2.155E+07	2.058E+07	1.987E+07	1.924E+07
6	4.00E-01	- 9.00E-01	4.932E+07	3.114E+07	2.555E+07	2.349E+07	2.242E+07	2.164E+07	2.095E+07
7	1.00E-01	- 4.00E-01	9.696E+06	6.108E+06	5.004E+06	4.600E+06	4.389E+06	4.235E+06	4.100E+06
8	1.70E-02	- 1.00E-01	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
9	3.00E-03	- 1.70E-02	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
10	5.50E-04	- 3.00E-03	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
11	1.00E-04	- 5.50E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
12	3.00E-05	- 1.00E-04	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
13	1.00E-05	- 3.00E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
14	3.05E-06	- 1.00E-05	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
15	1.77E-06	- 3.05E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
16	1.30E-06	- 1.77E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
17	1.13E-06	- 1.30E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
18	1.00E-06	- 1.13E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
19	8.00E-07	- 1.00E-06	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
20	4.00E-07	- 8.00E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
21	3.25E-07	- 4.00E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
22	2.25E-07	- 3.25E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
23	1.00E-07	- 2.25E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
24	5.00E-08	- 1.00E-07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
25	3.00E-08	- 5.00E-08	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
26	1.00E-08	- 3.00E-08	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
27	1.00E-11	- 1.00E-08	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
			2.763E+08	1.670E+08	1.340E+08	1.222E+08	1.165E+08	1.124E+08	1.089E+08

Figure S2.6.15 SAS2 neutron source spectrum

M I X I N G T A B L E

ENTRY	MIXTURE	ISOTOPE	NUMBER DENSITY	NEW IDENTIFIER
1	1	92234	1.10503E-06	92234
2	2	92234	1.10427E-06	1000002
3	1	92235	5.12253E-05	92235
4	2	92235	5.11902E-05	1000004
5	6	92235	1.31783E-04	28
6	1	92236	2.58307E-05	92236
7	2	92236	2.58130E-05	1000007
8	1	92238	5.89429E-03	92238
9	2	92238	5.89025E-03	1000009
10	6	92238	4.80619E-02	33
11	1	8016	1.25029E-02	8016
12	2	8016	1.24944E-02	1000012
13	9	8016	3.15067E-02	36
14	1	40302	3.52295E-03	40302
15	2	40302	3.52054E-03	1000015
16	1	54135	2.83519E-19	54135
17	2	54135	2.83325E-19	1000017
18	1	55133	1.29784E-05	55133
19	2	55133	1.29695E-05	1000019
20	1	93237	3.01271E-06	93237
21	2	93237	3.01064E-06	1000021
22	1	94238	9.51973E-07	94238
23	2	94238	9.51320E-07	1000023
24	1	94239	3.34067E-05	94239
25	2	94239	3.33838E-05	1000025
26	1	94240	1.11634E-05	94240
27	2	94240	1.11557E-05	1000027
28	1	94241	7.59665E-06	94241
29	2	94241	7.59144E-06	1000029
30	1	94242	3.13334E-06	94242
31	2	94242	3.13120E-06	1000031
32	1	95241	2.23368E-06	95241
33	2	95241	2.23215E-06	1000033
34	1	95243	6.29197E-07	95243
35	2	95243	6.28766E-07	1000035
36	1	96244	1.22156E-07	96244
37	2	96244	1.22073E-07	1000037
38	9	1001	6.30133E-02	61
39	3	5010	1.67345E-03	62
40	3	5011	6.79370E-03	63
41	1	24304	3.72536E-04	24304
42	2	24304	3.72536E-04	65
43	3	24304	3.78409E-04	66
44	5	24304	1.74286E-02	67
45	1	25055	3.71141E-05	25055
46	2	25055	3.71141E-05	69
47	3	25055	3.76992E-05	70
48	5	25055	1.73633E-03	71
49	1	26304	1.26877E-03	26304
50	2	26304	1.26877E-03	73
51	3	26304	1.28878E-03	74
52	5	26304	5.93579E-02	75
53	1	28304	1.65031E-04	28304
54	2	28304	1.65031E-04	77
55	3	28304	1.67633E-04	78
56	5	28304	7.72073E-03	79
57	1	7014	2.90138E-05	7014
58	2	7014	2.90138E-05	81
59	4	7014	4.30051E-22	82
60	3	6012	2.11679E-03	6012

Figure S2.6.16 BONAMI mixing table of cell-weighted case

```
THIS XSDRN WORKING TAPE WAS CREATED 06/14/93 AT 07:46:06
THE TITLE OF THE PARENT CASE IS AS FOLLOWS
THIS XSDRN WORKING TAPE WAS CREATED 06/14/93 AT 07:45:21
THE TITLE OF THE PARENT CASE IS AS FOLLOWS
SCALE4 - 27 NEUTRON 18 GAMMA GROUP SHIELDING LIBRARY
    TAPE ID                          8054036          NUMBER OF NUCLIDES                44
    NUMBER OF NEUTRON GROUPS              27          NUMBER OF GAMMA GROUPS            18
    FIRST THERMAL GROUP                   15          LOGICAL UNIT                       4
                                TABLE OF CONTENTS
  DOSE FACTORS                                    UPDATED 9/07/89                 ID      900
   HYDROGEN        ENDF/B-IV MAT 1269/THRM1002    UPDATED 10/13/89                ID       61
   BORON-10        ENDF/B-IV MAT 1273             UPDATED 10/13/89                ID       62
   BORON-11        ENDF/B-IV MAT 1160             UPDATED 10/13/89                ID       63
   CARBON-12       ENDF/B-IV MAT 1274/THRM1065    UPDATED 10/13/89                ID     6012
   NITROGEN-14     ENDF/B-IV MAT 1275             UPDATED 10/13/89                ID     7014
   NITROGEN-14     ENDF/B-IV MAT 1275             UPDATED 10/13/89                ID       81
   NITROGEN-14     ENDF/B-IV MAT 1275             UPDATED 10/13/89                ID       82
   OXYGEN-16       ENDF/B-IV MAT 1276             UPDATED 10/13/89                ID       36
   CHROMIUM(SS304)ENDF/B-IV MAT 1191              UPDATED 10/13/89                ID    24304
   CHROMIUM(SS304)ENDF/B-IV MAT 1191              UPDATED 10/13/89                ID       65
   CHROMIUM(SS304)ENDF/B-IV MAT 1191              UPDATED 10/13/89                ID       66
   CHROMIUM(SS304)ENDF/B-IV MAT 1191              UPDATED 10/13/89                ID       67
   MANGANESE       ENDF/B-IV MAT 1197             UPDATED 10/13/89                ID    25055
   MANGANESE       ENDF/B-IV MAT 1197             UPDATED 10/13/89                ID       69
   MANGANESE       ENDF/B-IV MAT 1197             UPDATED 10/13/89                ID       70
   MANGANESE       ENDF/B-IV MAT 1197             UPDATED 10/13/89                ID       71
   IRON(SS304)     ENDF/B-IV MAT 1192             UPDATED 10/13/89                ID    26304
   IRON(SS304)     ENDF/B-IV MAT 1192             UPDATED 10/13/89                ID       73
   IRON(SS304)     ENDF/B-IV MAT 1192             UPDATED 10/13/89                ID       74
   IRON(SS304)     ENDF/B-IV MAT 1192             UPDATED 10/13/89                ID       75
   NICKEL(SS304)   ENDF/B-IV MAT 1190             UPDATED 10/13/89                ID    28304
   NICKEL(SS304)   ENDF/B-IV MAT 1190             UPDATED 10/13/89                ID       77
   NICKEL(SS304)   ENDF/B-IV MAT 1190             UPDATED 10/13/89                ID       78
   NICKEL(SS304)   ENDF/B-IV MAT 1190             UPDATED 10/13/89                ID       79
   URANIUM-235     ENDF/B-IV MAT 1261             UPDATED 10/13/89                ID       28
   URANIUM-238     ENDF/B-IV MAT 1262             UPDATED 10/13/89                ID       33
   OXYGEN-16       ENDF/B-IV MAT 1276             UPDATED 10/13/89                ID     8016
   ZIRCALLOY       ENDF/B-IV MAT 1284             UPDATED 10/13/89                ID    40302
   XENON-135       ENDF/B-IV MAT 1294             UPDATED 10/13/89                ID    54135
   CESIUM-133      ENDF/B-IV MAT 1141             UPDATED 10/13/89                ID    55133
   URANIUM-234     ENDF/B-IV MAT 1043             UPDATED 10/13/89                ID    92234
   URANIUM-235     ENDF/B-IV MAT 1261             UPDATED 10/13/89                ID    92235
   URANIUM-235     ENDF/B-IV MAT 1163             UPDATED 10/13/89                ID    92236
   URANIUM-238     ENDF/B-IV MAT 1262             UPDATED 10/13/89                ID    92238
   NEPTUNIUM-237   ENDF/B-IV MAT 1263             UPDATED 10/13/89                ID    93237
   PLUTONIUM-238   ENDF/B-IV MAT 1050             UPDATED 10/13/89                ID    94238
   PLUTONIUM-239   ENDF/B-IV MAT 1264             UPDATED 10/13/89                ID    94239
   PLUTONIUM-240   ENDF/B-IV MAT 1265             UPDATED 10/13/89                ID    94240
   PLUTONIUM-241   ENDF/B-IV MAT 1266             UPDATED 10/13/89                ID    94241
   PLUTONIUM-242   ENDF/B-IV MAT 1161             UPDATED 10/13/89                ID    94242
  AM-241 1056 SIGP=5+4 NEWXLACS 218NGP P-3 293K                                    ID    95241
  AM-243 1057 218 GP WT F-1/E-M 090376 P3 293K                                     ID    95243
   CURIUM-244      ENDF/B-IV MAT 1162             UPDATED 10/13/89                ID    96244

    TAPE COPY USED      0 I/O'S, AND TOOK    2.00 SECONDS
```

Figure S2.6.17 NITAWL-II merged library contents edit

```
                    SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK
GENERAL PROBLEM DESCRIPTION DATA BLOCK

                              GENERAL PROBLEM DATA

IGE   1/2/3 = PLANE/CYLINDER/SPHERE          2      ISN  QUADRATURE ORDER                    8
IZM   NUMBER OF ZONES                        9      ISCT ORDER OF SCATTERING               3
IM    NUMBER OF SPACIAL INTERVALS           50      IEVT 0/1/2/3/4/5/6=Q/K/ALPHA/C/Z/R/H   0
IBL   0/1/2/3 = VACUUM/REFL/PER/WHITE        1      IIM  INNER ITERATION MAXIMUM        20
IBR   RIGHT BOUNDARY CONDITION               0      ICM  OUTER ITERATION MAXIMUM        12
MXX   NUMBER OF MIXTURES                     9      ICLC -1/0/N--FLAT RES/SN/OPT          0
MS    MIXING TABLE LENGTH                   60      ITH  0/1 = FORWARD/ADJOINT            0
IGM   NUMBER OF ENERGY GROUPS               45      IFLU NOT USED(ALWAYS WGID)            4
NNG   NUMBER OF NEUTRON GROUPS              27      IPRT -2/-1/0/N=MIXTURE XSEC PRINT    -2
NGG   NUMBER OF GAMMA GROUPS                18      ID1  0/1/2/3=NO/PRT ND/PCH N/BOTH   53
IFTG  NUMBER OF FIRST THERMAL GROUP          15      IPBT -1/0/1=NONE/FINE/ALL BAL. PRT    0

                                SPECIAL OPTIONS

IFG   0/1 = NONE/WEIGHTING CALCULATION       0      IPN  0/1/2 DIFF. COEF. PARAM          0
IQM   VOLUMETRIC SOURCES (0/N=NO/YES)        2      IDFM 0/1 = NONE/DENSITY FACTORS 38*   0
IPM   BOUNDARY SOURCES (0/N=NO/YES)          0      IAZ  0/N = NONE/N ACTIVITIES BY ZONE  2
IFN   0/1/2 = INPUT 33*/34*/USE LAST        53      IAI  0/1=NONE/ACTIVITIES BY INTERVAL  1
ITMX  MAXIMUM TIME (MINUTES)                14      IFCT 0/1=NO/YES UPSCATTER SCALING     0
IDT1  0/1/2/3=NO/XSECT/SRCE/FLUX--OUT        0      IPVT 0/1/2=NO/K/ALPHA PARAMETRIC SRCH 0
ISX   BROAD GROUP FLUXES                     0      ISEN OUTER ITERATION ACCELERATION     0
IBLN  ACTIVITY DATA UNIT                     0      NBND BAND REBALN PARAMETER           -1
JBKL  0/1/2 BUCKLING GEOMETRY                0

                            FLOATING POINT PARAMETERS

EPS   OVERALL CONVERGENCE        1.00000E-03      DY   CYL/PLA HT FOR BUCKLING   0.00000E+00
PTC   POINT CONVERGENCE          1.00000E-03      DZ   PLANE DEPTH FOR BUCKLING  0.00000E+00
XNF   NORMALIZATION FACTOR       0.00000E+00      VSC  VOID STREAMING CORRECTION 0.00000E+00
EV    EIGENVALUE GUESS           0.00000E+00      PV   IPVT=1/2--K/ALPHA         1.00000E+00
EVM   EIGENVALUE MODIFIER        0.00000E+00      EQL  EV CHANGE EPS FOR SEARCH  1.00000E-03
BF    BUCKLING FACTOR=1.420892   1.42089E+00      XNPM NEW PARAM MOD FOR SEARCH  7.50000E-01
     THIS CASE WILL REQUIRE       3640 LOCATIONS FOR MIXING
     THIS CASE HAS BEEN ALLOCATED 200000 LOCATIONS
```

Figure S2.6.18 XSDRNPM problem definition page of shipping cask case

SAS2 SAMPLE CASE 1: 33 MWD/KGU, 17*17 PIN, PWR, 1 CYC, DRY-FUEL CASK

13Q ARRAY HAS 60 ENTRIES.

14Q ARRAY HAS 60 ENTRIES.

15Q ARRAY HAS 60 ENTRIES.

DATA BLOCK 2 (MIXING TABLE, ETC.)

	NUCLIDES ON TAPE	CCCC IDENTIFICATION	MIXTURE	MIXING TABLE COMPONENT	ATOM DENSITY
1	61		1	92234	1.10503E-06
2	62		2	92234	1.10427E-06
3	63		1	92235	5.12253E-05
4	6012		2	92235	5.11902E-05
5	7014		6	28	1.31783E-04
6	81		1	92236	2.58307E-05
7	82		2	92236	2.58130E-05
8	36		1	92238	5.89429E-03
9	24304		2	92238	5.89025E-03
10	65		6	33	4.80619E-02
11	66		1	8016	1.25029E-02
12	67		2	8016	1.24944E-02
13	25055		9	36	3.15067E-02
14	69		1	40302	3.52295E-03
15	70		2	40302	3.52054E-03
16	71		1	54135	2.83519E-19
17	26304		2	54135	2.83325E-19
18	73		1	55133	1.29784E-05
19	74		2	55133	1.29695E-05
20	75		1	93237	3.01271E-06
21	28304		2	93237	3.01064E-06
22	77		1	94238	9.51973E-07
23	78		2	94238	9.51320E-07
24	79		1	94239	3.34067E-05
25	28		2	94239	3.33838E-05
26	33		1	94240	1.11634E-05
27	500000		2	94240	1.11557E-05
28	8016		1	94241	7.59665E-06
29	40302		2	94241	7.59144E-06
30	54135		1	94242	3.13334E-06
31	55133		2	94242	3.13120E-06
32	92234		1	95241	2.23368E-06
33	92235		2	95241	2.23215E-06
34	92236		1	95243	6.29197E-07
35	92238		2	95243	6.28766E-07
36	93237		1	96244	1.22156E-07
37	94238		2	96244	1.22073E-07
38	94239		9	61	6.30133E-02
39	94240		3	62	1.67345E-03
40	94241		3	63	6.79370E-03
41	94242		1	24304	3.72536E-04
42	95241		2	65	3.72536E-04
43	95243		3	66	3.78409E-04
44	96244		5	67	1.74286E-02
45			1	25055	3.71141E-05
46			2	69	3.71141E-05
47			3	70	3.76992E-05
48			5	71	1.73633E-03
49			1	26304	1.26877E-03
50			2	73	1.26877E-03
51			3	74	1.28878E-03
52			5	75	5.93579E-02
53			1	28304	1.65031E-04
54			2	77	1.65031E-04
55			3	78	1.67633E-04
56			5	79	7.72073E-03
57			1	7014	2.90138E-05
58			2	81	2.90138E-05
59			4	82	4.30051E-22
60			3	6012	2.11679E-03

ELAPSED TIME 0.06 MIN.

Figure S2.6.19 Mixing table of shipping cask case

DETECTOR 3 (R= 2.73220E+02, Z= 1.82880E+02)

MT= 9029 ANSI STANDARD NEUTRON FLUX-TO-DOSE-RATE FACTORS (REM/HR)/(NEUT/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE	
1	3.48448E-01	1.49160E-04	5.19746E-05	
2	1.32192E+00	1.44640E-04	1.91203E-04	
3	1.62559E+00	1.27010E-04	2.06466E-04	
4	8.71729E-01	1.28110E-04	1.11677E-04	
5	1.20979E+00	1.29770E-04	1.56994E-04	
6	2.79266E+00	1.02810E-04	2.87113E-04	
7	2.48317E+00	5.11830E-05	1.27096E-04	
8	1.65637E+00	1.23190E-05	2.04048E-05	
9	1.16133E+00	3.83650E-06	4.45544E-06	
10	1.17959E+00	3.72470E-06	4.39363E-06	
11	1.24667E+00	4.01500E-06	5.00539E-06	
12	9.89035E-01	4.29260E-06	4.24553E-06	
13	9.80778E-01	4.47440E-06	4.38839E-06	
14	1.14775E+00	4.56760E-06	5.24246E-06	
15	5.74692E-01	4.55810E-06	2.61950E-06	
16	3.46089E-01	4.51850E-06	1.56380E-06	
17	1.61769E-01	4.48790E-06	7.26001E-07	
18	1.43230E-01	4.46650E-06	6.39736E-07	
19	2.68011E-01	4.43450E-06	1.18850E-06	
20	8.95137E-01	4.32710E-06	3.87335E-06	
21	2.84516E-01	4.19750E-06	1.19425E-06	
22	7.71004E-01	4.09760E-06	3.15926E-06	
23	6.94834E+00	3.83900E-06	2.66747E-05	
24	1.40935E+01	3.67480E-06	5.17908E-05	
25	9.24969E+00	3.67480E-06	3.39908E-05	
26	7.58962E+00	3.67480E-06	2.78903E-05	
27	1.21468E+00	3.67480E-06	4.46369E-06	
			1.34043E-03	(TOTAL)

Figure S2.6.20 XSDOSE neutron dose rates at 2 m

DETECTOR 3 (R= 2.73220E+02, Z= 1.82880E+02)

MT= 9504 ANSI STANDARD GAMMA-RAY FLUX-TO-DOSE-RATE FACTORS (REM/HR)/(PHOTONS/CM**2/SEC)

GRP	SCALAR FLUX	DOSE FACTOR	CALCULATED DOSE	
28	6.30648E+00	8.77160E-06	5.53179E-05	
29	1.37594E+01	7.47850E-06	1.02899E-04	
30	6.78255E+00	6.37480E-06	4.32374E-05	
31	4.27727E+00	5.41360E-06	2.31554E-05	
32	5.97535E+00	4.62210E-06	2.76187E-05	
33	6.70765E+00	3.95960E-06	2.65596E-05	
34	1.46592E+02	3.46860E-06	5.08467E-04	
35	6.87653E+01	3.01920E-06	2.07616E-04	
36	2.63696E+02	2.62760E-06	6.92887E-04	
37	3.12846E+02	2.20510E-06	6.89856E-04	
38	1.90931E+02	1.83260E-06	3.49900E-04	
39	1.91132E+02	1.52280E-06	2.91056E-04	
40	2.08456E+02	1.17250E-06	2.44415E-04	
41	1.12042E+02	8.75940E-07	9.81419E-05	
42	1.33512E+02	6.30610E-07	8.41940E-05	
43	1.68484E+02	3.83380E-07	6.45933E-05	
44	6.17935E+00	2.66930E-07	1.64946E-06	
45	1.59007E-02	9.34720E-07	1.48627E-08	
			3.51158E-03	(TOTAL)

Figure S2.6.21 XSDOSE gamma dose rates at 2 m

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S2.A DESCRIPTION AND EXAMPLES OF INPUT LEVEL-3

During the development of the SCALE-4 version of SAS2, it was expedient to read the case data used by the neutronics codes in the additional pass (path B) with the NAMELIST method. Once the new SAS2H procedure was developed, the simplified free form of input and associated processing of the input was added. Only the simplified input described in Table S2.5.1 is used, if INPLEVEL is set to 0, 1, or 2. However, if the user wants to supply any different data to the neutronics codes than that automatically derived by SAS2H for INPLEVEL=2, the user can specify INPLEVEL=3 and supply input using the following procedure:

1. First, set up the SAS2H input exactly as it should be done for an INPLEVEL=2 case, except change the "=2" to "=3." The code sets up data for the three neutronics codes with the level-2 input, but then permits additional data to override it.

2. Using the input descriptions for BONAMI-S, NITAWL-II, and XSDRNPM-S given in Sects. F1, F2, and F3, respectively, decide which data arrays are to be altered. It may be helpful to look at the printout of the SAS2H case using level-2 and PARM=HALT00 to determine the default input before changing the data.

3. Change the format from that of FIDO (FIDAS) requirements, where integer arrays or floating- point arrays are denoted by i$$ or j**, respectively (e.g., 1$$ or 24**). Replace the dollar signs with an equal sign "=" and place the letter "I" on the left (e.g., I1= or I14=). Replace the asterisks with "=" and place an "X" on the left (e.g., X24= or X35=). The data entries following the equal sign may be separated by a comma or one or more spaces. Note that any data array automatically supplied by SAS2H that is satisfactory does not need to be repeated. If no data change is required for the code input, no input data array is needed for the code. The only exception to this rule is that the XSDRNPM title card is required. The SCALE free-form input rules (see Sect. M3) replace those of the FIDO input system. The complete length of the data array is not required.

4. The entire input data for each code must be enclosed between a keyword for the code and an END. The END may not start in column one. The code keywords are the first three letters of the code's name, or BON, NIT, and XSD. The XSDRNPM-S title record should immediately follow a separate data record with the XSD keyword. The XSDRNPM-S title card must remain (as in FIDO input) as a single card image. If no data are input for the code, only the code's 3-letter name and END are required. The complete set of data for the three codes must follow SAS2 input entries for Data Block 8 of Table S2.5.1. The level-3 input must be in the order of data for BONAMI-S, NITAWL-II, and XSDRNPM-S. The data required by Table S2.5.1 should continue with entries for Data Block 9.

5. The feature to change data between cycles, MXREPEATS=0, may also be used with input level-3. In these cases, the combination of both the data for Data Block 8 plus the data for the three codes for the cycle must be included for NCYCLES*NLIB/CYC number of times before continuing with POWER, etc.

Three examples of level-3 input are given in Figs. S2.A.1 through S2.A.3. The main difference between the first two examples and the same cases submitted by input level-2 is the mesh interval structure. The cases are examples only and are not intended as an improvement over the input level-2 data. The input of the first case (Fig. S2.A.1) is very short. The second case (Fig. S2.A.2) shows a much more extensive input and includes input for mixing table data, mesh intervals, and other data.

The third example of level-3 input (Fig. S2.A.3) is a special case designed to determine an axially power-weighted moderator density to be input as the water density in the fuel-pin cell of a BWR assembly case. The example may be used for the slab-geometry case producing (after fission weighting slab moderator

densities) the final water density (DEN=0.5039) applied in sample case 4 (Sect. S2.6.7). The first estimate of the moderator density (VF=0.4323) in the case is the simple volume-weighted density. Other details of the input may be observed from the case data below. Because power-volume weighting of the slab zone water densities is the objective of the case, the "power-volume" product may be replaced conveniently by the "integrated fission source" (listed on line for "group" 28) produced in the zone balance tables of XSDRNPM-S printout. The advantage of using SAS2 in the case, over the use of functional modules throughout the analysis, is the use of the more simplified unit-pin-cell input.

Limits on Using Input Level-3

A few limitations are not given in the above five-step procedure on using input level-3. The size parameters input, or those derived from input level-2, must correspond to sizes of associated arrays. Also, there are maximum size limits to data arrays. Limits are 20 zones, 200 intervals, 100 resonance nuclides, 1000 total nuclides (or mixing table size), 249 energy groups, 600 activity processes, and 80 values corresponding to an angular quadrature of 16. These and other array sizes are used in: label commons /XSD/ and /NIT/; the subroutines S2HBON, S2HNIT, S2HXSD, and MTAB2H; and the BLOCK DATA initialization statements for /XSD/. Thus, a few simple "patches" in the code would be required as a method of increasing these limits, if the need should ever be required.

There are certain data, not expected to be wanted in input level-3 cases, that may not be input. The -1$ data, for core allocation, may not be used. All other data arrays may be used in the BONAMI-S input. All data arrays, except the -1$ data and 6$ data, may be used in the NITAWL-II input. The only data arrays that may be used in the XSDRNPM-S input are those denoted by: 0$, 1$, 2$, 3$, 4$, 5*, 13$, 14$, 15*, 35*, 36$, 38*, 39$, 40$, 41*, 42*, 43*, 46$, 47*, 48*, 49$, 50$, 51$, and 52$. The SCALE free-form input system (in Sect. M3) is used in place of the FIDO input system. FIDO-type features (e.g., skipping entries or interpolations) may not be used because they are presently not incorporated into the SCALE free-form input system. Note that without the entry-skipping option, the default values do not apply for parameters in the array being input.

```
=SAS2      PARM='HALT03,SKIPSHIPDATA'
SAS2H, (FOR APPENDIX CASE 1) 33 GWD/MTU PWR, 3.1% U235
27GROUPNDF4    LATTICECELL
UO2  1 0.945 811  92235 3.1  92238 96.8725  92234 0.0275   END
ZIRCALLOY  2 1  620   END
BORON   3  1.58587-4  570  END
H2O  3 0.7295  570 END
CO-59  3 0 1-20 570 END
END COMP
SQUAREPITCH  1.25984 0.81915 1 3 0.94996 2 0.83566 0  END
MORE DATA  SZF=0.7  END
NPIN/ASSM=264 FUELNGTH=787.2856   NCYCLES=3 NLIB/CYC=1
PRINTLEVEL=4
LIGHTEL=16  INPLEVEL=3  NUMZONES=4  END
3  0.57150  2 0.61214  3 0.71079  500 2.46
 BON     IO= 12, 17, 18, 1      END
 NIT    IO= 1, 3, 0, 4  END
XSD
SAS2H - (17X17) PWR TYP. IRR. HIST., 3.1% ENRICH - 33 GWD/MTU, CYC 1
 I1= 2, 4, 29
 X35= 0.0,0.1,0.2,0.3,0.4,   0.5,0.5715,0.59,0.61214,0.64,
0.68,0.71,0.8,0.9, 1.0,     1.1, 1.2, 1.3, 1.4, 1.5,
 1.6, 1.7, 1.8, 1.9, 2.0,   2.1, 2.2, 2.3, 2.4, 2.5
 I36= 1 1 1 1 1 1  2 2  3 3 3 4 4 4 4 4 4
 4 4 4 4 4 4 4 4 4 4 4 4
   END
POWER=37.36  BURN=293.3333  DOWN=1-20       END
POWER=37.36  BURN=293.3333  DOWN=1-20       END
POWER=37.36  BURN=293.3333  DOWN=1826.25    END
C  0.13   N  0.07   O  134   AL  0.10
SI  0.14   P  0.31   TI  0.11   CR  5.0
MN  0.24   FE  9.9   CO  0.072   NI  9.5
ZR  217   NB  0.71   MO  0.39   SN  3.6
END
```

Figure S2.A.1 Example 1 of level-3 input

```
=SAS2      PARM='HALT03,SKIPSHIPDATA'
SAS2H, (FOR APPENDIX CASE 2) 33 GWD/MTU PWR, 3.1% U235
27BURNUPLIB    LATTICECELL
UO2  1 0.945 811  92235 3.1  92238 96.8725  92234 0.0275   END
U-233  1 0 1-20 811  END
KR-85  1 0 1-20 811  END
SR-90  1 0 1-20 811  END
Y-89   1 0 1-20 811  END
ZR-94  1 0 1-20 811  END
ZR-95  1 0 1-20 811  END
NB-94  1 0 1-20 811  END
TC-99  1 0 1-20 811  END
EU-155 1 0 1-20 811  END
RU-106 1 0 1-20 811  END
RH-103 1 0 1-20 811  END
RH-105 1 0 1-20 811  END
XE-131 1 0 1-20 811  END
XE-132 1 0 1-20 811  END
XE-135 1 0 1-20 811  END
XE-136 1 0 1-20 811  END
CS-134 1 0 1-20 811  END
CS-137 1 0 1-20 811  END
BA-136 1 0 1-20 811  END
LA-139 1 0 1-20 811  END
CE-144 1 0 1-20 811  END
PR-143 1 0 1-20 811  END
ND-143 1 0 1-20 811  END
ND-145 1 0 1-20 811  END
ND-147 1 0 1-20 811  END
PM-147 1 0 1-20 811  END
SM-149 1 0 1-20 811  END
SM-151 1 0 1-20 811  END
SM-152 1 0 1-20 811  END
EU-153 1 0 1-20 811  END
EU-154 1 0 1-20 811  END
ZIRCALLOY  2 1  620   END
BORON   3  1.58587-4  570  END
H2O  3 0.7295  570 END
CO-59  3 0 1-20 570 END
END COMP
SQUAREPITCH  1.25984 0.81915 1 3 0.94996 2 0.83566 0  END
MORE DATA  SZF=0.7  END
NPIN/ASSM=264 FUELNGTH=787.2856   NCYCLES=3 NLIB/CYC=1
PRINTLEVEL=4
LIGHTEL=16  INPLEVEL=3  NUMZONES=4  END
3  0.57150  2 0.61214  3 0.71079  500 2.46
 BON    I1= 2, 3, 6, 0, 0, 9  X2=1.0E-3, 1.35  I3= 1 1 1 1 1  2
 I4 = 92235, 1001, 8016, 5010, 5011, 40302
 X5 = 8.0E-4, 4.870-2, 2.435-2, 4.426-6, 1.797-5, 4.252E-2
 I6= 1, 2, 1  X7=0.65024, 0.69342, 0.806802   X8=591 591 591 X9=0 0 0
 I10= 200, 201, 202, 203, 204, 205  I11= 0, 1, 0   END
 NIT   I0= 1, 3, 0, 4  I1= 0, 5, 53, 0 0 0 0 0 0 0 0 0
 I2= 201, 202, 203, 204, 205,
  92235, 92238, 92234, 92236,  8016,     5,
  40302,  1001,  5010,
   5011, 27059, 54135, 55133,
  93237, 94238, 94239, 94240, 94241,
  94242, 95241, 95243, 96244,   999,
 92233,36085,38090,39089,40094, 40095,41094,43099,63155,44106,
 45103,45105,54131,54132,54136, 55134,55137,56136,57139,58144,
 59143,60143,60145,60147,61147, 62149,62151,62152,63153,63154
    END
```

Figure S2.A.2 Example 2 of level-3 input

```
XSD
SAS2H - (17X17) PWR TYP. IRR. HIST., 3.1% ENRICH - 33 GWD/MTU, CYC 1
 I1= 2, 4, 29, 1, 3,  3, 58, 8, 3, 1,  20, 25, 0, 0, 0
 X5= 1.0E-4, 1.0E-4, 1.0, 0.0, 0.0,  1.420892, 365.76, 219.3, 0 1
 1.0E-3, 0.75
 I13= 1 1 1 1 2 3 3 3
 3 3 3 3 3  3 3 3 3 3
 3 3 3 3 3  3 3 3 3 3
 3 3 3 3 3  3 3 3 3 3
 3 3 3 3 3  3 3 3 3 3
 3 3 3 3 3  3 3 3 3 3
 I14= 201, 202, 203, 204, 205,
  92235, 92238, 92234, 92236,  8016,     5,
  40302,  1001,  5010,
   5011, 27059, 54135, 55133,
  93237, 94238, 94239, 94240, 94241,
  94242, 95241, 95243, 96244,   999,
 92233,36085,38090,39089,40094, 40095,41094,43099,63155,44106,
 45103,45105,54131,54132,54136, 55134,55137,56136,57139,58144,
 59143,60143,60145,60147,61147, 62149,62151,62152,63153,63154
 X15= 4.870-2, 2.435-2, 4.426-6, 1.797-5, 4.252E-2,
  2.408-4, 7.429-3, 2.145-6, 1.00-22, 1.534-2, 1.348-2,
  4.294-3, 2.695-2, 2.450-6, 9.946-6, 1-22 1-22 1-22
 1-22 1-22 1-22 1-22 1-22
 1-22 1-22 1-22 1-22 1-22
 X35= 0.0,0.1,0.2,0.3,0.4,   0.5,0.5715,0.59,0.61214,0.64,
0.68,0.71,0.8,0.9, 1.0,     1.1, 1.2, 1.3, 1.4, 1.5,
 1.6, 1.7, 1.8, 1.9, 2.0,   2.1, 2.2, 2.3, 2.4, 2.5
 I36= 1 1 1 1 1 1  2 2  3 3 3 4 4 4 4 4 4
 4 4 4 4 4 4 4 4 4 4 4 4 4
 I39= 1, 2, 1, 3          END
POWER=37.36  BURN=293.3333  DOWN=1-20       END
POWER=37.36  BURN=293.3333  DOWN=1-20       END
POWER=37.36  BURN=293.3333  DOWN=1826.25    END
C  0.13   N  0.07   O  134   AL  0.10
SI  0.14   P  0.31   TI  0.11   CR  5.0
MN  0.24   FE  9.9   CO  0.072   NI  9.5
ZR  217   NB  0.71   MO  0.39   SN  3.6
END
//
```

Figure S2.A.2. (continued)

```
=SAS2     PARM='HALTOO,SKIPSHIPDATA'
APPENDIX CASE 3, SAS2, SLAB FOR AXIAL FISSION-WEIGHTED H2O DENSITY   USED
27BURNUPLIB   LATTICECELL
UO2  1 0.940  840 92235 2.64 92238 97.3366  92234 0.0234   END
ZIRCALLOY  2 1  620   END
BORON   3  1.0000-22  558  END
H2O  3 0.4323  558 END
CO-59  3 0 1-20 558 END
SS304  5 1   END
END COMP
SQUAREPITCH   1.6256 1.05664 1 3 1.25222 2 1.0795 0  END
MORE DATA  SZF=0.7  END
NPIN/ASSM=59  FUELNGTH=2128.424   NCYCLES=3 NLIB/CYC=1
PRINTLEVEL=4
LIGHTEL=3  INPLEVEL=3 NUMZONES=4  END
3  0.5   2  0.6   3  0.7   500  2.0
  BON    I1= 2, 4, 8, 0, 0, 0, X2=1.0E-3, 1.35, I3= 5*1, 2, 3, 3,
 I4= 92235, 92238, 26304, 28304, 8016, 40302, 8016, 1001,
 X5= 5.24-4, 2.20-2, 9.62-5, 8.59-5, 4.64-2,  4.25-2,
 .02,.05 I6= 3 2 3 1 X7=0.5 0.6 0.7 2 X8= 558.,620.,558.,840.
 X9= 4*0.0,
 I10=  201, 202, 203, 204, 205, 206, 207, 208, I11= 1, 2, 1, 0,  END
  NIT   I1= 0, 8, 2, 9*0,
 I2= 201, 202, 203, 204, 205, 206, 207, 208,
  92235, 92238,
     END
 XSD
SAS2H,  (8X8) BWR POW-WTED MOD-DEN, 2.64% ENRICH, 27.5GWD/MTU,  CYC 1
       I1=  1, 12, 120, 0, 0,  12, 43, 8, 3, 1,  20, 55, 0, 0, 0,
    I4= 1, 3, 0, -1, 3,   4, 0, -1, 0,  I3= 1, 0, 0, 14, 12, 7*0,
 X5= 2*1.0E-4, 1.0, 0.0, 1.0,  1.420892, 416., 416.,    0.0, 1.0,
 1.0E-3, 0.75,
  I13= 1, 1, 3*2,
  4*3, 4*4, 4*5, 4*6, 4*7, 4*8, 4*9, 4*10, 4*11, 2*12,
  I14= 207, 208, 207, 208, 203,
  92235,92238,207,208, 92235,92238,207,208,
 92235,92238,207,208, 92235,92238,207,208,
 92235,92238,207,208, 92235,92238,207,208,
 92235,92238,207,208, 92235,92238,207,208,
  207, 208, 203, 206, 207, 208,
 X15=                        0.28748E-01, 0.57495E-01,
                             0.21561E-01, 0.43121E-01, 0.21026E-01,
 0.14594E-03, 0.53120E-02, 0.25956E-01, 0.30069E-01,
 0.14594E-03, 0.53120E-02, 0.24128E-01, 0.26414E-01,
 0.14594E-03, 0.53120E-02, 0.22773E-01, 0.23705E-01,
 0.14594E-03, 0.53120E-02, 0.21789E-01, 0.21736E-01,
 0.14594E-03, 0.53120E-02, 0.21061E-01, 0.20279E-01,
 0.14594E-03, 0.53120E-02, 0.20409E-01, 0.18976E-01,
 0.14594E-03, 0.53120E-02, 0.19834E-01, 0.17825E-01,
 0.14594E-03, 0.53120E-02, 0.19450E-01, 0.17059E-01,
         0.15794E-01, 0.31589E-01, 0.42052E-02, 0.29760E-02,
                             0.21059E-01, 0.42119E-01,
   X35=   0.0,   2.54,  5.08,  7.62, 10.16, 12.70, 15.24, 17.78,
  20.32,  22.86,  25.40,  28.45,  31.50,  34.54,  37.59,  40.64,
  43.69,  46.74,  49.78,  52.83,  55.88,  63.71,  71.54,  79.37,
  87.20,  95.03, 102.86, 110.70, 118.53, 126.36, 134.19, 137.32,
 140.46, 143.59, 146.73, 149.86, 152.99, 156.13, 159.26, 162.40,
 165.53, 168.66, 171.80, 174.93, 178.06, 181.19, 184.32, 187.45,
 190.59, 193.72, 196.85, 199.98, 203.11, 206.25, 209.38, 212.51,
 215.64, 218.77, 221.90, 225.04, 228.17, 231.30, 234.44, 237.57,
 240.71, 243.84, 246.97, 250.11, 253.24, 256.38, 259.51, 264.21,
 268.91, 273.61, 278.31, 283.01, 287.71, 292.40, 297.10, 301.80,
 306.50, 312.77, 319.03, 325.29, 331.56, 337.82, 344.08, 350.35,
 356.61, 362.87, 369.14, 375.40, 381.67, 387.94, 394.20, 400.47,
 406.74, 413.00, 419.27, 425.53, 431.80, 436.88, 441.96, 447.04,
 452.12, 457.20, 462.28, 467.36, 472.44, 477.52, 482.60, 485.14,
 487.68, 490.22, 492.76, 495.30, 497.84, 500.38, 502.92, 505.46,
 508.00,
 I36=  10*1, 10*2, 10*3, 10*4, 10*5, 10*6, 10*7, 10*8,
  10*9, 10*10, 10*11, 10*12,
  I39= 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, I51= 27*1,    END
POWER=26.13    BURN=353.9257  DOWN=1-20      END
POWER=26.13    BURN=353.9257  DOWN=1-20      END
POWER=26.13    BURN=353.9257  DOWN=1826.25   END
ZR  564   FE  43   NI  3.9
END
//
```

Figure S2.A.3 Example 3 of level-3 input

S2.B FORMAT OF FUEL ATOM DENSITIES AND RADIATION SOURCES

A formatted (BCD) data set is output on unit No. 72 to preserve significant atom densities and neutron and photon source spectra of the spent fuel. The data are stored at the time of starting the burnup of the loaded assembly, at the time of reactor shutdown of each cycle (as input to SAS2), and at the end of the spent fuel cooling time for shipment (as specified to SAS2).

In order to keep the same format throughout, the arrays for photon and neutron spectra and neutron source strengths are always included. However, they are valid only at the last time (after the cooling time). They are zero or meaningless values, which were not computed, at the other times. Each card-image record uses 80 columns, with the last card-image padded to the end with either zeros or blanks as indicated by the format.

Except for the first and last records (each a single card image), the remainder of the written records include the identical type of data (sometimes converted to different units) as written (in binary) on unit No. 71. Only zeros and blanks are added. The order is the same as that on unit No. 71, except that nuclide IDs and atom densities are in pairs instead of two separate arrays. The value of making the unit No. 72 data set is that the card-image output can be transported to other computers and applications should be easier than using the machine-specific binary input written on unit No. 71.

The isotopic quantity values written on unit No. 72 for the final decay case are converted from the g-atoms/assembly read from unit No. 71 to atoms/b-cm, consistent with the dimensions or units used at the earlier times. Other data of the decay case remain in units per assembly. Densities of light-element nuclides that are outside the fuel zone and depleted during the burnup analyses passes are converted from adjusted densities (scaled for fuel volume equivalence) to their actual density used by the neutronics codes. This conversion provides the adjustment in the light-element densities required by ORIGEN-S to compute the total removable fission energy plus (n,γ) reaction energy per fission.

The format of the data set for each time step written is presented below. Each write statement is given separately as a different write number and its format. Each variable is listed by a position number, the variable name, and a comment or definition. If the variable is an array, the variable giving its size is shown in parentheses. Where scalar variables are not used as a size, the comment usually refers to the data array in ORIGEN-S input that fully defines it.

In all cases, for either neutron or photon spectra, the value in the first position in the spectrum array pertains to the group bounded by the first two values in the corresponding group structure arrays, etc. Thus, note carefully the order for ENER and ENEUTS in using spectral data.

Write No. 1; FORMAT(2I10,6(1X,1P,E9.3)).

1. LPASS: library pass No. used for ORIGEN-S case

2. MTIME: position No. of data from unit No. 71

3. TW: time from start of assembly burnup, d

4. BURMTU: accumulated burnup at TW, kWd/kg heavy metal (current weight)

5. BURASM: accumulated burnup at TW, MWd/assembly

6. PWMTU: specific power of cycle, kW/kg heavy metal (current heavy metal)

7. PWASM: specific power of cycle, MW/assembly

8. WTMTU: current metric ton heavy metal, t heavy metal/assembly

Write No. 2; FORMAT(8I10/8I10/8I10/6I10,2(1X,1P,E9.3)/1P,E10.3,6X,A4,6(1X,1P,E9.3)).

1. ITOT: total No. of nuclides in complete library

2. IL: No. of light-element-library nuclides

3. IA: No. of actinide-library nuclides

4. IF: No. of fission-product-library nuclides

5. NRFLAG: =0, for SCALE-3 and later SAS2 versions

6. MSUB: time step No. of ORIGEN-S case

7. NSTEPO: step position No. in subcase on unit No. 71

8. KASEPO: case position No. on unit No. 71

9. JOBPOS: =1, the job position No. on unit No. 71

10. NOCS: =1, subcase number

11. NOBLND: see 1$ data (in ORIGEN-S input; and, also, below)

12. NDSET: see 3$ data

13. NTYPE: see 3$ data

14. NGRP: number of neutron spectrum energy groups (see SPNEUT)

15. NELEM: see 3$ data

16. NVERT: see 3$ data

17. NG: No. of total gamma spectrum energy groups (see DSAV and ESAV)

18. MMN: see 56$ data

19. MOUT: see 56$ data

20. INDEX: see 56$ data

21. MSTAR: see 56$ data

22. NUNIT: = 4, meaning TW time of data is given in d

23. KBLEND: see 56$ data

24. NENLE: No. of groups in light-element spectrum (see SPECLE)

25. NENAC: No. of groups in actinide spectrum

26. NENFP: No. of groups in fission-product spectrum

27. L1: maximum of NENLE and 1, or MAX(NENLE,1)

28. L2: MAX(NENAC,1)

29. L3: MAX(NENFP,1)

30. L4: MAX(IA,1)

31. TMO: time at start of cycle, d

32. FRACPW: see 57* data

33. TCONST: see 57* data

34. TUNIT: see NUNIT = 6 in 56$ data

35. TWRITE: = TW, time from start of assembly burnup, d

36. PW: assembly specific power in time step, MW/b-cm

37. FW: reactor thermal flux in time step, n/s-cm^2

38. ZER: zero written three times

Write No. 3; FORMAT(4(I8,2X,1P,E10.4))

1. NUCL(1): ORIGEN-S nuclide ID as ZAS (note, S = 0 or 1 for ground or excited state) for first nuclide

2. D(1): density of NUCL(1), atoms/b-cm

3. NUCL(2): same as NUCL(1) for second nuclide

4. D(2): same as D(1) for second nuclide

5. etc. for all library nuclides through D(ITOT), see ITOT in Write No. 2

Write No. 4; FORMAT(20A4)

1. TITLE(20): ORIGEN-S case title, same as SAS2 title

Write No. 5; FORMAT(20A4)

1. BASIS(10): ORIGEN-S case BASIS input; see case printouts

2. BASIS(11 to 20): blank characters

Write No. 6; FORMAT(1P,8E10.4)

1. EGROUP(NENLE+1): see 37* data

2. EACTGP(NENAC+1): see 36* data

3. EFPGRP(NENFP+1): see 39* data

4. SPECLE(L1): break down into light-element spectrum

5. SPECAC(L2): break down into actinide spectrum

6. SPECFP(L3): break down into fission-product spectrum

7. ENER(NG+1): total gamma spectrum group structure in ascending order, MeV

8. DSAV(NG): total SAS2 gamma spectrum, photons/s-assembly

9. ESAV(NG): total gamma energy spectrum, MeV/s-assembly

Write No. 7; FORMAT(20A4)

1. TISAV: ORIGEN-S title of total SAS2 gamma spectrum

Write No. 8; FORMAT(1P,8E10.4)

1. SPNNUC(L4): nuclide neutron spontaneous fission source, n/s-assembly

2. ALPNUC(L4): nuclide (α,n) source, n/s-assembly

3. SPNEUT(NGRP): total neutron spectrum, n/s-assembly

4. SPECAN(NGRP): (α,n) neutron spectrum, n/s-assembly

5. SPECSP(NGRP): spontaneous fission neutron spectrum, n/s-assembly

6. ENEUTS(NGRP+1): neutron spectrum group structure in descending order, eV

Write No. 9 with no list;

FORMAT(' ------- END OF STEP DATA ------- ',50X)
(Note: These dashes provide an easy way to search to end of the step data.)

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Computing Applications Division

SAS3: AN AUTOMATED MONTE CARLO SHIELDING ANALYSIS MODULE

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ABSTRACT

SAS3 is the SCALE Shielding Analytical Sequence for three-dimensional geometry problems. The system incorporates the input and cross-section processing capabilities found in CSAS with the radiation transport capabilities of the MORSE-SGC Monte Carlo code. Three-dimensional geometry features of the combinatorial MARS (Multiple Array System) package can be used within the MORSE model specification. The SAS3 control module executes in sequence BONAMI, NITAWL-II, XSDRNPM (optionally), ICE, and the MORSE-SGC codes.

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ACKNOWLEDGMENTS

The SAS3 sequence is the result of the efforts of many individuals on the SCALE development team. The standard composition input processor reflects the contributions of R. M. Westfall, J. R. Knight, J. A. Bucholz, L. M. Petrie, and N. F. Landers. The interest and motivation of R. M. Westfall at ORNL and R. H. Odegaarden, formerly of the U.S. Nuclear Regulatory Commission, significantly accelerated the development of the SAS3 system. The SCALE subroutine library developed by L. M. Petrie made many of the SAS3 features possible, such as dynamic memory allocation, free-form input, and random-access disk utilization. J. R. Knight, J. A. Bucholz and N. F. Landers are responsible for much of the development of the criticality sequences from which much of the SAS3 programming was taken. Their help is especially appreciated.

S3.1 INTRODUCTION

The SAS3 control module executes Shielding Analysis Sequence No. 3 for automating cross-section processing and performing shielding analysis. The programs executed in the SAS3 sequence are BONAMI, NITAWL-II, XSDRNPM (optionally), ICE, and MORSE-SGC. The BONAMI program is used to correct cross sections with Bondarenko self-shielding factors. NITAWL is used to perform resonance self-shielding. XSDRNPM may be optionally used to generate cell-weighted cross sections for use by MORSE. MORSE-SGC is the SCALE version of the MORSE family of Monte Carlo programs. It contains the MARS geometry system (see Sect. M9) with combinatorial geometry. This geometry system allows ease in modeling multiple-array systems by using a repeating array feature along with an unlimited array-nesting capability. MORSE-SGC incorporates supergroup cross-section storage and tracking. This feature is advantageous in running problems requiring extensive cross-section storage due to many media, high-order Legendre expansion of the scattering cross section, or a fine energy group mesh. Execution is controlled by a simple input processor, which reads the standard composition input (see Sect. C4) and the additional input required to run MORSE. The MARS geometry system in MORSE-SGC is very versatile in modeling complicated lattice geometry. Execution of MORSE-SGC in SAS3 requires the following input:

1. combinatorial MARS geometry input,
2. fixed source terms for each energy group,
3. energy importance weights for each group if running a coupled neutron gamma problem,
4. splitting and Russian roulette parameters by importance region and energy group,
5. MORSE-SGC control parameters for problem input, and
6. CSAS standard composition input and geometry options for calculating the Dancoff factor.

S3.1.1 MORSE-SGC PROBLEM SETUP IN SAS3

This version of SAS3 assumes all shielding calculations are fixed-source problems. Criticality problems may be run for models containing fissile material, but it is not possible to run a criticality calculation simultaneously with a shielding calculation. SAS3 runs MORSE-SGC in a "fully coupled" mode for neutron-gamma problems. This mode treats the gamma production as an energy transfer, as opposed to a true secondary particle. This method makes the neutron nonabsorption probability greater than 1. To enhance neutron transport and encourage gamma production, energy biasing is invoked to bias selection of the scattered particle energy. The following biasing features are available in MORSE:

1. Russian roulette,
2. importance splitting,
3. pathlength stretching,
4. source angular biasing, and
5. energy biasing.

The following analysis systems are available in SAS3:

1. point detector response,
2. array collision edits by location and media, and
3. boundary crossing estimates that require a user-supplied subroutine.

The source description in SAS3 is composed of:

1. defining the source volume, XMIN, XMAX, YMIN, YMAX, ZMIN, ZMAX,
2. defining the source in each energy group, and
3. optionally defining the source media.

MORSE-SGC is configured to reduce the necessity of user-supplied subroutines. SAS3 with MORSE-SGC offers the user many input options to simplify his problem setup.

S3.1.2 SAS3 VERSUS SAS3X

SAS3 has the ability to optionally generate cell-weighted cross sections for use by MORSE. This option is initiated by executing the SAS3X sequence, instead of the SAS3 sequence. The cell-weighted cross sections are for an LWR or BWR fuel pin cell. The flux weighting of the cross sections is performed by XSDRNPM. Normally in a SAS3 execution, XSDRNPM is not executed. The cell-weighted cross sections generated by XSDRNPM are given the last media number in a run. For example, for a SAS3X run with seven mixtures, the cell-weighted cross sections would be available in MORSE-SGC as media No. 8. SAS3X and SAS3 may generate resonance-corrected fuel cross sections for only one fuel enrichment.

S3.2 BIASING TECHNIQUES IN SAS3

Monte Carlo calculations represent a statistical model of physical particle transport. As a statistical calculation, the results have a deviation associated with them which is a function of the number of estimates made. Each particle track has a weight associated with it from which estimates of different types can be made. If the distribution of the particle weights is small in a particular energy range located in a portion of the geometry model, then the estimate distribution for that energy range and region will have a small variance associated with it. To achieve a small variance from random samples requires a balance between the number of particles tracked in a given portion of the geometry and the weight distribution of the particles in each energy range. The user assigns a set of weights for biasing in each geometry zone. All the geometry zones using the same set of biasing weights compose an importance region. Each region's weight distribution and particle population in each energy group may be controlled by Russian roulette and splitting techniques. The biasing techniques discussed below are presented in more detail in Sect. F9.3 which also provides helpful guidelines for biasing shielding problems.

S3.2.1 RUSSIAN ROULETTE

Russian roulette is a way of terminating a particle's history when its weight is too small to contribute meaningfully to a particular estimate being made. Russian roulette, escape, and time are the only three ways a particle's history may be terminated. The user must enter both a Russian roulette cutoff weight and a survival weight for each energy group and importance region in the model.

The cutoff weight is the weight at which Russian roulette is initiated. When a particle's weight, WATE, is reduced below the cutoff weight, then Russian roulette is played to determine if the particle's history will be terminated. The particle's weight is compared with the product of a random number and the Russian roulette survival weight. If the particle's weight is greater than this product, then the particle survives the Russian roulette game and is given the survival weight. If the particle weight is less than this product, then the particle history is terminated. The frequency with which Russian roulette is played in a given energy group and importance region is determined by the Russian roulette cutoff weights, WTLOW. The frequency particles survive the Russian roulette game is WATE/WTAVE, where WTAVE is the survival weight. Playing Russian roulette in this way is an efficient way of reducing the number of particles being tracked in a given energy group of a particular geometry region.

S3.2.2 PARTICLE SPLITTING

Particle (or importance) splitting is another method used to control the size of a particle's weight. As a result of pathlength stretching, source angular biasing, or a high probability of multiple-particle generation at a collision site (i.e., n,2n and n,γ reactions for neutrons, or pair production for gammas) the particle weight may increase at a collision. To keep the distribution of particle weights from becoming too large in a geometry region, a particle may be split into two particles, each with half the original particle weight and, thereby, conserving the original particle weight. The disadvantage of this process is that, after splitting, MORSE must track two particles from the collision site instead of one. The advantage of splitting is keeping the particle weights uniformly distributed and increasing the number of collision estimates in a part of the geometry as a result of tracking split particles. Splitting gives a way to increase the particle population in parts of the geometry where collisions may be significant to the final result. For deep-penetration problems, splitting is a useful and necessary tool.

The user should be careful not to oversplit or the computational time for his problem may increase rapidly. Similarly the user should not set his Russian roulette cutoff weight, WTLOW, so low that much calculational time is spent tracking particles of low weight. No easy and clear prescription is available for determining the Russian roulette and splitting weights for a problem. The user should be aware that

overbiasing a problem may lead to erroneous results. Overbiasing may provide results with small standard deviations but incorrect answers. Monte Carlo biasing techniques are an art and as such require user awareness and thought.

S3.2.3 DIRECTION BIASING OPTIONS FOR PATHLENGTH STRETCHING

In many shielding problems, it is desirable to increase the number of collisions near a detector. One way to accomplish this is to stretch the pathlength of particles traveling in the direction of the point detector and shrink the pathlength of particles traveling away from the point detector. This is a means of encouraging particles to travel towards and have collisions near the detector. Whenever the pathlength of a particle is altered, the particle weight must be corrected for the bias applied to the particle pathlength.

In the older versions of MORSE, the user had to supply a subroutine called DIREC. It was to return the amount of pathlength alteration upon its call. DIREC computed the angle θ between the particle trajectory and the preferred direction of travel. It returned the cosine of this angle.

The current version of MORSE-SGC/S gives the user many options for biasing the pathlength of a particle without requiring a user-supplied subroutine. The current subroutine DIREC gives the user an input option to choose which method of pathlength stretching to apply. This often eliminates the need for the user supplying his own subroutine.

The extent of pathlength stretching is determined by the parameter "PATH." This information is entered as a function of both energy group and importance region. Each particle whose path has been altered by pathlength stretching must have its weight adjusted to compensate for the bias. The particle pathlength will be stretched by a factor "BIAS", where

BIAS = 1.0 / (1.0 - PATH(IG,NREG)*DIREC)

Figure S3.2.1 is a polar diagram of BIAS versus θ for various values of PATH. DIREC is taken to be the cosine of θ. For large values of PATH, large degrees of pathlength stretching will occur, and correspondingly large changes in a particle's weight will occur.

Pathlength stretching is often referred to as the "exponential transform method." It should be used very cautiously. Overbiasing with pathlength stretching can lead to erroneous results. Whenever pathlength stretching is invoked, it modifies the particle weight distribution and changes the effect of the Russian roulette and splitting parameters. This change occurs as a result of the weight correction applied to particles due to the pathlength stretching. Pathlength stretching should be applied only when absolutely necessary. The user should apply Russian roulette and splitting and then, as a "last resort" apply pathlength stretching. Splitting is preferred for deep-penetration problems instead of pathlength stretching to increase the number of collisions near a detector.

S3.2.4 ENERGY BIASING IN SAS3

Since MORSE runs in a "fully coupled" mode in SAS3, the neutron nonabsorption probability is greater than 1 when running neutron-gamma problems. The definition of a nonabsorption probability is the ratio of the scattered cross section to the total cross section. In the "fully coupled" case for MORSE, the scattering cross section includes neutron-to-gamma transfers; therefore, the total scattering cross section will be larger than the total cross section. This causes particles to increase in weight at collision sites, until they transfer into the gamma groups. Energy biasing is a technique to preferentially select a downscatter group. The particle weight is corrected for the bias applied to the selection. By encouraging the neutrons to scatter into the gamma groups, the calculation can be accelerated. Again, as in all kinds of biasing, be careful not to overbias. One of the most important means of reducing the number of particles tracked is with Russian roulette. Unfortunately, in a "fully coupled" mode it is not possible to easily kill particles with Russian

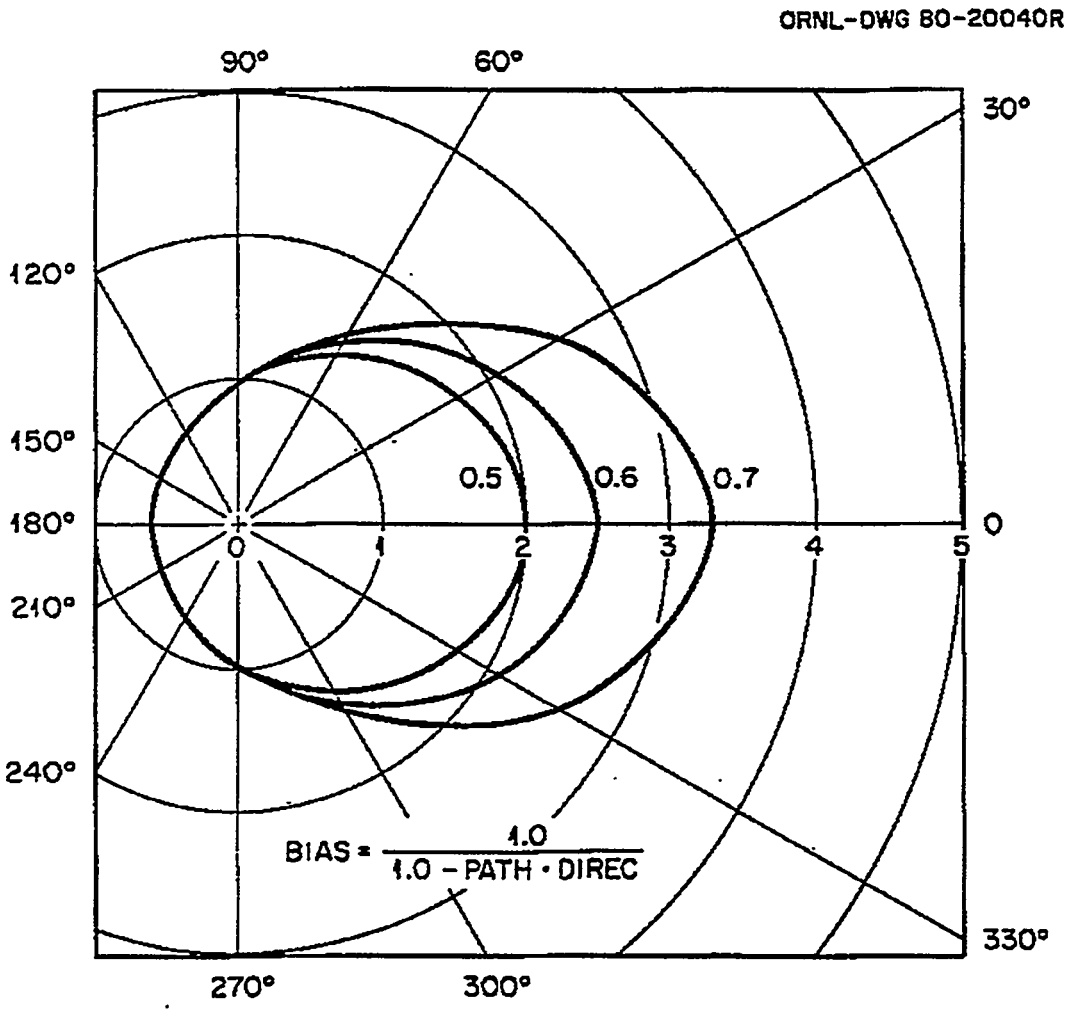

Figure S3.2.1 Polar diagram of BIAS versus θ

roulette. Extending the life of a particle may significantly increase computer time requirements. Therefore, biasing particles into the gamma groups is one way of attempting to make the calculation more efficient and cost effective.

S3.2.5 SOURCE ANGULAR BIASING

Source angular biasing is a method of affecting particle migration by attempting to have particles start their history in a preferred direction. This method affects only the particle's initial weight and initial direction. It is only applicable to problems with isotopic sources. The source angular biasing function applied in SAS3 is

$$P(\theta) = \alpha e^{-\alpha\theta}/(1 - e^{-\alpha\pi})$$

The larger the value of α, the more forward peaked is the angular distribution of P. Similarly, the larger the value of α, the larger the weight correction applied to a particle whose direction has been biased.

Appendix F9.B describes the exponential angular biasing scheme available in MORSE-SGC. The preferred direction is automatically set to the coordinates of the first point detector. This particular method for angular biasing was demonstrated to the author by Dave Collins of Radiation Research Associates in Fort Worth, Texas. *Source angular biasing should be used with care.* (See Sect. F9.3.3).

S3.3 SOURCE SAMPLING AND ANALYSIS TECHNIQUES

In running a Monte Carlo calculation, one must take many factors into consideration to describe a problem. The source sampling technique, the biasing games played, and the analysis methods applied are several important considerations in using any general Monte Carlo transport code. This section describes the source sampling technique available in MORSE-SGC and several of the analysis approaches operational in MORSE-SGC.

S3.3.1 VOLUMETRIC SOURCE SAMPLING IN SAS3

In SAS3 the user inputs a source volume space defined with bounds XMIN, XMAX, YMIN, YMAX, ZMIN, and ZMAX. The source subroutine in MORSE uniformly samples locations within this defined volume. If the SAS3 user specified a source media (MSM in SAS3 input), the code accepts only points found in the source media. If a source media is not given, then all points sampled in the defined source volume are assumed to be valid source points. For shielding calculations, this process occurs at the beginning of every batch. For criticality calculations, this process occurs only at the beginning of the first batch. Subsequent batch source particles are generated by fission collision sites from the previous batch.

The user is given the option of having the source particles started with a uniform isotropic angular distribution or having the initial source direction sampled from the biased distribution described in the previous section.

For shielding problems in SAS3, the user must give the particle source for each energy group. The source is summed over all energy groups, and a normalized distribution is computed. The user must enter a source multiplication constant. This constant is multiplied by the source sum. The product must be in units of particles/second. Each detector response is multiplied by this factor to compute absolute reaction rates properly normalized for the problem source description. Point-source problems may be run by setting XMAX equal to XMIN, YMAX equal to YMIN, and ZMAX equal to ZMIN. Planar source may be run in a similar manner. Hemispherical angular sampling is not available in the current source routine. Also nonuniform sampling distributions are not available in the current version of MORSE-SGC.

S3.3.2 POINT DETECTOR ESTIMATES

MORSE-SGC allows the user two methods of computing the reaction rate at a point detector. Either a single or multiple estimate may be made to each point detector from each collision site. These estimates are made by subroutine RELCOL or RELCOA. For some problems, making multiple estimates from each possible downscatter group at a collision site to the point detector will improve the standard deviation of a response. The user decides which method to use by setting IFLAG(9) in the MORSE input. Subroutine RELCOA makes multiple estimates from a collision site. It is called when IFLAG(9) is set to +1. Subroutine RELCOL makes a single estimate to each point detector from each collision site when IFLAG(9) is set to -1. When IFLAG(9) is set to zero, then no point detector estimates are made from collision sites.

On some problems it is possible to compute negative fluxes with the collided point detector estimators. When this occurs, the problem has yielded erroneous results. Negative estimates can result from negative angular scattering probabilities. When the point detector results are negative, the user should modify his problem and/or his biasing schemes.

When making point detector estimates, subroutine SDATA makes uncollided flux estimates from source locations. It is important for the user to remember that this version of MORSE-SGC is set up to compute the uncollided flux and collided flux responses separately and they are not added together. The total flux response printed out by MORSE is the total collided flux response. The actual total response is the sum of the collided flux response and the uncollided flux response.

S3.3.3 MARS ARRAY ANALYSIS

The MARS geometry system in MORSE-SGC provides the user with the ability to model very complicated lattice arrays with minimum effort. In Monte Carlo tracking, the user should be aware of where particles are tracked and the number of collisions occurring throughout the user's model. This information is necessary to properly determine if the calculational results are realistic or in error. MORSE-SGC contains a collided flux editor for the MARS system. This editor allows the user to obtain reaction rates throughout his array geometry as a function of array or universe (cell type) and as a function of media. The collided flux editor for MARS is described in detail in Sect. M9.4. The Collided Flux Edit system (CFE) provides the user with valuable information without adding additional computation time. The MARS user in MORSE-SGC should utilize the CFE feature where possible to obtain the maximum amount of information from his calculation.

S3.3.4 AUTOMATED RESPONSES IN SAS3

SAS3 is set up to automatically retrieve standard neutron and gamma ANSI standard dose responses from the SCALE master cross-section libraries. Table S3.3.1 lists the response ID Number and corresponding units for each of the responses available in the SCALE libraries. At present not all SCALE cross-section libraries contain these responses. The responses are present as a fake material ID 500000.

Table S3.3.1 SCALE standard response sets

Dose factor ID No.	Identification	Units
9001	Hurst	(mrad/h)/(neutrons/cm^2-s)
9002	Snyder-Neufeld	(mrad/h)/(neutrons/cm^2-s)
9026	Snyder-Neufeld Conversion from flux to biological dose	(mrem/h)/(neutrons/cm^2-s)
9027	Henderson conversion from flux to absorbed dose rate in tissue	(rad/h)/(neutrons/cm^2-s)
9028	Straker-Morrison	(mrem/h)/(neutrons/cm^2-s)
9029	ANSI standard neutron	(rem/h)/(neutrons/cm^2-s)
9501	Straker-Morrison	(mrad/h)/(photons/cm^2-s)
9502	Henderson	(rad/h)/(photons/cm^2-s)
9503	Claiborne-Trubey	(rad/h)/(photons/cm^2-s)
9504	ANSI standard Gamma-ray	(rem/h)/(photons/cm^2-s)

The ANSI standard neutron and gamma-ray dose conversion factors (IDs 9029 and 9504) are selected as the default SAS3 responses. See the Input Description for "NRE=". SAS3 will not allow the user to run without any responses in the problem. The user may optionally enter a set of responses, which will be added to the standard responses retrieved from SCALE libraries. These rules apply to both criticality and shielding problems. If the user utilizes the point detector estimator, then for each point detector he will receive results for all responses in his problem.

S3.4 SAS3 SUBROUTINE DESCRIPTION

Many of the subroutines in the SAS3 driver are from CSAS4 (see Sect. C4). The subroutines described in this section are subroutines added to CSAS4 to incorporate MORSE-SGC. SAS3 utilizes the SCALE Subroutine Library extensively. Both subroutines in CSAS4 and in the SCALE library are described in other sections of the SCALE documentation.

Figure S3.4.1 shows the SAS3 execution sequence as executed by SAS3 and SAS3X. The SAS3 input processor is called before any of the SCALE modules are executed. SAS3 and SAS3X are identical, with the exception that SAS3X executes XSDRNPM. The choice between SAS3 and SAS3X is made in the input data (=SAS3 or =SAS3X). The SAS3 input processor program flow is shown in Fig. S3.4.2. The individual subroutines shown in the figure are described below.

ACTIE is called from MANRY. ACTIE reads the SCALE master cross-section library and retrieves the ANSI standard neutron and gamma dose responses in the fake material set 500000. If no standard dose responses are found, a warning message is printed out. If the user receives the warning and enters no responses of his own, his job is aborted.

CPYJOM is called from RINPUP. It copies MARS data to unit 95.

DPDATA is a utility routine for SAS3. RINPUP writes binary files using DPDATA for later use by subsequent programs.

JOMIN is called by RINPUP to process MARS geometry input data. It calls JOMIN1, JOMIN2, AZIP, RESTOR, and SAZAR.

MANRY is called from OAKTRE to manipulate the reading of the responses from both the SCALE cross-section library and from user input. MANRY calls ACTIE to retrieve responses and RESPTI to obtain titles for the responses retrieved. It reads user responses and prints out all responses and titles.

OAKTRE is called from SAS3. The MORSE SAS3 control options are read in this routine. Most of the input in block 1 of MORSE is initialized in OAKTRE.

RESPTI is called from MANRY. It returns titles for standard responses retrieved from SCALE cross-section library files.

RINPUP prints out the edit of the MORSE input and controls the MORSE input setup. RINPUP is a modified version of RINPU1 in MORSE-SGC. It calls CPYJOM, DPDATA, FREAD, JOMIN, and STORK.

SAS3 is the main controlling routine for SAS3 execution. SAS3 calls C4DATA to control the CSAS input processing and calls OAKTRE to control the MORSE input processing.

STORK is called from RINPUP to write out in binary the MARS combinatorial geometry data and labeled commons for later use by MORSE. The records written by STORK are read by RESTOR in MORSE. STORK returns to RINPUP the number of regions in the problem geometry.

ORNL-Dwg. 81-4004R

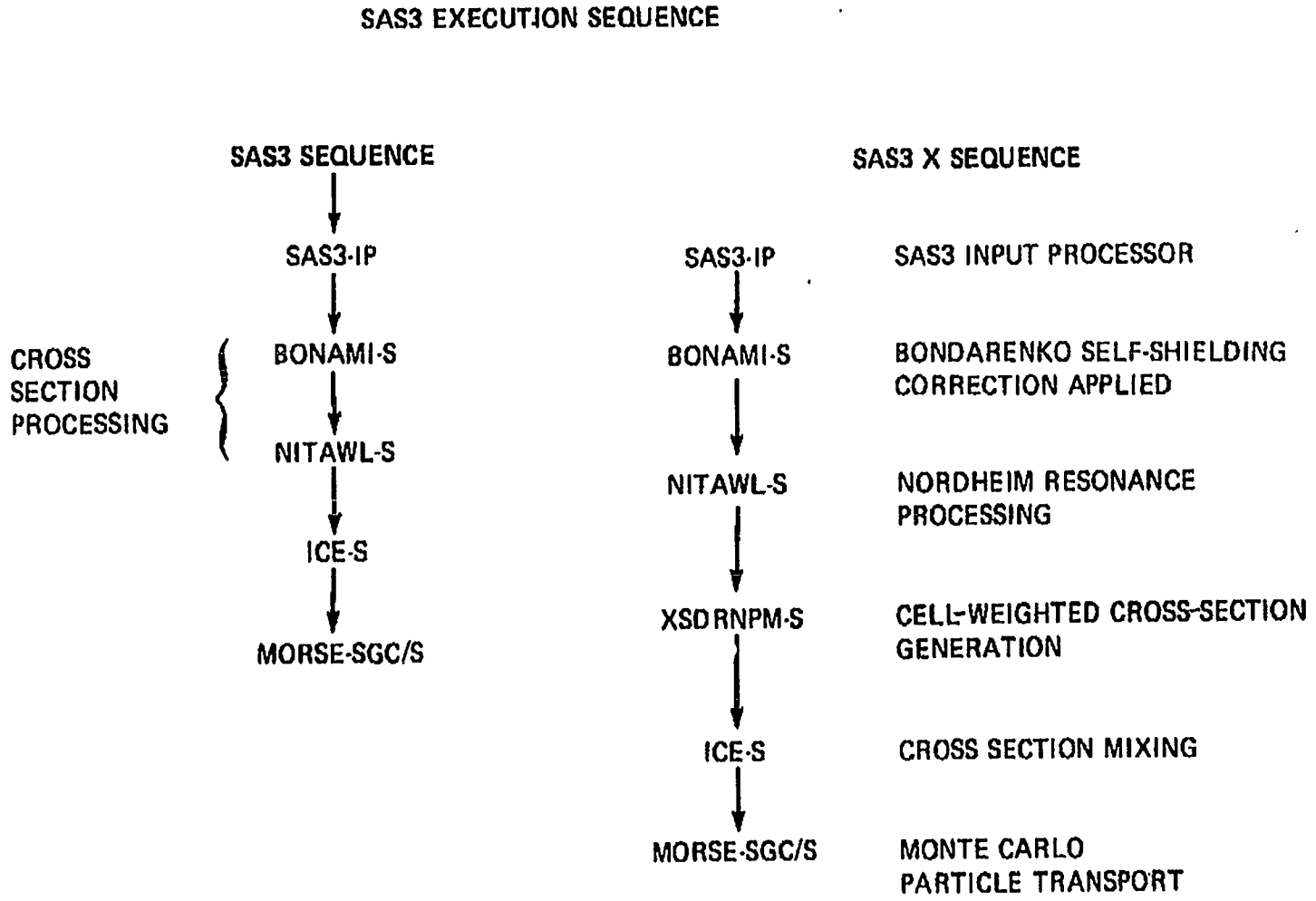

Figure S3.4.1 SAS3 and SAS3X program execution sequence

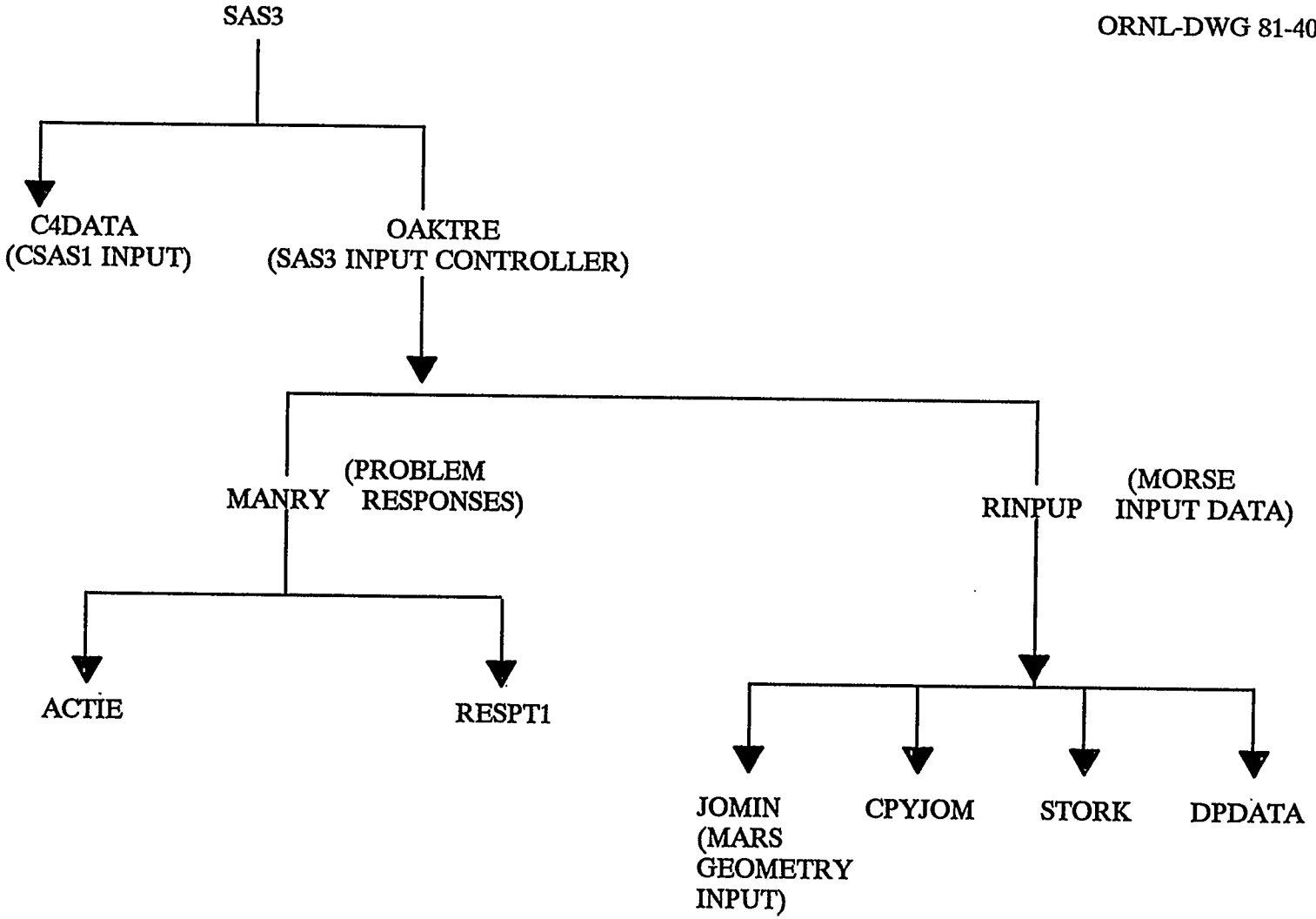

Figure S3.4.2 SAS3 input processor flow chart

S3.5 SAS3 INPUT DESCRIPTION

All the SAS3 input is free form. The first portion of the input is the standard composition input as described in Sect. C4.4. This information is followed by a SAS3 title card. The next portion of the SAS3 input is the SAS3 parameter input. The combinatorial MARS geometry is entered after the parameter input. See Sect. M9.A for a description of the geometry input. The MARS geometry input is followed by some miscellaneous Monte Carlo input requirements for use by MORSE-SGC. This input description concerns SAS3 requirements. The user is referred to Sect. C4.4 for the standard composition input description and to Sect. M9.A for the combinatorial MARS input description.

The SAS3 user must enter either the "NOD=" parameter for point detector problems or the "NKC=" parameter for criticality problems. Under no circumstances should both parameters be entered. The SCALE user is strongly recommended to use CSAS for his criticality problem instead of SAS3, whenever possible. It requires much less computer time, and the KENO geometry is much less susceptible to geometry tracking errors than the combinatorial MARS system. For these reasons, where the criticality lattice model permits, run CSAS instead of SAS3. Furthermore, the user is recommended to model as many of his universes in MARS as "simple" rather than "comjom." The simple universe simulates KENO tracking and requires less computer time than the comjom universes. See Sect. M9 for a more detailed discussion on combinatorial MARS geometry modeling.

SAS3 Input Requirements:

**** Material Information Processor Input (see Sects. C4.4.2 and S3.4)****

SAS3 Title Card (80 col.)

SAS3 Parameter Input

... Input format is "XXX=Y," where XXX is a variable name and Y is the value XXX is being assigned. Either "NOD=" or "NKC=" is required; all other variables are optional. Variable names in parentheses indicate the corresponding MORSE-SGC names.

PARAMETER NAME	DESCRIPTION
NOD=	Number of point detectors for a fixed-source shielding problem
NKC=	The number of the first batch to be included in the estimate of k; if less than or equal to zero, no estimate of k is made. This parameter must be entered for criticality problems
NST=	(NSTRT) Number of particles per batch (default is 100)
NMO=	(NMOST) Maximum number of particles allowed for in the bank(s); may equal NSTRT+1 if no splitting, fission, and secondary generation (default is 200)
NIT=	(NITS) Number of batches (default is 100)
NKI=	(NKILL) Set greater than zero if Russian roulette is allowed (default is 1)
NSR=	(NSPLT) Set greater than zero if splitting is allowed. If NSR=-1, then the user must input splitting, Russian roulette, and direction biasing parameters (default is 1)

NOP= Number of user input responses

NRE= Library Response Flag Option

NRE>0	Number of response IDs requested User must enter response ID required immediately following parameter input See Table S3.3.4 for available response IDs Not all SCALE libraries contain responses
NRE=0	Default ID requested for standard neutron and gamma dose IDs requested are 9029 and 9504
NRE=-1	All available response IDs requested
NRE=-2	All available neutron responses requested
NRE=-3	All available gamma responses requested

MAL= (MEDALB) Specular Reflection Media

NDS= Number of array analysis edits requested

RAN= User input random number seed (Z12 Format)

IST= (ISTR) Switch to print cross sections

IMO= (IMOM) Switch to print moments of angular distribution

MSM= SOURCE MEDIA Flag; if set to a valid media number, then all source particles will start in MSM

IPR= (IPRIN) Switch to print angles and probabilities

NPA= Set greater than zero if pathlength stretching (exponential transform) is invoked

NDG= Used only when NPA is set greater than zero. Selects the option for direction biasing to be used

IPU= (IPUN) Switch to print results of bad Legendre coefficients

MAX= (MAXGP) Group number of last group for which Russian roulette, splitting, or exponential transform is to be performed.

IFM= (IFMU) Switch to print intermediate results of the scattering angles calculated from the Legendre coefficients if >0

END TERMINATES INPUT OF VARIABLES

If NRE>0, then NRE response IDs are entered.

If NOP>0, then NOP responses and titles are entered as follows.

NOP response sets are entered, one entry for each energy group for each set. Enter first response set, all groups, second response set, all groups... NOP response set, all groups.

NOP title cards are entered

Note, all responses are normalized to the source volume.

****** MARS Combinatorial Geometry INPUT (See Sect. M9.A) ******

The following eight variables are required input.

TMAX - Maximum computer time for MORSE execution (min.)

NABP - Neutron angular biasing parameter to bias source particles to the first point detector location. Enter zero for no neutron angular biasing

NABOG - Gamma angular biasing parameter. Not used in SAS3. Enter 0

XMIN, XMAX, YMIN, YMAX, ZMIN, and ZMAX - Source volume boundaries

If NSR=-1, then the following splitting, Russian roulette, and pathlength stretching parameters must be entered.

((WTHI(I,J),I=1,MAXGP), J=1,MXREG) Weight above which splitting will occur

((WTLOW(I,J),I=1,MAXGP), J=1,MXREG) Weight below which Russian roulette is played

((WTAVE(I,J),I=1,MAXGP), J=1,MXREG) Weight parameters for particles surviving Russian roulette.

((PATH(I,J),I=1,MAXGP), J=1,MXREG) Pathlength stretching parameters for use in exponential transform.

Energy bias factors are required input if running a coupled neutron gamma problem.

((EPROB(I,J),I=1,NNGA+NGGA), J=1,MXREG). Values of the relative importance of particles leaving a collision in region J going to enter energy group I.

Source energy distribution (NNGA+NGGA+1 entries required). This input should not be entered for criticality problems where NKC is greater than zero. The appropriate fission spectrum will be automatically selected by SAS3. This input is required for shielding problems where NOD (number of detectors) is greater than zero. Enter one value for each energy group and a source normalization factor. The units are arbitrary providing:

$$\text{Total source in particles/s} = N \sum_{i=1}^{NNGA+NGGA} X_i$$

where

i = energy group number i
X_i = source fraction in energy group i
N = source normalization factor
NNGA = number of neutron energy groups
NGGA = number of gamma energy groups

If NOD>O, then NOD point detector locations must be entered.

XDET, YDET, ZDET (Absolute coordinates)
If NOD was not entered or is zero, then enter three zeroes for a detector coordinate.

END CARD *****

"END" in Column 1 will terminate input processing for SCALE SAS3.

S3.6 SAS3 SAMPLE PROBLEM - TANK SHIELDING PROBLEM

S3.6.1 OBJECT AND CALCULATIONAL PROCEDURE

Object:

Determine the neutron and gamma dose per source neutron from a tank containing 9 g/L Pu-Nitrate solution at nine point locations.

Procedure:

Point detector results at nine locations were computed with MORSE-SGC in the SCALE SAS3 system by sampling from a uniformly distributed source in the Pu-Nitrate solution. Uncertainty in the MORSE results leads to a simpler approach to determine an upper limit on the dose at the nine point detectors. The upper limit was obtained by running the MORSE problem with a point source in a void tank as opposed to a distributed source, and computing results for all point detectors.

S3.6.2 TANK MODEL AND CALCULATIONAL ASSUMPTIONS

The atomic number densities used in the calculation are given in Table S3.6.1. The geometry model is given in Fig. S3.6.1 and was modeled in combinatorial geometry for MORSE, as shown in Figs. S3.6.2 and S3.6.3. The cross-section library used is the 27 neutron 18 gamma SCALE library based on ENDF/B-IV data. The cross sections are corrected automatically by SAS3 for resonance self-shielding using the Nordheim Integral treatment in the NITAWL code. The cross sections were mixed in the ICE code and then used by MORSE for the particle transport.

For the tank calculation, MORSE sampled source particles from a uniform distribution within the tank solution. The sampling process involved defining a rectangular volume of space containing the tank. Uniform samples were obtained within this volume and only samples found in the tank solution were accepted as source locations. For the point source calculation, MORSE sampled source particles from a point (0,0,63.69) at the center of the voided tank. The source energy spectrum used was a ^{235}U fission spectrum given in Table S3.6.2.

The ANSI standard neutron and gamma dose response functions were used to obtain the neutron and gamma dose results at the point detector locations. The response functions are given in Table S3.6.3, where RESP(1) is the neutron dose response and RESP(2) is the gamma dose response set. The units on the response function times the flux are REM/HOUR.

A fully coupled MORSE calculation was performed where the secondary gamma particles are treated as an energy downscatter. Bias techniques employed in this problem were Russian roulette, splitting, and energy biasing. The energy biasing scheme biased the possible downscatter groups to accelerate the tracking procedure and reduce the number of thermal scatterings. The complete SAS3 input for the point source calculation is given in Table S3.6.4.

S3.6.3 CALCULATIONAL DIFFICULTY AND CONCLUSIONS

Monte Carlo point detector estimates are made from each source location and from each collision site. As a result, statistical fluctuations are aggravated by large distributed sources and by detector locations near a large scattering source. Most of the tank calculation involved making estimates from collision sites in the Pu-Nitrate solution. Many collision and source estimates are required to accurately calculate the leakage flux to a point detector location. The closer the detector is to the scattering source, the more difficult it is to

Table S3.6.1 Mixture atomic compositions

Media No.	Nuclide	Atom density (atom/barn.cm)	Description
1	H	0.066522	Plutonium
1	N	9.0675 E-05	Nitrate
1	O	0.033533	Solution
1	Pu-240	1.129 E-06	
1	Pu-239	2.154 E-05	
2			Stainless Steel 304
3	H	0.054782	Benelex
3	C	0.033852	
3	O	0.023862	
4	H	0.014868	Concrete
4	C	0.003814	
4	O	0.041519	
4	Ca	0.011588	
4	Si	0.006037	
4	Mg	0.000587	
4	Fe	0.000968	
4	Al	0.000735	
4	Na	0.000304	

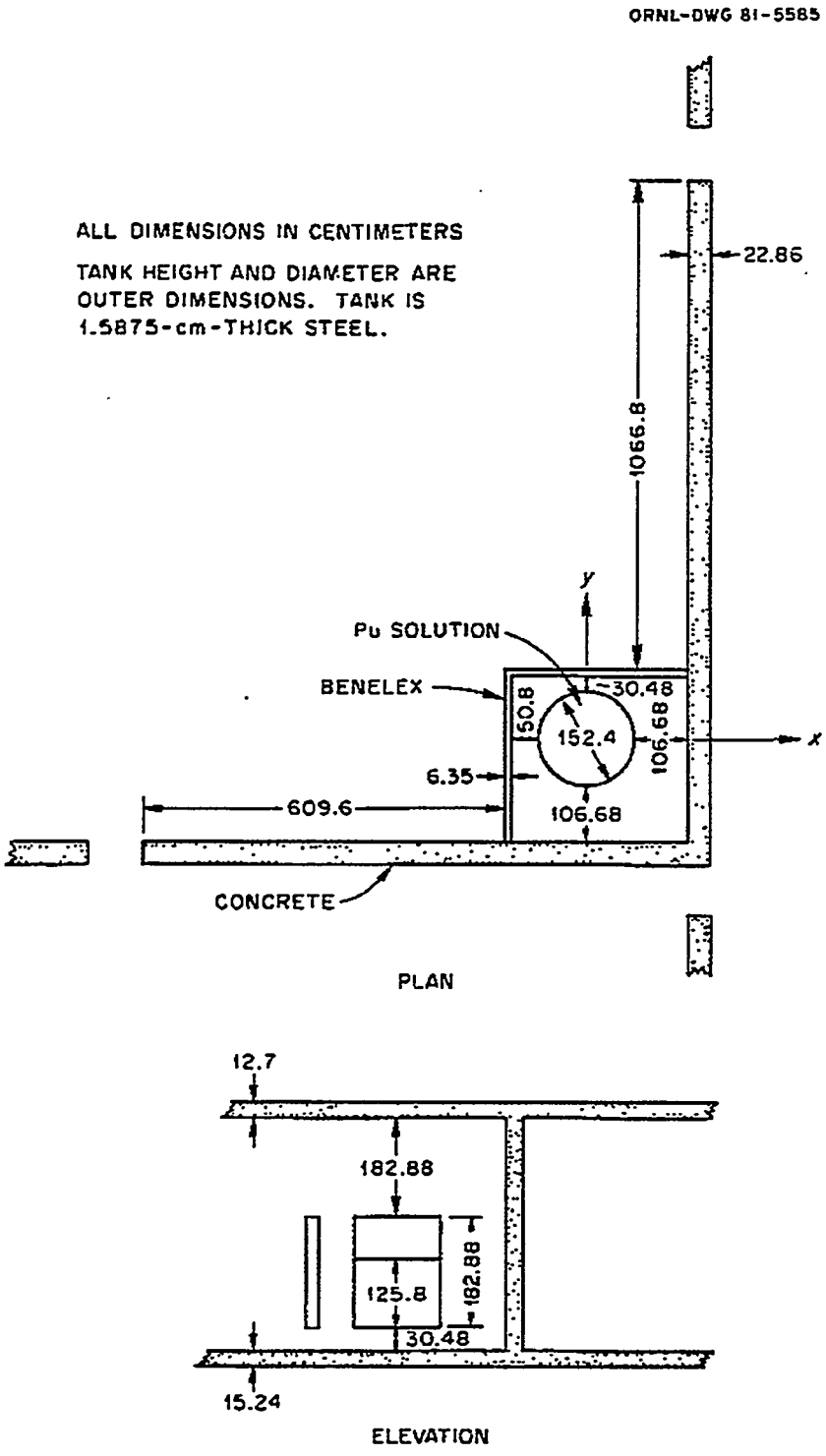

Figure S3.6.1 Geometry for the tank shielding problem

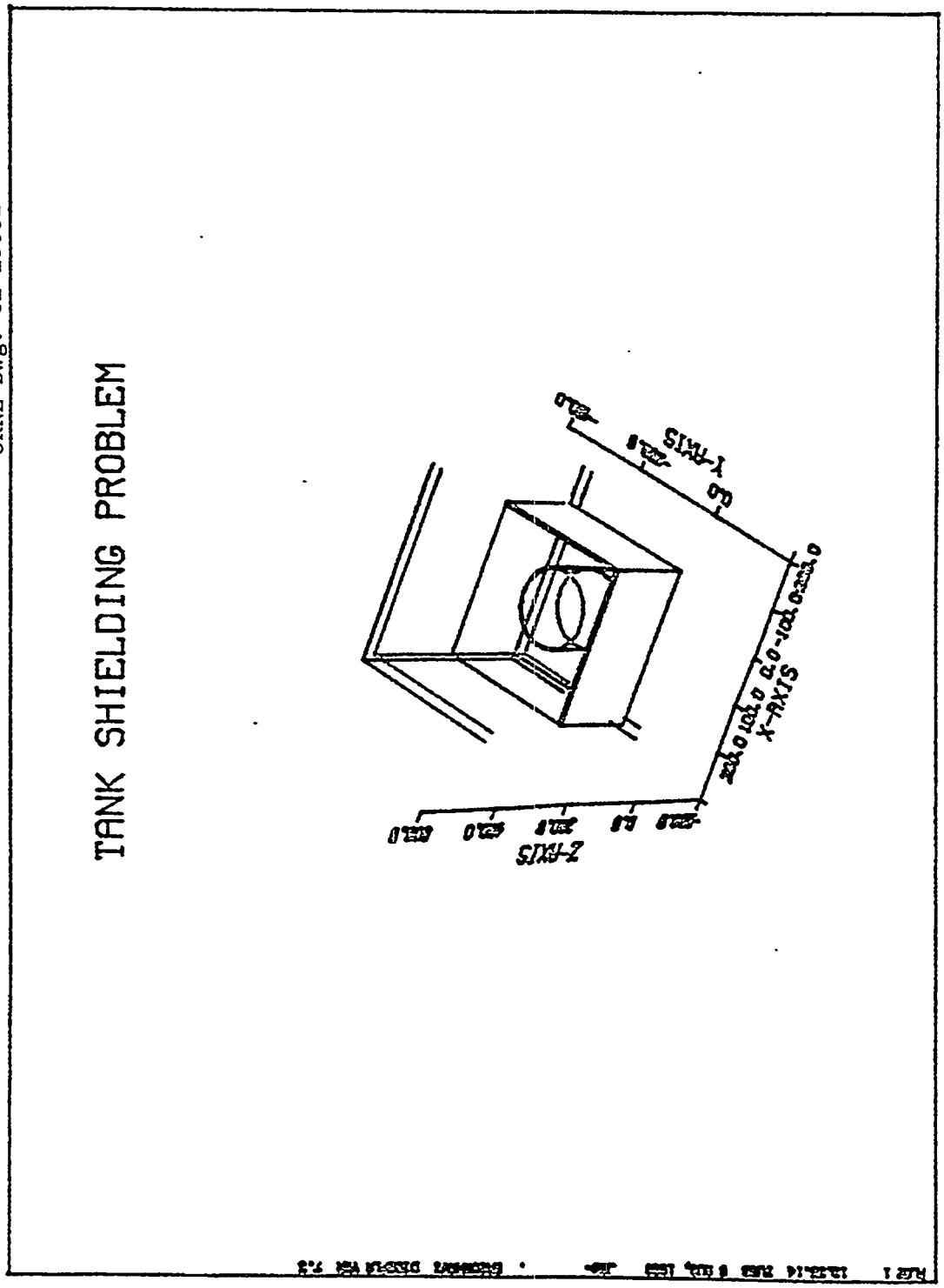

Figure S3.6.2 Tank shielding problem for SAS3

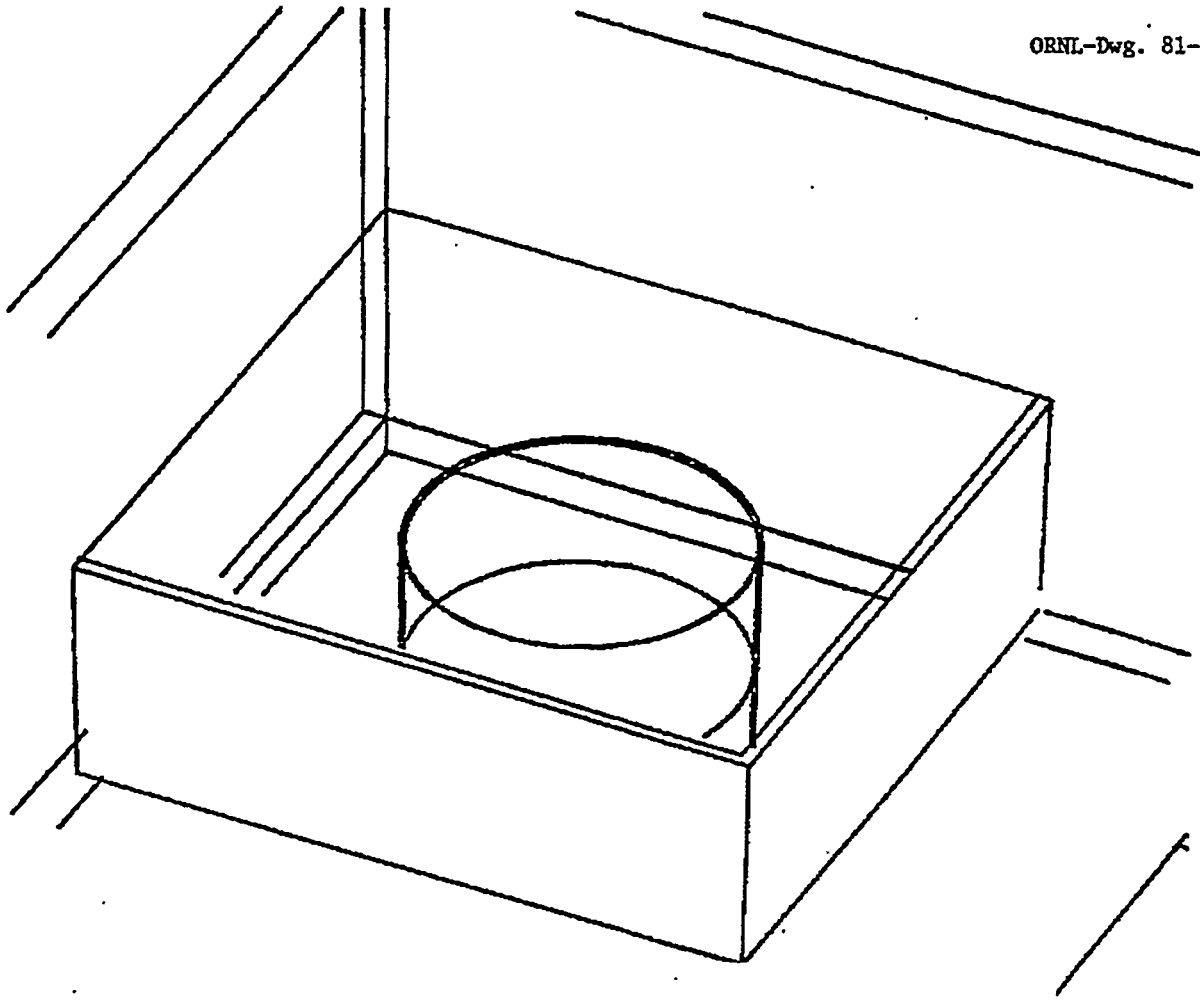

Figure S3.6.3 Tank shielding model for SAS3

Table S3.6.2 Neutron source spectrum

Group No.	Energy (eV)	Fractional source spectrum
	2.000 + 07	
1	6.434 + 06	0.02107
2	3.000 + 06	0.1883
3	1.850 + 06	0.2149
4	1.400 + 06	0.1245
5	9.000 + 05	0.1662
6	4.000 + 05	0.1805
7	1.000 + 05	0.08965
8	1.700 + 04	0.01385
9	3.000 + 03	0.001006
10	5.50 + 02	7.470 E-03
11	1.00 + 02	5.877 E-04
12	3.00 + 01	4.128 E-05
13	1.00 + 01	0
14	3.05 + 00	0
15	1.77 + 00	0
16	1.30 + 00	0
17	1.13 + 00	0
18	1.00 + 00	0
19	0.800	0
20	0.400	0
21	0.325	0
22	0.225	0
23	0.100	0
24	0.050	0
25	0.030	0
26	0.010	0
27	1.000-05	0

Table S3.6.3 Neutron and gamma dose response sets

Group	Neutron Response RESP(1)	Gamma Response RESP(2)
1	0.1492 E-03	0.0
2	0.1446 E-03	0.0
3	0.1270 E-03	0.0
4	0.1281 E-03	0.0
5	0.1298 E-03	0.0
6	0.1028 E-03	0.0
7	0.5118 E-04	0.0
8	0.1232 E-04	0.0
9	0.3836 E-05	0.0
10	0.3725 E-05	0.0
11	0.4015 E-05	0.0
12	0.4293 E-05	0.0
13	0.4474 E-05	0.0
14	0.4568 E-05	0.0
15	0.4558 E-05	0.0
16	0.4518 E-05	0.0
17	0.4486 E-05	0.0
18	0.4466 E-05	0.0
19	0.4434 E-05	0.0
20	0.4327 E-05	0.0
21	0.4197 E-05	0.0
22	0.4098 E-05	0.0
23	0.3839 E-05	0.0
24	0.3675 E-05	0.0
25	0.3675 E-05	0.0
26	0.3675 E-05	0.0
27	0.3675 E-05	0.0
28	0.0	0.8772 E-05
29	0.0	0.7478 E-05
30	0.0	0.6375 E-05
31	0.0	0.5414 E-05
32	0.0	0.4622 E-05
33	0.0	0.3960 E-05
34	0.0	0.3469 E-05
35	0.0	0.3019 E-05
36	0.0	0.2628 E-05
37	0.0	0.2205 E-05
38	0.0	0.1833 E-05
39	0.0	0.1523 E-05
40	0.0	0.1173 E-05
41	0.0	0.8759 E-06
42	0.0	0.6306 E-06
43	0.0	0.3834 E-06
44	0.0	0.2669 E-06
45	0.0	0.9347 E-06

Table S3.6.4 SAS3 sample input for tank shielding problem

```
TANK SHIELDING PROBLEM, JIM WEST, ORNL, AUGUST, 1980
27N-18COUPLE    INFHOMMEDIUM
H         1       0.0                 0.066522 END
N         1       0.0                 9.0675E-05END
O         1       0.0                 0.033533 END
PU-240    1       0.0                 1.129E-06END
PU-239    1       0.0                 2.154E-05END
SS304     2       1.0                     END
H         3       0.0                 0.054782 END
C         3       0.0                 0.033852 END
O         3       0.0                 0.023862 END
H         4       0.0                 0.014868 END
C         4       0.0                 0.003814 END
O         4       0.0                 0.041519 END
CA        4       0.0                 0.011588 END
SI        4       0.0                 0.006037 END
MG        4       0.0                 0.000587 END
FE        4       0.0                 0.0001968END
AL        4       0.0                 0.000735 END
NA        4       0.0                 0.000304 END

         END COMP
SHIELDING PROBLEM
RAN=35A467B NOD=9 NIT=25 END
SHIELDING PROBLEM
0 0 0 0

RCC       0.0 0.0 1.5875 0.0 0.0 179-715 74.6125
RCC       5*0.0 182.88 76.2
RPP       -100-0 100.0 -100.0 100.0 -100.0 76.2
RPP       -1500.0 182.88 -182.88 1500.0 -30.48 396.24
RPP       -1500.0 205-74 -205-74 1500.0 -30.48 396.24
RPP       -127.0 183.00 -183-00 106.68 0.0 182.88
RPP       -133-35 183-00 -183-00 113-03 0.0 182.88
RPP       -1.0E+05 1.0E+05 -1.0E+05 1.0E+05 -1.0E+05 1.0E+05
RPP       -1500.0 1500.0 -1500.0 1500.0 -30.48 396.24
RPP       -1500.0 1500.0 -1500.0 1500.0 -45-72 408.94
      END
SOL       +1 +3
AIR       +1 -3
TNK       +2 -1
WAL       +5 -4
SMW       +7 -6 +4
AIR       +6 -2 +4 OR +9 -7 +4 OR +9 -5
SPC       +8 -10
TBC       +10 -9
          END
 3*1      5*2
 8*0
 1000 1000 2 4 3 1000 0 4
 0
 70.0 2*0.0 4*0.0 2*63.69
 8*1.0 12*0.5 7*0.3 13*0.8 5*0.5
 8*1.0 12*0.5 7*0.3 13*0.8 5*0.5
 .2107E-01 .1883 .2149 .1245 .1662 .1805 .8965E-01 .1385E-01 .1006E-02
 .7470E-04 .5877E-05 .4128E-G6 33*0.0 1.0
 -134.0 0.0 64.49
  0.0 -206. 64.49
 206. -194-31 64.49
 243.84 0.0 64.49
-742.95 0.0 64.49
 448.58 -205.74 64.49
 0.0 1179.83 64.49
 0.0 0.0 379.
 END
```

obtain satisfactory statistics with a reasonable amount of computer time. Thus, the tank calculation required 4 h of IBM-3033 time, whereas the point source calculation required only 27 min of IBM-3033 computer time.

The final results output from MORSE for the point-source neutron and gamma dose are shown in Table S3.6.5. A comparison of these results with the tank calculation is shown in Tables S3.6.6 and S3.6.7. Recall that the point-source, void-tank values represent an upper limit on the dose.

Table S3.6.5 MORSE output for the point-source neutron and gamma dose

ANSI STANDARD NEUTRON DOSE RATE (REM PER HOUR)

DETECTOR	RESPONSES (DETECTOR) UNCOLL RESPONSE	FSD UNCOLL	TANK SHIELDING PROBLEM TOTAL RESPONSE	FSD TOTAL
1	4.2984E-11	0.02132	9.3314E-11	0.05789
2	5.9913E-11	0.02132	1.9688E-10	0.33128
3	2.0028E-12	0.02448	4.8434E-11	0.12591
4	3.4093E-13	0.02639	2.1431E-11	0.07242
5	1.2785E-14	0.02897	2.9475E-11	0.06539
6	1.3984E-12	0.02132	1.0885E-11	0.06716
7	3.4556E-27	0.02962	4.8769E-12	0.05091
8	5.5451E-13	0.02132	3.8151E-12	0.07494
9	4.2215E-11	0.01328	1.4278E-10	0.11259

ANSI STANDARD GAMMA DOSE RATE (REM PER HOUR)

DETECTOR	RESPONSES (DETECTOR) UNCOLL RESPONSE	FSD UNCOLL	TANK SHIELDING PROBLEM TOTAL RESPONSE	FSD TOTAL
1	0.0	0.0	1.6067E-11	0.48253
2	0.0	0.0	1.0102E-11	0.24655
3	0.0	0.0	3.4994E-12	0.47029
4	0.0	0.0	6.5317E-13	0.09756
5	0.0	0.0	8.8504E-13	0.09943
6	0.0	0.0	5.13OOE-13	0.10769
7	0.0	0.0	1.5479E-13	0.09657
8	0.0	0.0	2.0327E-13	0.10860
9	0.0	0.0	4.7293E-12	0.25422

Table S3.6.6 Neutron dose results per source neutron (collided + uncollided)

Detector	MORSE point source REM/h/N	FSD	MORSE tank source REM/h/N	FSD
1	1.36 E-10	(0.04)	1.05 E-11	(0.28)
2	2.57 E-10	(0.25)	8.67 E-12	(0.10)
3	5.04 E-11	(0.12)	3.49 E-13	(0.20)
4	2.18 E-11	(0.07)	1.11 E-12	(0.92)
5	2.95 E-11	(0.07)	6.98 E-13	(0.18)
6	1.23 E-11	(0.06)	1.75 E-12	(0.15)
7	4.88 E-12	(0.05)	2.73 E-13	(0.21)
8	4.37 E-12	(0.07)	4.51 E-13	(0.14)
9	1.85 E-10	(0.09)	1.58 E-12	(0.55)

Table S3.6.7 Gamma dose results per source neutron

Detector	MORSE point source REM/h/N	FSD	MORSE tank source REM/h/N	FSD
1	1.61 E-11	(0.48)	5.60 E-12	(0.13)
2	1.01 E-11	(0.25)	1.42 E-11	(0.57)
3	3.50 E-12	(0.47)	3.92 E-13	(0.25)
4	6.53 E-13	(0.10)	2.90 E-12	(0.97)
5	8.85 E-13	(0.10)	7.36 E-13	(0.29)
6	5.13 E-13	(0.11)	2.05 E-13	(0.063)
7	1.55 E-13	(0.10)	1.12 E-13	(0.12)
8	2.03 E-13	(0.11)	8.57 E-14	(0.093)
9	4.73 E-12	(0.25)	2.82 E-13	(0.090)

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SAS4: A MONTE CARLO CASK SHIELDING ANALYSIS MODULE USING AN AUTOMATED BIASING PROCEDURE

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ABSTRACT

The SAS4 control module performs a three-dimensional Monte Carlo shielding analysis of a spent fuel shipping cask using an automated biasing procedure. Biasing parameters required by the Monte Carlo calculation are generated from results of a one-dimensional adjoint discrete-ordinates calculation. SAS4 performs resonance self-shielding treatment with either the BONAMI or NITAWL-II functional module and cell weighting with the XSDRNPM functional module; then it carries out adjoint discrete-ordinates and Monte Carlo calculations, respectively, with the XSDRNPM and MORSE-SGC functional modules.

Similar to other control modules in the SCALE system, simplified input is adopted in SAS4. In particular, for MORSE-SGC the user is neither required to specify all biasing parameters nor to set up the detailed MARS geometry input for the Monte Carlo calculation.

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S4.1 INTRODUCTION

The primary function of the Shielding Analysis Sequence No. 4 (SAS4) control module is to perform a three-dimensional (3-D) Monte Carlo shielding analysis of a spent nuclear fuel shipping or storage cask using an automated biasing procedure.[1] To carry out a Monte Carlo shielding calculation of a cask, the user is confronted by three major input tasks: (1) the preparation of cross-section data; (2) the preparation of biasing parameters such as Russian roulette and splitting weights, path-length stretching parameters, source biasing parameters, etc.; and (3) the setup and verification of geometry input. The preparation of cross-section data is done in SAS4 using the methods and input data for the Material Information Processor (see Sect. M7.2 for techniques and Sect. M7.4 for input data), which is used by CSAS and other SCALE control modules. SAS4 assists the user with the other tasks by using a procedure that automatically calculates biasing parameters for a Monte Carlo calculation and by using a geometry input processor that generates detailed MARS geometry input (see Sect. M9) of a cask model from simplified user input. Simplified input is also adopted for the other portions of the control module.

The SCALE functional modules executed by SAS4 (and the function of each) are given sequentially below:

BONAMI performs resonance self-shielding calculations for nuclides that have Bondarenko data associated with their cross sections. (See Sect. F1 for a module description.)

NITAWL-II applies a Nordheim resonance self-shielding correction to nuclides having resonance parameters. (See Sect. F2 for a module description.)

XSDRNPM provides cell-weighted cross sections based, for the LATTICECELL option, on the specified unit cell. (See Sect. F3 for a module description.)

XSDRNPM performs an adjoint calculation to generate biasing parameters for the Monte Carlo analysis.

MORSE-SGC performs a Monte Carlo simulation of the radiation transport through a cask and evaluates the dose rates exterior to the cask. (See Sect. F9 for a module description.)

SAS4 is able to compute neutron or gamma dose rates at any user-specified points outside a cask. By default, four surface-averaged dose rates are calculated on the outside surface of the cask and at 1, 2, and 3 m from this surface. The source energy spectrum can be input directly or read from an ORIGEN-S source file (see Sect. F7). The response function (dose factor) can be input directly or read from the standard response functions available in some of the SCALE cross-section libraries. For geometry checking by the PICTURE functional module (see Sect. M13), the user has the option of saving the detailed MARS geometry input generated by the input processor.

Finally, a cask model has been developed to implement the automated biasing procedure and the simplified geometry input option. The cask model has the following common features found in many shipping and storage casks: a radial water jacket for neutron shielding, axial impact limiters, corner coolant holes, and a fuel basket (or insert). For the fuel region, homogeneous and heterogeneous models are allowed. This cask model, combined with the available fuel configurations, should cover a broad class of cask shielding problems. However, as a last resort, an option is provided for the user to supply a detailed MARS geometry input directly to SAS4.

S4.2 METHODS AND TECHNIQUES

In a Monte Carlo shielding analysis of a deep-penetration problem such as a spent fuel cask, variance reduction techniques must be used to calculate reasonably good results at an affordable cost. Generation of biasing parameters and application of the parameters to solve a particular problem are no trivial tasks. Nevertheless, a systematic approach has been developed recently for biasing a Monte Carlo transport calculation of a spent fuel cask.[1] This approach uses adjoint fluxes from a one-dimensional (1-D) discrete-ordinates calculation performed with the XSDRNPM code to generate the biasing parameters for a Monte Carlo analysis by the MORSE-SGC code. The entire procedure for cross-section preparation, adjoint flux calculation, automatic generation of Monte Carlo biasing parameters, and a Monte Carlo calculation has been implemented in this control module to provide calculated radiation dose levels exterior to a cask at a reasonable computational cost.

This section details the method used by SAS4 in performing a 3-D Monte Carlo shielding analysis of a nuclear fuel cask using the automated biasing procedure. The techniques of cross-section preparation and input data generation for execution of the functional modules are presented. The cask geometry model and the different options of calculating neutron or gamma-ray doses outside a cask are described.

S4.2.1 GENERAL DESCRIPTION OF THE SAS4 METHODOLOGY

SAS4 calculates radiation doses exterior to a nuclear fuel shipping cask with the Monte Carlo method. The method uses the existing functional modules and cross-section and subroutine libraries in the SCALE system to carry out the analysis. The functional modules executed by SAS4 are BONAMI, NITAWL-II, XSDRNPM, and MORSE-SGC, along with the Material Information Processor described in Sect. M7. An outline of the SAS4 calculational sequence is shown in Fig. S4.2.1. The basic function of each functional module, as applied to SAS4, is described below.

BONAMI applies the Bondarenko method for resonance self-shielding calculations for nuclides whose cross sections include Bondarenko data. BONAMI is described in Sect. F1, and the Bondarenko method is discussed in Sect. M7.2.5.1.

NITAWL-II performs the Nordheim resonance self-shielding corrections to cross sections for nuclides whose cross sections include resonance parameters. NITAWL-II is described in Sect. F2, and additional information on the Nordheim integral treatment is provided in Sect. M7.2.5.2.

XSDRNPM performs two 1-D discrete-ordinates calculations to provide two very different functions in SAS4. First, it is used to produce cell-weighted cross sections if the LATTICECELL option is input for the fuel lattice type. Then, it is executed in the adjoint mode with a slab geometry to calculate adjoint fluxes that are used to generate biasing parameters for the Monte Carlo analysis. More details on XSDRNPM can be found in Sect. F3.

MORSE-SGC performs a Monte Carlo fixed-source analysis that calculates dose rates outside a transport or storage cask. All the standard biasing options in the MORSE code, including source biasing, splitting and Russian roulette, path-length stretching, and collision energy biasing, are invoked. All the required biasing parameters are derived from results of the adjoint XSDRNPM calculation and are automatically input to MORSE so that the user is rid of this difficult input task. For more details on the MORSE code, refer to Sect. F9 and Ref. 2.

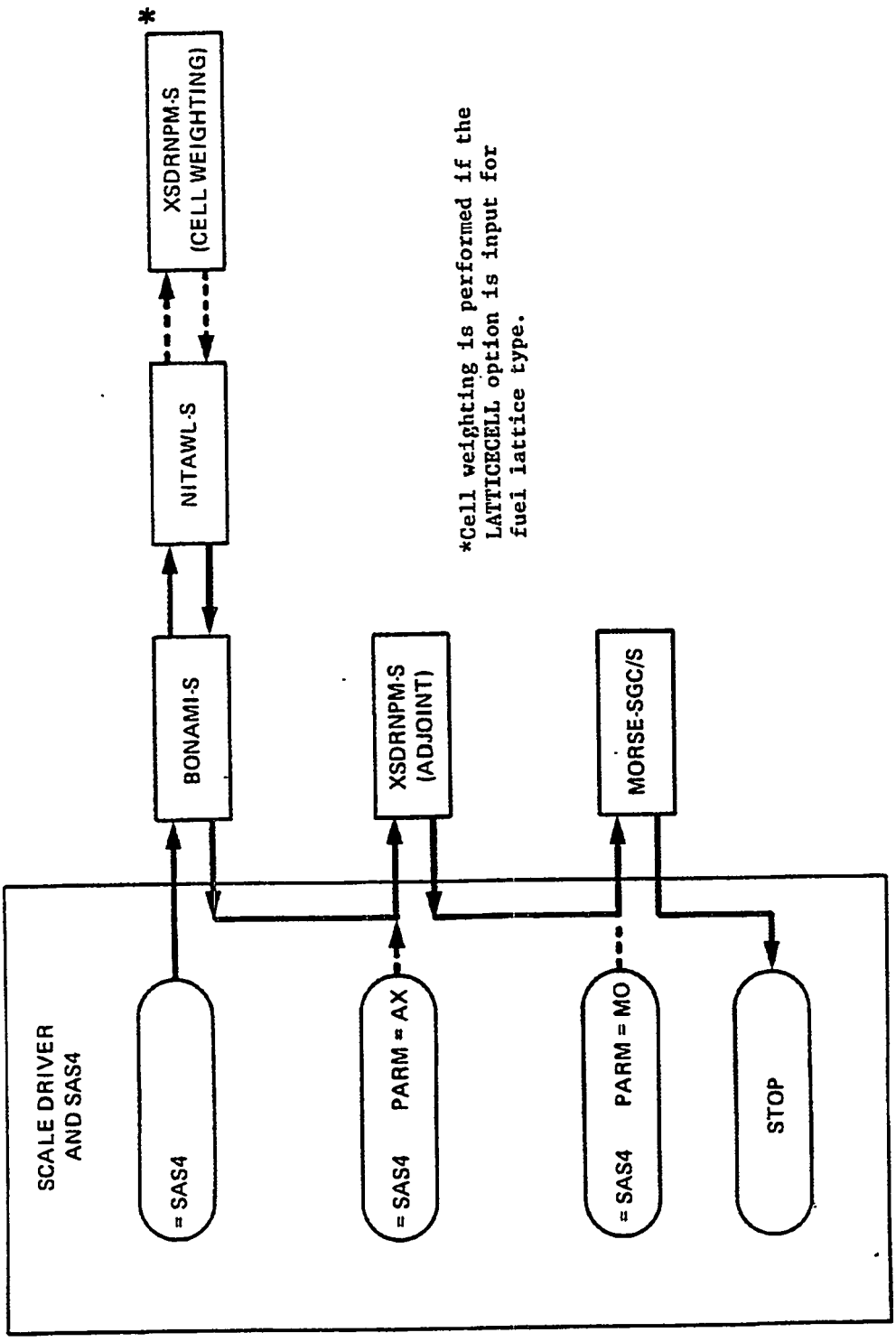


Figure S4.2.1 Outline of the SAS4 analytic sequence

SAS4 uses a simplified input procedure similar to other control modules in SCALE. The input to SAS4 basically consists of three parts: (1) the material information data, (2) the adjoint discreteordinates input data, and (3) the Monte Carlo input data. A cask model has been developed to facilitate implementation of the simplified geometry input and the automated biasing procedure in MORSE-SGC calculations.

The preceding description gives a brief summary of the SAS4 methodology. Detailed discussions of the techniques employed by SAS4 are presented in the following sections.

S4.2.2 DESCRIPTION OF THE SAS4 CASK MODEL

A great deal of consideration was given to the development of the SAS4 cask model. Three basic criteria to be satisfied by the cask model were the following:

1. The model should be quite general and should include most, if not all, of the common features in current cask design so that this control module would be of practical value and useful for shielding analysis.

2. The cask model must be able to incorporate the automated biasing procedure so that accurate and reliable results could be obtained, even by an inexperienced Monte Carlo user, at a reasonable computing cost.

3. Simplified geometry input would be used to describe the model.

With these conditions in mind, a cask model (Fig. S4.2.2) was developed. This cask model basically consists of a container region and a source region. The cask is composed of right circular cylinders of shielding materials with a central cavity to accommodate the source region. The cask is symmetrical about the cask midplane. Because most spent fuel casks are tall cylinders, more than 4 m in height, this assumption on symmetry should not introduce significant error to the results of the calculation. There are two reasons for applying symmetry to this model: (1) symmetry improves the calculational efficiency and, more importantly, (2) the symmetry is necessary to implement the automated biasing procedure in the Monte Carlo analysis. In the Monte Carlo analysis, the entire cask is modeled in the geometry.

In more detail, the container of the cask model consists of an insert (fuel basket), a cavity, an inner liner, an outer liner, three radial shields, three axial shields, impact limiters, a water jacket, and corner holes. This model is a rather elaborate container geometry and probably has more components than typically needed. However, with the default features, this cask model can easily describe casks with less complicated geometries. The user can specify a cask geometry using the simplified geometry input option, which is invoked by setting the parameter IGO $\leq$ 3 in the Monte Carlo input data. The IGO parameter performs two input functions: (1) it signals whether the geometry is to be input with the simplified geometry input option (IGO $\leq$ 3) or with the MARS geometry input option (IGO = 4) and (2) if the simplified geometry input option is chosen, the value of IGO specifies the geometry of the source region.

The simplified geometry input option allows four different geometric configurations for the source region. The four source region geometries corresponding to IGO = 0, 1, 2, and 3 are illustrated in Figs. S4.2.3 and S4.2.4. Note that for all the geometries, the source region is divided into three axial sections in which the fuel hardware is located on both ends of the active fuel. The fuel hardware represents such materials as cladding, plenum spring, end fitting, etc. Activation products (^{60}Co in particular) in the fuel hardware can be a significant source of gamma-ray doses at the ends of a cask.

For IGO = 0, the source region (fuel and fuel hardware) is a cylinder of radius FRD; for IGO = 1, the source region is two or three concentric cylinders. For IGO = 2 and 3, the source region is filled with identical fuel units A fuel unit consists of a fuel assembly surrounded by an extra space. As shown in Fig. S4.2.3, the fuel pins in an assembly are homogenized inside the fuel channel for IGO = 2 and represented explicitly for IGO = 3. The fuel unit is defined solely for modeling convenience. The lateral dimensions of

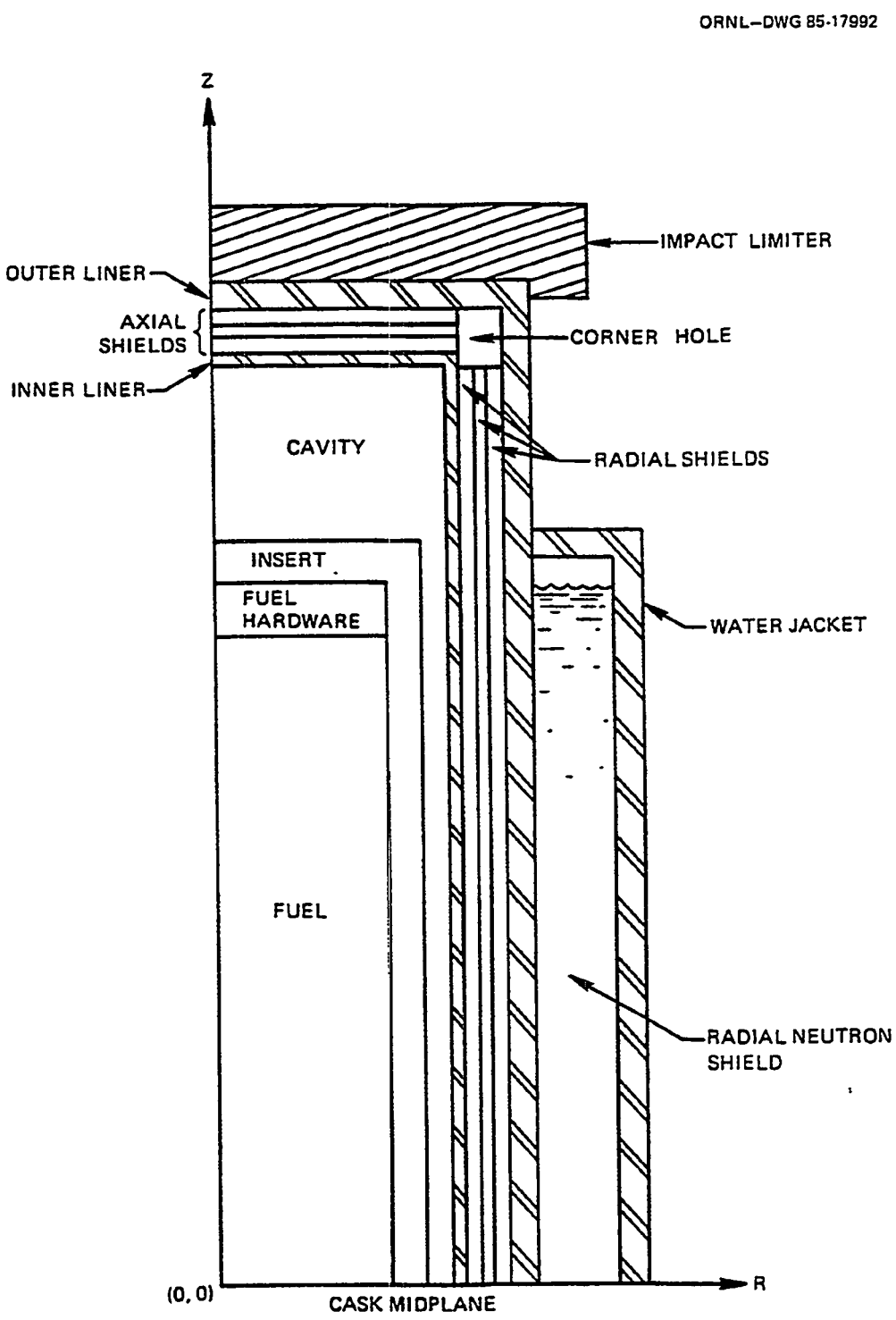


Figure S4.2.2 SAS4 cask model for IGO = 0

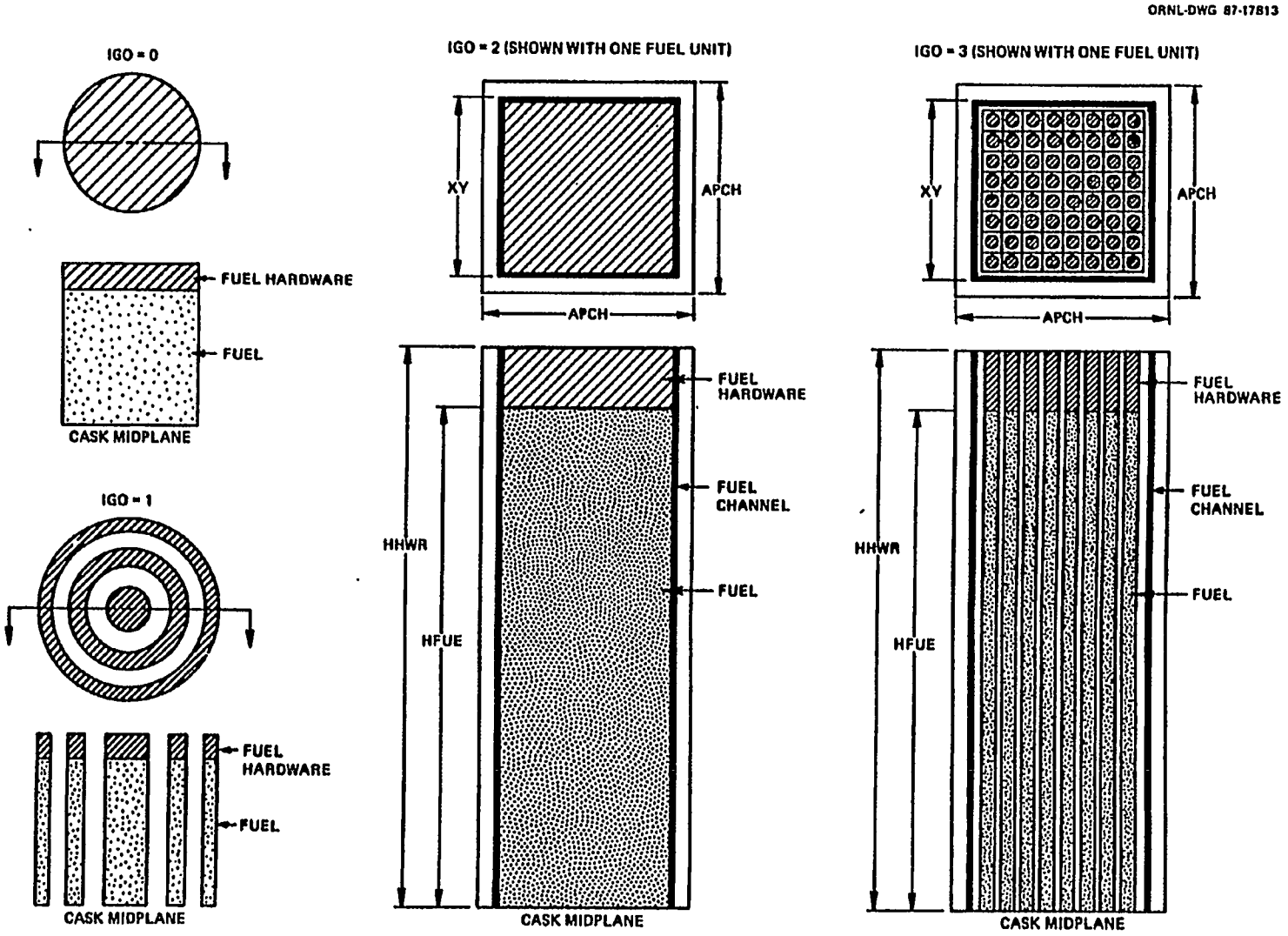


Figure S4.2.3 Geometry options of source region for simplified geometry input

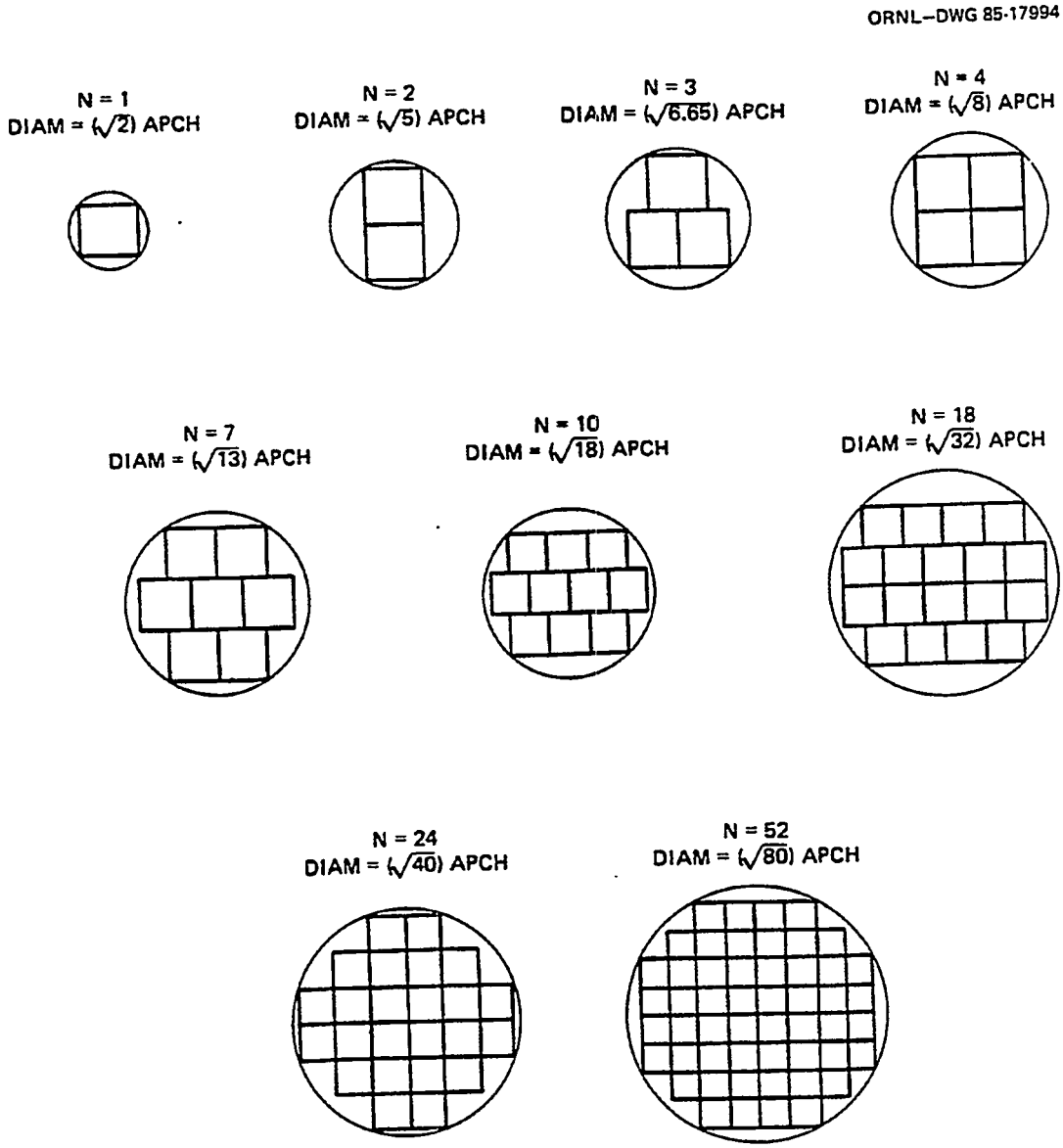


Figure S4.2.4 Packing arrangements of fuel units for goemetry options IGO = 2 and 3

a fuel unit are APCH × APCH, and the axial dimension is 2*HHWR. The center-to-center separation of fuel units is APCH cm. The number of fuel units allowed for these two options is 1, 2, 3, 4, 7, 10, 18, 24, and 52. The packing arrangements of the fuel units are shown in Fig. S4.2.4. Note that for modeling convenience, for IGO = 3 all lattice cells in the model are assumed to be completely filled with fuel rods; any vacant cells in the actual assemblies are accounted for by reducing the radial dimensions of the fuel rods to conserve the mass of the materials in each assembly.

It is believed that this cask model with the simplified geometry input is applicable to a wide variety of nuclear cask designs because it possesses many common features found in existing casks. With some imagination and consideration, the user can use this cask model to perform Monte Carlo analyses of most nuclear fuel cask shielding problems.

Finally, for IGO = 4, the user can model any casks using the detailed MARS geometry input. When modeling cask geometries with this option, the following four conditions must still be satisfied: (1) the entire cask must be modeled in the geometry, (2) the geometry must be symmetrical about the cask midplane, (3) the source region must be axially divided into the fuel section and the hardware sections at both ends, and (4) the geometry must include surfaces for the four default surface detectors described in Sect. S4.2.4. The reader is referred to the input description in Table S4.4.3 (Sect. S4.4.1), sample problem 4 in Sect. S4.5, and Sect. M9 of the SCALE system for more information on setting up MARS geometries for Monte Carlo analyses.

Although it appears that the SAS4 cask model is developed only for intact fuel assemblies, actually the model can also be used to analyze casks loaded with consolidated fuel or other forms of fuel arrangements. For the intact fuel assemblies loading, the LATTICECELL option should be input for cross-section processing in the material information processor; all the geometry options IGO = 0, 1, 2, 3, and 4 are permitted. For a tightly packed fuel loading such as consolidated fuel, the INFHOMMEDIUM option should be input; only the geometry options IGO = 0, 1, and 4 are allowed. More discussions regarding the LATTICECELL and INFHOMMEDIUM options are presented in the next section.

S4.2.3 CROSS-SECTION PREPARATION AND APPLICATION

As described in Sect. S4.2.1, input to SAS4 is composed of three parts: (1) the material information data, (2) the adjoint discrete-ordinates input data, and (3) the Monte Carlo input data. SAS4 makes use of the Material Information Processor (see Sect. M7.4) to read the material information data and to carry out resonance self-shielding treatment and cell-weighting calculation (if required).

The SAS4 cask model can be loaded with intact nuclear fuel assemblies, consolidated fuel rods, or homogeneous fuel. For the intact assemblies loading, the user describes a unit cell geometry using the LATTICECELL option for the fuel lattice type in the material information processor data. For this option, fuel-rod materials are resonance corrected using the unit cell geometry, while other resonance materials are treated using an infinite homogeneous geometry. A cell-weighting calculation is performed on the fuel-rod materials by the XSDRNPM functional module. All five Monte Carlo geometry input options (IGO = 0, 1, 2, 3, and 4) are permitted for the LATTICECELL option. For consolidated fuels or other tightly packed fuels, the user can use the INFHOMMEDIUM option for the fuel lattice type, which performs resonance treatment for all resonance materials with an infinite homogeneous geometry. For this option, only IGO = 0, 1, and 3 are allowed in the Monte Carlo geometry input.

An outline of the calculational sequences in SAS4, along with the units that transfer data among the functional modules, is presented in Fig. S4.2.5. The resonance-corrected microscopic cross-section data in working library format are written on logical unit 4 by the NITAWL-II functional module. This library is subsequently read by the XSDRNPM function module to perform a cell-weighting calculation if the LATTICECELL option is specified for the fuel (see Table S4.4.2 in Sect. S4.4.7). However, if the INFHOMMEDIUM option is chosen, the cell-weighting calculation is omitted. In either case, XSDRNPM is called to perform an adjoint slab-geometry transport calculation in the radial or axial direction that produces adjoint angular fluxes on logical unit 12. Finally, SAS4 processes the adjoint angular fluxes into various

biasing parameters, which are subsequently transmitted to MORSE-SGC via the input processor and logical unit 96. MORSE-SGC reads the appropriate microscopic cross-section data from either logical unit 3 or 4 and receives a mixing table generated by the SAS4 input processor. The entire processes of cross-section data preparation and data transmission are carried out automatically within the SAS4 control module.

After defining the mixtures in the material information data, the user must apply them in the unit cell specification (if needed) and in the adjoint discrete-ordinates and Monte Carlo calculations. The mixtures in SAS4 can be separated into two categories: (1) fuel materials and (2) cask materials. The fuel materials are used to describe the source region, and the cask materials are used for the insert, the cavity, and the rest of the geometry shown in Fig. S4.2.2. The mixture numbers and densities of the cask materials remain constant throughout the control module. Therefore, their applications in the adjoint discrete-ordinates and Monte Carlo calculations are straightforward. The applications of the fuel materials in the source region are complicated by the fuel lattice types and the source region geometry options.

For the LATTICECELL option, mixtures used to define the fuel materials should not be used for the cask materials, and vice versa. This rule must be observed because the fuel materials have been processed to account for resonance and cell-weighting effects and will be homogenized or mixed for a particular source region geometry option (IGO = 0, 1, 2, or 3). Among these processes, the fuel materials (including the fuel hardware) are given different mixture numbers. Hence, their applications in the adjoint discrete-ordinates and Monte Carlo calculations are more involved. However, for source region geometry options IGO = 0, 1, 2, and 3, SAS4 automatically assigns the appropriate mixture numbers of the fuel materials to the two calculations. For IGO = 4, the user should use the mixture numbers MFUEL and MHW, respectively, for the fuel and fuel hardware in the Monte Carlo calculation. More detailed descriptions are presented in Sect. 4.4.1 (Tables S4.4.2 and S4.4.4) and in Sect. S4.4.

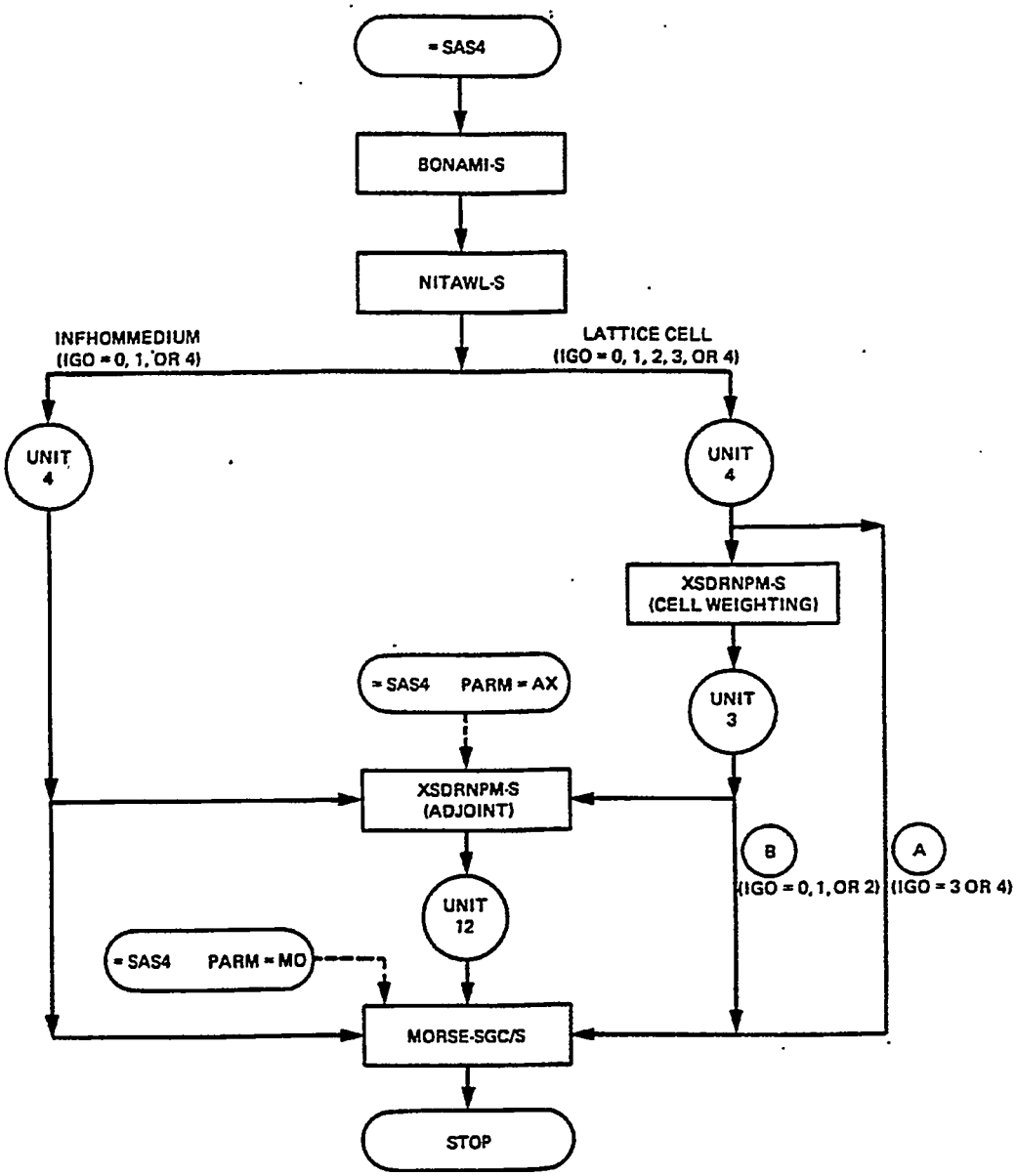
For the INFHOMMEDIUM option, SAS4 does not perform any homogenization or mixing of the fuel materials. The user must define all materials via the material information data and apply them accordingly in the adjoint discrete-ordinates calculation as well as the Monte Carlo calculation. Again, refer to Sect. S4.4.1 (Tables S4.4.2 and S4.4.4) and Sect. S4.4.2 for more details.

S4.2.4 SOURCE AND DETECTOR OPTIONS

In a Monte Carlo shielding calculation, the user must define the source parameters (position, energy, and direction) and the detector conditions (location, geometric shape, and response function) of the problem. SAS4 assumes source particles start isotropically in the source region (consisting of the active fuel and fuel hardware) with an energy spectrum specified by the user. The source spatial distribution is uniform in the hardware but may have an axial profile in the active fuel. SAS4 also provides four surface detectors in addition to the point detectors input by the user.

The cask model (described in Sect. S4.2.2) consists of the container and the source region. Although the source region may have many radial configurations, it is axially separated into three sections—the active fuel section and the fuel hardware sections on both ends of the active fuel. For the Monte Carlo calculation, source particles start in the volume of one of the two materials (active fuel and fuel hardware) in the source region. The user indicates his choice of starting material by supplying a value for the parameter ISO of the Monte Carlo input in Sect. S4.4.1 (Table S4.4.2). The source strength is assumed to be axially uniform over the fuel hardware, but for the active fuel an axial profile may be input via the IPF parameter in the Monte Carlo input data in Sect. S4.4.1 (Table S4.4.2). The IPF parameter determines the axial distribution of the active fuel region. It allows the user to select a distribution from the following three options: (1) a uniform distribution (IPF = 0); (2) a typical PWR axial profile for gamma or neutrons (IPF = $\pm$1); or (3) a user input axial profile (IPF > 1).

The IGO parameter of the Monte Carlo input in Sect. S4.4.1 (Table S4.4.2) satisfies two input functions: (1) it signals whether the simplified geometry input option (IGO $\leq$ 3) or the MARS geometry input option (IGO = 4) is to be used for geometry input; (2) if the simplified input is used, IGO indicates



For LATTICECELL option:

(A)– Cross-section data for explicit fuel-pin modeling in MORSE calculation with IGO=3 or 4 are read from Unit 4.

(B)– Cross-section data for homogenized-fuel modeling in MORSE calculation with IGO=0, 1, or 2 are read from Unit 3.

Figure S4.2.5 Calculational sequences of LATTICECELL and INFHOMMEDIUM options and data transfer among functional modules

the source region configuration for the problem. For IGO = 0 and 1, the radial position of source particles is sampled uniformly over the cross-section area of the source region. For IGO = 2, 3, and 4, a rejection procedure is used whereby source particle coordinates are determined by sampling uniformly within an appropriate volume and only points inside the correct material (active fuel or fuel hardware) are accepted.

The source energy spectrum is supplied to SAS4 either by direct input or from a file generated by ORIGEN-S. When the source energy spectrum is input via an ORIGEN-S file, it is imperative that the input file contain the appropriate neutron and/or gamma-ray spectra represented in the same multigroup cross-section structure used in the calculation.

Sometimes cask analysts exclude fission neutrons from the transport process and instead add them initially to the fixed source. The option of excluding fission neutrons in the transport process is allowed in SAS4. The user may invoke this option by setting IFS > 0 in the parameter card of the adjoint discrete-ordinates input. This approach of treating fission neutrons is an approximation and, although it perhaps may save some computing cost, it is discouraged because the correct treatment of fission is straightforward and handled directly in the SAS4 shielding calculation.

Two types of detectors are used in the Monte Carlo calculation: surface detectors and point detectors. The surface detectors are analog detectors that calculate averaged responses based on particles crossing the detector surfaces. The accuracy and precision of the responses depend on the number of particles and their respective weights crossing the detector surfaces. Four surface detectors are automatically implemented in the SAS4 Monte Carlo calculation. Depending on the direction of the transport calculation indicated by the IDR parameter in the adjoint discrete-ordinates input data (IDR = 0 for a radial calculation and IDR > 0 for an axial calculation), the surface detectors are located radially or axially on the outermost surface of the cask and 1, 2, and 3 m from this outermost surface.

The axial detectors are circular disks with radii FR1*RCAV cm for the first detector and are, respectively, FR2*(RCAV + 100), FR3*(RCAV + 100), and FR4*(RCAV + 100) cm for the other three detectors, where FR1, FR2, FR3, and FR4 are input parameters that allow the user to specify the size of the surface detectors, and RCAV is the radius of the cavity input by the user. The value of FR1, FR2, FR3, and FR4 should be greater than 0 and less than 1. Two sets of axial surface detectors are arranged symmetrically on the top and bottom ends of the geometry. Flux estimates are made on both sets of surfaces, and the averaged responses are computed for each detector in the Monte Carlo analysis. A similar method is used for the axial point detectors when IDR = 1. In Fig. S4.2.6, the top axial detectors are shown and labeled as detectors 1a through 4a. The radial detectors are side surfaces of cylinders having appropriate radii. As shown in Fig. S4.2.6, the radial detectors are detectors 1b through 4b. The heights of the radial detectors are, respectively, FR1*2*(HFUE), FR2*2*(HFUE + 100), FR3*2*(HFUE + 100) and FR4*2*(HFUE + 100) cm, where HFUE is the height of the active fuel measured from the midplane of the cask. The values of FR1, FR2, FR3, and FR4 should be such that sufficient histories will cross the surface detectors to obtain reasonable uncertainty. For axial detectors, 1.0 is recommended for all four. For radial detectors, recommended values are 1.0 for FR1 and 0.7 for the others.

In the Monte Carlo calculation, the four surface detectors are numbered as detectors 1 to 4 and the point detectors (if input) are numbered as detectors 5 to NOD+4, where NOD is the number of point detectors input in the parameter card of the Monte Carlo input data. Because of the method of particle tracking used by MORSE-SGC, a surface detector must be part of a surface between two different media or two different importance regions. In the geometries automatically generated by SAS4 for the simplified geometry input option (IGO ≤ 3), the four default surface detectors (radial or axial) are located on surfaces between different importance regions. As shown in Fig. S4.2.2, the surfaces of the impact limiters (top and bottom) are the outermost axial surfaces of the cask, and the surface of the water jacket is the outermost radial surface. Thus, the axial and radial surface doses, respectively, are scored on these surfaces. Similarly, the surface doses at 1, 2, and 3 m are scored on surfaces at the respective distances from the appropriate cask surface. To correctly calculate the cask surface doses, the following conditions must be satisfied: for an axial calculation, if the impact limiters are input by the user (see the cask geometry cards in Table S4.4.3 in

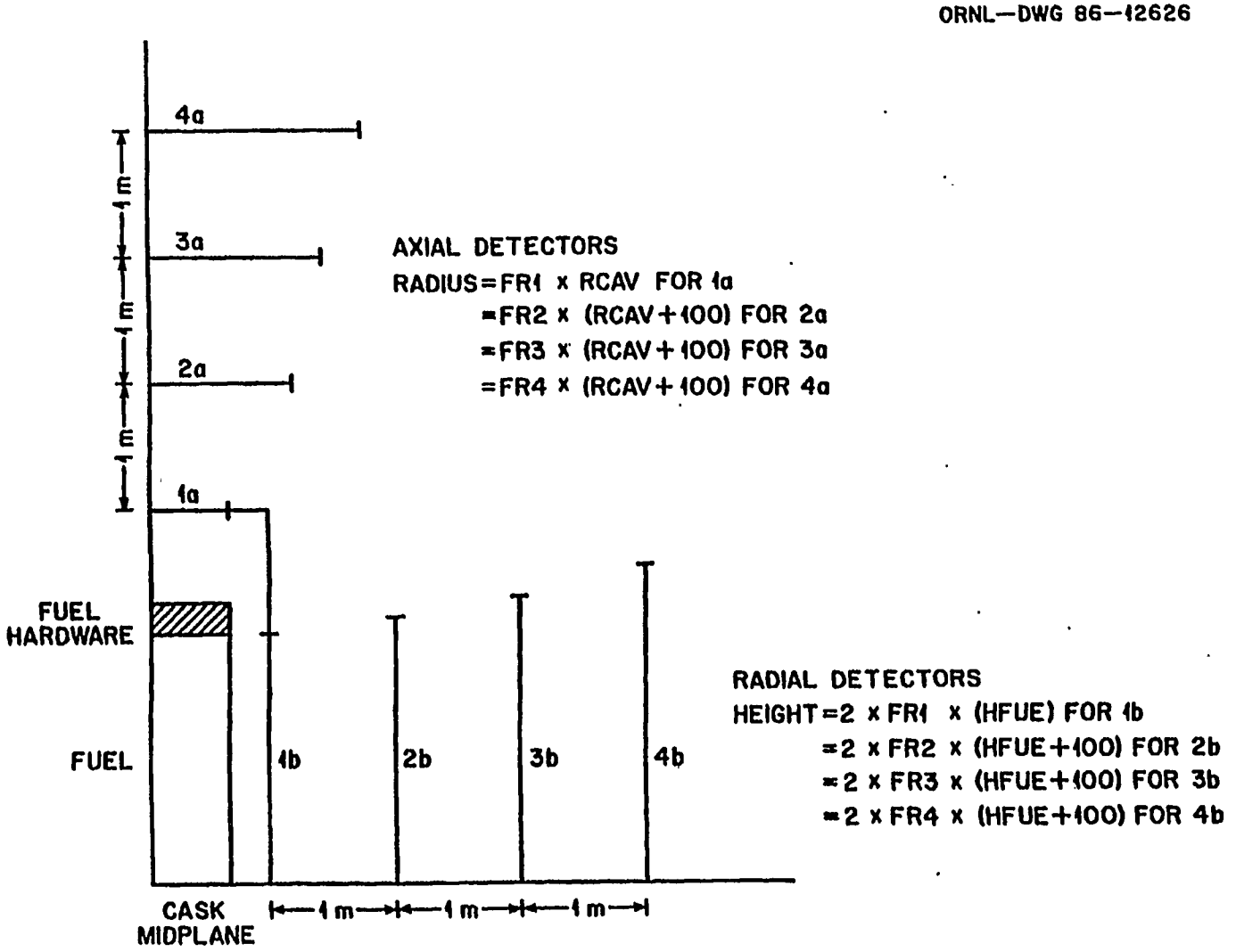


Figure S4.2.6 SAS4 default axial and radial surface detectors (only the top half is shown)

Sect. S4.4.1), the radius of the limiters RIMP must be greater than FR1*RCAV. For a radial calculation, if the water jacket is input, the height of the jacket HJAC must be greater than FR1*HFUE.

When using the geometry input option IGO = 4 to explicitly model a shipping cask, the user must include in the cask an outermost radial surface at radius RMAX and an outermost axial surface at height HMAX (see the source volume boundary array card in Table S4.4.2 of Sect. S4.4.1). Also, the height of the outermost radial surface must be greater than FR1*HFUE, and the radius of the outermost axial surface must be greater than FR1*RCAV. Furthermore, the user must include in the geometry three cylindrical surfaces with radii and heights, respectively, 1, 2, and 3 m away from the outermost cask surfaces. These surfaces should be enclosed in an internal void zone, which in turn is surrounded by an external void zone. Finally, the zones sharing any one of these four surfaces should be given different importance region numbers, preferably regions 1 and 2. The user is referred to sample problem 4 in Sect. S4.5 for an example of MARS geometry input.

The point detectors are input by the user. The user indicates the number of point detectors and their coordinates in the Monte Carlo input data. It is important that the positions of the point detectors (radial or axial) are consistent with the direction of the transport calculation indicated by the IDR parameter. For point detectors that lie within the axial projection of the cask cylinder, IDR should be set greater than zero to indicate a calculation with axial biasing. For point detectors located outside this projection, IDR should be zero, indicating a calculation with radial biasing. In a radial biasing calculation, next-event estimations are made from all collision and source points to the point detectors. In an axial biasing calculation, two options are available for next-event estimation to point detectors. The first option is IDR = 1, and next-event estimations are made from points that lie in the half (top of bottom half) of the cask nearest the detectors. This procedure assumes that contributions from collision and source points in the opposite half of the cask are negligible. The second option is IDR = 2, and next-event estimations are made from all points to the point detectors. With this option, source axial location biasing is not used, but particle transport is still biased axially away from the midplane and toward the top and bottom of the cask.

It is appropriate to discuss the application of the two axial options, IDR = 1 and 2. For spent fuel casks, the IDR = 1 option has calculated good results for axial point detectors. This is not surprising because spent fuel casks generally have large axial dimensions (greater than 4 m) and are filled with high-density materials. Therefore, the contribution from the opposite half of the cask can be ignored. Hence, this option is appropriate only for systems similar to spent fuel casks. For smaller systems with axial dimensions less than 3 m, or systems filled with low-density materials, the IDR = 2 option should be a better choice. Finally, note that of the two axial options the IDR = 2 option may consume a great deal more computation time due to estimation from the whole geometry.

The user is reminded that next-event estimations to point detectors can be very time consuming, especially if a heterogeneous fuel model is used. In a next-event estimation, tracking is made from a source or collision point to point detectors which are many mean-free paths away. Since tracking is the most time-consuming portion of Monte Carlo transport analysis, next-event estimation will significantly add on to the cost of a calculation.

The response functions are fluence-to-dose-rate conversion factors. The user can choose one from the SCALE standard response functions described in Table S4.2.1 or can specify a response function in the input.

Note that when neutron response is desired, only the neutron source spectrum is input. However, both neutron and gamma-ray source spectra must be input when the total gamma-ray response is to be calculated. Clearly, if the user wishes to calculate only the primary gamma-ray dose (dose contributed only by the gamma-ray source), the neutron source spectrum should be set to 0. On the other hand, if the secondary gamma-ray dose (dose contributed by neutron-captured gamma rays) is desired, the gamma-ray source spectrum should be set to 0.

Because of the automated biasing procedure in SAS4, neutron and gamma doses are computed in separate calculations. Also, different calculations are required for radial and axial detectors. Therefore, to obtain a full characterization of a spent fuel cask by SAS4, the user must perform at least four calculations. Two more calculations are needed if estimates of gamma doses contributed by the fuel hardware material are

Table S4.2.1 SCALE standard response function ID numbers

ID No.	Response function	Availability[a]
9001	Hurst dose factors (mrad/h)/(neutrons/cm^2/s)	1, 2, 5
9002	Snyder-Neufeld dose factors (mrad/h)/(neutrons/cm^2/s)	1, 2, 5
9026	Snyder-Neufeld conversion from flux to biological dose (mrem/h)/(neutrons/cm^2/s)	1, 2, 5
9027	Henderson conversion from neutron flux to absorbed dose rate in tissue (rad/h)/(neutrons/cm^2/s)	1, 2, 5
9028	Straker-Morrison conversion factors (mrem/h)/(neutrons/cm^2/s)	1
9029	ANSI standard neutron flux-to-dose-rate factors (rem/h)/(neutrons/cm^2/s)	1, 2, 3, 5, 6
9501	Straker-Morrison conversion factors (mR/h)/(photons/cm^2/s)	1, 4
9502	Henderson conversion factors (rad/h)/(photons/cm^2/s)	1, 2, 4
9503	Claiborne-Trubey conversion factors (rad/h)/(photons/cm^{2}2/s)	1, 2, 4
9504	ANSI standard gamma-ray flux-to-dose-rate factors (rem/h)/(photons/cm^2/s)	1, 2, 4

[a]Reference numbers of cross-section libraries:
1. 22N-18COUPLE
2. 27N-18COUPLE
3. 27BURNUPLIB
4. 18GROUPGAMMA
5. 123GROUPGMTH
6. 27GROUPNDF4

desired. Finally, the normal results output by MORSE-SGC are given in response-per-source-particle-per-second. To obtain the total response, the user must multiply MORSE's results by the total source strength in source-particles-per-second. For source particles originating from the active fuel, the total source strength is the source intensity in the full length of the fuel. For source particles originating from the fuel hardware, the total source strength is two times the source intensity in one end (top or bottom) of the fuel hardware being analyzed. In SAS4, a source strength factor, SFA, is included in the parameter card of the Monte Carlo input data. The MORSE-SGC results are automatically multiplied by this factor. Therefore, if SFA is set equal to the total source strength in source-per-second, all of the results output by MORSE-SGC are per total source strength.

S4.2.5 THE AUTOMATED BIASING PROCEDURE

This section is devoted to describing the automated biasing procedure in the MORSE-SGC calculation and explaining the setup of the adjoint XSDRNPM calculation with respect to the spent fuel cask geometry and the MORSE-SGC calculation. The reader is referred to Ref. 1 for the detailed theoretical developments on generation of the various biasing parameters from the adjoint fluxes and application of the biasing parameters in the MORSE-SGC code. The automated biasing procedure basically involves

1. calculation of adjoint fluxes of a simplified 1-D slab model of a cask using the XSDRNPM functional module,

2. processing of the adjoint fluxes into different biasing parameters by the SAS4 control module,

3. application of the biasing parameters to particle random walk in MORSE-SGC calculation, and

4. estimation of radiation doses exterior to the cask.

For Monte Carlo shielding analysis of a spent fuel cask, the purpose of biasing (or importance sampling) is to encourage and increase the propagation of radiation particles toward the cask outer surface so that better estimates of exterior doses can be obtained. Because nuclear fuel casks generally have a long, cylindrical shape, it is difficult to effectively bias particles toward all three sides of a cask. For this reason, the SAS4 Monte Carlo cask model is assumed to be symmetrical about the midplane. Even with the symmetric cask model, the characteristics of particle transport radially and axially may be drastically different because of the geometric shapes, the shielding materials, and possibly the streaming effect in the fuel materials. Because of these complications, the biasing procedure in the Monte Carlo calculation is applied separately for radial and axial detectors. For radial detectors, particle transport is biased radially toward the side. For axial detectors, particle transport is biased axially away from the midplane and toward the top or bottom surfaces.

For calculation of axial doses, the user should indicate an axial transport calculation in the input by setting the parameter IDR > 0 in the adjoint discrete-ordinates input. The adjoint XSDRNPM calculation will start with an adjoint source on the outermost axial surface, using the response function as the adjoint source spectrum. For calculation of radial doses, IDR is set to 0 and the adjoint source starts on the outermost radial surface. In either case, a 1-D slab geometry model is used in XSDRNPM, and each layer of material is identified as a zone. Hence, axially the user needs to input as many zones as the number of material layers along the axial direction starting from the midplane of the cask. The thickness of the first zone should be the height of the fuel measured from the midplane. Radially the entire source region is considered one zone and other material layers make up other zones in the radial direction. The thickness of the first zone should be the radius of the source region. For example, in Fig. S4.2.2, if the inner liner, the shields, and the outer liner are made of one material, they are treated as one zone in the adjoint XSDRNPM geometry. SAS4 uses the SAS2 automatic mesh generator (see Sect. S2.2.9) to generate spatial meshes for the adjoint XSDRNPM calculation. XSDRNPM outputs the adjoint angular fluxes and flux moments on logical unit 12,

which are subsequently converted by the control module to the appropriate biasing parameters for MORSE-SGC.

MORSE-SGC has several standard biasing options available to the user: source energy biasing, energy biasing at collision sites, splitting and Russian roulette, and path-length stretching. The efficiency of a calculation is determined by the proper specification of the biasing parameters. It has been shown[3,4] that a near-optimal importance function for selection of emergent particle parameters, that is, energy and direction of a particle emerging from a source or a collision point, is the adjoint flux. The event-value function has been shown[5,6] to be the proper biasing function for path-length selection. In SAS4, these adjoint functions in the form of angular fluxes and flux moments are calculated by the adjoint XSDRNPM using a slab geometry cask model and are used to specify the appropriate parameters for all the biasing schemes in MORSE-SGC.

SAS4 invokes most of the standard biasing options in MORSE-SGC for the cask shielding calculation. The importance regions in MORSE-SGC are determined by the control module, using the adjoint XSDRNPM zone boundaries as a starting point. Each zone in XSDRNPM corresponds to one or more importance regions in MORSE-SGC, depending on the approximate optical thickness of a zone. The importance functions are calculated from the adjoint functions and are spatially averaged over each importance region. The detailed generation of the importance functions is presented elsewhere. The importance functions for the biasing options are transmitted directly to MORSE-SGC by the input file, whereas the source position biasing function for axial calculation and the estimation probabilities for next-event estimations to point detectors are passed to MORSE-SGC through logical unit 96. The application of estimation probabilities to next-event estimations is a time-saving procedure and has been explained thoroughly in Ref. 1. Finally, for situations where azimuthal symmetry exists, point detectors are replaced by ring detectors to improve the efficiency of the calculation. This technique is explained elsewhere.

S4.3 PROGRAM FLOW AND SUBROUTINE DESCRIPTION

This section describes the logical flow of information through the SAS4 analytic sequence and the subroutines of this control module. The calculational sequence of this control module is outlined in Fig. S4.2.1. To accomplish the objectives of SAS4, more than 20 subroutines were written for the control module and about 10 subroutines in MORSE-SGC were modified or created. The subroutines of the control module are described in Sect. S4.3.1, and the subroutines of the MORSE-SGC functional module are presented in Sect. S4.3.2. The input/output units used by SAS4 are explained in Sect. S4.3.3.

S4.3.1 DESCRIPTION OF SAS4 SUBROUTINES

Subroutines of the SAS4 control module are presented in this section. Excluding the input/output (I/O) routines of the SCALE subroutine library, SAS4 is composed of 29 subroutines. Figure S4.3.1 provides a flow diagram of the SAS4 subroutines. The user is referred to the subroutine library in Sect. M2 for a detailed description of the following I/O routines: ALOCAT, AREAD, CLEAR, ERRO, FREAD, IREAD, LREAD, RSTPTR, SCANON, SCANOF, STOP, and ZREAD. The rest of the routines in Fig. S4.3.1 are described according to their logical order, starting with subroutine SAS4.

SAS4 is the executive routine for this control module. It calls C4DATA, READIN, AXDINP, and MORINP. It also checks the 'PARM=' parameter of the module specification card to allow two other entry points into SAS4 and to set the maximum number of words given to each functional module for execution.

C4DATA is described in detail in Sect. C4.3.3. It activates the Material Information Processor and opens the units that will be used to pass data to the functional modules. It has been modified to call AXSDRN.

AXSDRN is called by C4DATA to store material data on 11 records of logical unit 92. These data are needed for preparing input to the adjoint XSDRNPM and MORSE-SGC calculations.

VOLFRC is called to determine the volume fraction of a mixture in the unit cell.

READIN reads adjoint discrete-ordinates input and Monte Carlo input and writes them back on logical unit 91. It counts the number of input cards of both input streams and records them on logical unit 92.

AXDINP prepares input for the adjoint XSDRNPM calculation. The input is in binary format and is written on logical unit 98. It calls subroutines RESPFN, SIZCHK, MESHGE, and WRITXD.

RESPFN is called by AXDINP to read a response function from the SCALE response functions described in Table S4.2.1 of Sect. S4.2.4.

SIZCHK compares the size of the storage array with the storage size needed during setup of the storage area. If insufficient storage is encountered, error messages are printed indicating the additional needed storage and the exact location where the problem occurs.

MESHGE automatically generates spatial meshes for the adjoint XSDRNPM transport calculation, given the material and dimension of each zone.

WRITXD is called by AXDINP to write binary input on logical unit 98 for the adjoint XSDRNPM calculation.

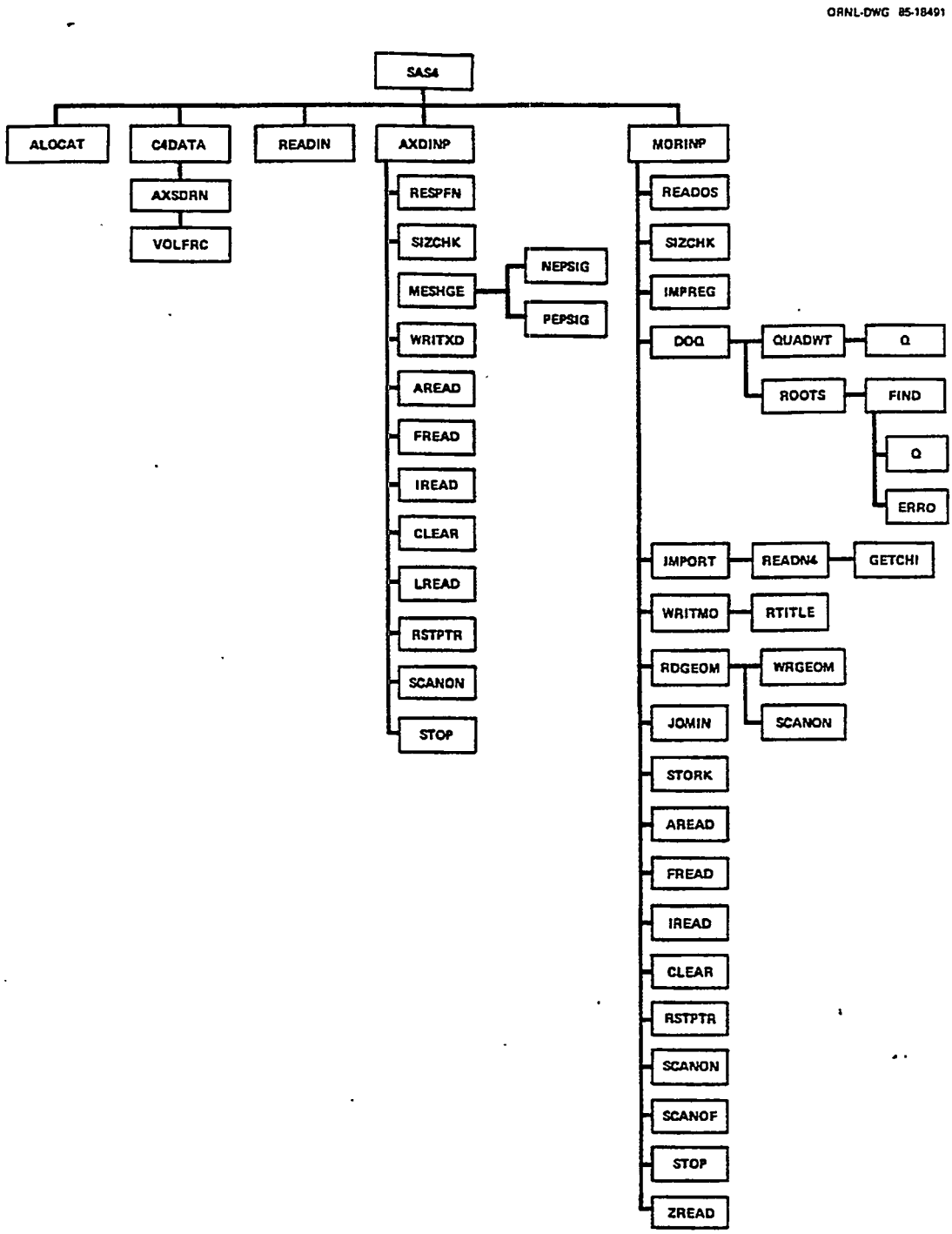


Figure S4.3.1 Flow diagram of SAS4 subroutines

NEPSIG is called by MESHGE to compute the epithermal asymptotic diffusion length of each mixture.

PEPSIG is called by MESHGE to compute a single total photon cross section (at 0.5 MeV) for each mixture.

MORINP is the input processor routine for the MORSE-SGC calculation. It reads SAS4 Monte Carlo input from logical unit 91, material mixing data from logical unit 92, and XSDRNPM adjoint fluxes from logical unit 12. Then it generates biasing parameters from the adjoint fluxes. Finally, it prepares binary MORSE-SGC input on logical unit 95. MORINP calls the following routines besides the SCALE I/O routines: READOS, SIZCHK, IMPREG, DOQ, IMPORT, WRITMO, RDGEOM, STORK, and JOMIN.

READOS is called by MORINP to read ORIGEN-S source spectra from logical unit 30.

IMPREG is called by MORINP. It subdivides any important regions, except region 1, which have numbers of intervals greater than MAXIN. MAXIN is initially set to 10, but may increase (if necessary) so that the number of subregions for each region will never be more than 4.

DOQ, QUADWT, Q, ROOTS, and FIND compute a quadrature set of the order specified through the arguments. Their description can be found in Sect. F3.3.

IMPORT generates biasing parameters for MORSE-SGC. It reads the adjoint angular fluxes and moments from logical unit 12. Then it calculates the region-averaged weight standards, path-length parameters, and source and collision energy biasing parameters. Finally, it writes on logical unit 96 six records of data which are used by MORSE-SGC for source spatial biasing and next-event estimation probability.

READN4 is called by IMPORT to read from logical unit 4 a fission spectrum of the uranium isotopes ^{235}U, ^{238}U, or ^{233}U. If a fission spectrum cannot be found, the spectrum array is set to 0.0.

GETCHI is called by READN4 to transfer data from one array to another array.

WRITMO is called by MORINP to write binary input for MORSE-SGC on logical unit 95.

RTITLE is called by WRITMO to provide the title of the response function IRF.

RDGEOM is called by MORINP to read the simplified geometry input and generates a detailed MARS geometry input of the cask for use by MORSE-SGC.

WRGEOM is called by RDGEOM to write the detailed MARS geometry input in card image on logical unit 91.

JOMIN is called by MORINP to read card-image MARS geometry data from logical unit 91 and to process the data into binary data.

STORK is called by MORINP to write two binary records of geometry data on logical unit 95.

S4.3.2 DESCRIPTION OF MORSE/SGC-S ROUTINES

To perform the Monte Carlo analysis of a shipping cask in SAS4, three new subroutines have been added to MORSE-SGC and nine subroutines have been modified. The new subroutines are SOURS4, NETLEV, and O0O106. The modified subroutines are DIREC, RELCOA, SDATA, SGAM, BDRYX,

NXTCOL, SOURCE, MAIN, O0O006, NDBTCH. When MORSE-SGC is called from SAS4, the variable JYPE in COMMON/SCALOP/ is set equal to 1. Through the value of JTYPE, MORSE-SGC will perform the special functions such as source sampling and biasing, importance region determination, and special estimation techniques required by SAS4. A detailed description of each of the 12 subroutines is given below. An additional description of the modified subroutines can be found in Sect. F9.B.1.

O0O106 is a new routine. It is the entry point to MORSE-SGC from SAS4. In this routine, JTYPE is set equal to 1 and ITYPE is set equal to 1.

O0O006 has been modified by setting JTYPE=0. O0O006 is the entry point to MORSE-SGC from the SAS3 control module.

MORSE has been modified by adding a statement JTYPE=0. It is the normal entry point to MORSE-SGC.

SOURCE has been modified to call SOURS4 if JTYPE=1. Other normal functions are unchanged.

SOURS4 is a new subroutine called by SOURCE. It generates source particle parameters for the cask model according to the source region geometry option IGO. The source particle distribution is uniform in the radial direction, but axially the source is uniform in the hardware and may have a profile in the active fuel. For an axial calculation with IDR = 1 and source particles originating from the fuel (ISO = 0), the axial position of the source particles is sampled from a biased distribution.

NXTCOL has been modified. Besides its normal function of determining the next collision site and optionally calling BDRYX, it determines for SAS4 the importance region of a collision point according to the distance from the point to the outer boundary of the cask.

NETLEV is a new subroutine. It converts the coordinates of a point from the global to the local coordinate system or vice versa, depending on the arguments it receives.

NDBTCH has been modified to print out responses by response functions and detectors at the end of each batch.

SDATA makes uncollided flux estimates from a source point to each detector. It has been modified to include an estimation probability when MORSE-SGC is executed through SAS4.

SGAM is similar to SDATA but an uncollided flux estimate is made from each secondary particle production point. Secondary particles are fission neutrons and captured gamma rays. SGAM has been modified to include an estimation probability when MORSE-SGC is executed by SAS4.

RELCOA makes next-event estimation from a collision point to each detector. For neutron collisions, estimates are made to each possible energy group. For gamma-ray collisions, a pair-production Klein-Nishina estimator is used. It has been modified to include an estimation probability when MORSE-SGC is executed by SAS4.

BDRYX is specifically written for SAS4. It returns immediately if JTYPE$\neq$1. It scores surface-averaged fluxes at four surfaces. Refer to Fig. S4.2.6 and Sect. S4.2.4 for more details of the surface detectors.

DIREC has been modified to accommodate the SAS4 module. Other normal functions remain unchanged.

S4.3.3 INPUT/OUTPUT LOGICAL UNITS AND CONTENTS

Fifteen logical units are used by SAS4. Table S4.3.1 gives a summary of these units and their creation and usage by various modules. Contents of logical units 92 and 96 are presented in Tables S4.3.2 and S4.3.3. The user might want to save the data in logical units 3, 4, and 12 because they are needed for execution of SAS4 via two other entry points. See Sect. S4.4.1 (Table S4.4.1) and Sect. S4.2.3 (Fig. S4.2.5) for the application of these units. If the user desires to examine the MARS geometry with the functional module PICTURE, the user must save the card-image geometry data in unit 91. At this point, the geometry data are put in the input stream of the PICTURE module for execution.

Table S4.3.1 Description of logical units used by SAS4

Unit No.	Type of data	Creating module	User module
1	AMPX master library	BONAMI	NITAWL-II
3	AMPX cell-weighted library	XSDRNPM	XSDRNPM, MORSE-SGC
4	AMPX working library	NITAWL-II	XSDRNPM, MORSE-SGC
5	Card input	DRIVER	
6	Printed output	All functional modules	All functional modules
12	XSDRNPM adjoint angular flux output	XSDRNPM-S	MORSE-SGC
16	MORSE geometry storage	MORSE-SGC	MORSE-SGC
17	MORSE scratch file	MORSE-SGC	MORSE-SGC
30	Source spectrum	ORIGEN-S	Control module
91	Scratch file to store card input later read by XSDRNPM and MORSE; also used by WRGEOM to store card-image MARS input	Control module	MORSE-SGC XSDRNPM
92	Scratch file to transfer cross-section and other data to XSDRNPM and MORSE	Control module	Control module
95	MORSE binary input	Control module	MORSE-SGC
96	BONAMI binary input; later used to transfer data to MORSE	Control module	BONAMI, MORSE-SGC
97	NITAWL binary input	Control module	NITAWL-II
98	XSDRNPM binary input	Control module	XSDRNPM

Table S4.3.2 Contents of logical unit 92[a]

Record No.	Contents	Comments
1	MMTBA,NNG,NGG,MXX,MXX1, MS,NNUC,(TITLE(I),I=1,20)	Written by AXSDRN
2	MFUEL,MMOD,MCLAD,MGAP,FUELOD, CLADOD,GAPOD,PITCH,IGEOM	Written by AXSDRN
3	LMIX(I),I=1,MS	Records 3 to 5 written by AXSDRN before cell averaging; they are used to form mixing tables for geometry options IGO = 3 and 4 of LATTICECELL option and all and all IGO options of INFHOMMEDIUM option
4	LMID(I),I=1,MS	
5	ADEN(I),I=1,MS	
6	LMIX(I),I=1,MS	Records 6 to 8 written by AXSDRN after cell averaging; they are used to form mixing tables for geometry options IGO = 0, 1 and 2 of LATTICECELL option records 9 to 11 written by AXSDRN; they are used to generate spatial meshes for adjoint XSDRN
7	LMID(I)I=1	
8	ADEN(I),I=1,MS	
9	FSIGS(I),I=1,MS	
10	FSIGT(I),I=1,MS	
11	FAM(I),I=1,MS	
12	ISCARD,MOCARD	Written by READIN
13	NASY,NCEL,NVAC,MSPA,MCAN, MBET,MZ1,MHWR,TCAN,XY,FR	Records 13 to 22 are written by AXDINP
14	ACEL,AARR,AFCL,AVAC,ASPA,ACAN	
15	IDR,ITY,IRF,IGRESP,IM,IZM,ISN, IFS,MSP,MXXP	
16	D(LRES+I-1),I=1,IGRESP	
17	D(LRN+I-1),I=1,IMP1	
18	D(LNZ+I-1),I=1,IM	
19	D(LZB+I-1),I=1,IZM	
20	LMIX(I),I=1,MSP	Records 20 to 22 are written after cell averaging and fuel zone homogenization; they are used to form mixing table for geometry opton IGO = 0 of LATTICECELL option
21	LMID(I),I=1,MSP	
22	ADEN(I),I=1,MSP	

[a]Note: AXDINP reads the first 12 records, and MORINP reads all the records.

Table S4.3.3 Contents of logical unit 96[a]

Record No.	Contents	Comments
1	IDR,IRF,IZM,IGO,INTFZ, ISO,MFUEL,MHWR	Records 1 to 6 are written by IMPORT
2	ZB(I),I=1,IZM	
3	PROB(I),I=1,IZM	
4	DEL(IM),IM=1,INTFZ	
5	RN(IM),IM=1,INTFZ	
6	FLUX(IM,IG),IM-1,INTFZ,IG=1,NGPFS	
7	If IGO=0, RFUE,HFUE,HHWR	Written by RDGEOM
	If IGO=1, RIN(I),ROUT(I),HFUE,HHWR, I=1,3	Written by RDGEOM
	If IGO=2 or 3, APCH,HFUE,HHWR,MXX	Written by RDGEOM
	If IGO=4, XMIN,XMAX,YMIN,YMAX, ZMIN,ZMAX,HFUE	Written by MORINP
8	RJAC,RCAV,HIM1,SFA,FR1,FR2, FR3,FR4,MSM,IPF	Written by MORINP
	If IPF.GT.0	
9	D(LBUB+I-1),I=1,IPF	Written by MORINP
10	D(LBUF+I-1),I=1,IPF	Written by MORINP

[a]Note: All ten records are read by SOURS4 in MORSE-SGC.

S4.4 INPUT DATA DESCRIPTION

This section describes input data for the SAS4 control module. Similar to other control modules in SCALE, the input data of SAS4 begin with the module specification card and end with the module termination card. The bulk of the input is composed of the Material Information Processor data, the adjoint discrete-ordinates data, and the Monte Carlo data. Table S4.4.1 gives a summary of the input data, and Fig. S4.2.1 illustrates the various calculational paths of the SAS4 module. There are three entry points into the SAS4 analytic sequence. Figure S4.2.5 and Table S4.4.1 illustrate these entry points and the necessary logical units for data transfer among the functional modules.

All data are entered in free form (i.e., alphanumeric, floating-point, and integer data can be entered in an unstructured manner). All 80 columns of any card may be used. Data can usually start or end in any column. Each data entry must be followed by one or more blanks (a comma can also be used in place of a blank for numeric entries) to terminate the data entry. Integers may be entered for floating values. For example, 10 will be interpreted as 10.0. Imbedded blanks are not allowed within a data entry unless an E precedes a single blank as in an unsigned exponent in a floating-point number. For example, 1.0E 4 would be correctly interpreted as 1.0×10^4.

Multiple entries of the same data value can be achieved by entering the number of repeats, followed by either R, *, or $, followed by the data value to be repeated. Imbedded blanks are not allowed between the number of repeats and the repeat flag. For example, 5R12, 5*12, 5$12, or 5R 12, etc., will enter five successive 12s in the input data. Multiple zeroes can be specified as nZ, where n is the number of zeroes to be repeated. The SCALE free-form reading routines are described in more detail in Sect. M3.

S4.4.1 INPUT DATA SUMMARY

SAS4 uses a simplified input procedure similar to other control modules in SCALE. The input to SAS4 basically consists of three parts: (1) material information data, (2) adjoint discrete-ordinates input data, and (3) Monte Carlo input data. Input data for SAS4 are outlined in Table S4.4.1 and are elaborated in Tables S4.4.2 and S4.4.3. Cask and fuel assembly models corresponding to the geometric input are provided in Figs. S4.4.1 and S4.4.2. Basically, the SAS4 control module is made up of five functional modules, namely: BONAMI, NITAWL-II, XSDRNPM, XSDRNPM, and MORSE-SGC. The BONAMI and NITAWL-II functional modules perform resonance self-shielding calculations. The first XSDRNPM functional module performs cell-weighting calculations for the LATTICECELL option. The second XSDRNPM functional module performs an adjoint 1-D slab geometry transport calculation, which provides the adjoint functions necessary for generating importance sampling parameters for subsequent Monte Carlo analysis. The MORSE-SGC functional module performs a Monte Carlo shielding analysis of a cask.

Besides the basic calculational sequence through the functional modules described in the preceding, SAS4 can be executed via two other entry points, indicated in Figs. S4.2.1 (Sect. S4.2.1) and S4.2.5 (Sect. S4.2.3), by using the PARM= feature in the module specification card. This feature allows users to start SAS4 calculations without having to repeat the functional modules that have been previously executed. The module specification card, the functional modules executed, and the logical units required to transfer data for all entry points are described in Table S4.4.1 and Fig. S4.2.5 (Sect. S4.2.3). Except for the module specification card, the same input data are required for the same problem for SAS4 regardless of the entry point to the module. Finally, if the user desires to save the MARS geometry input generated by SAS4 for use in the PICTURE functional module, the user must save the content of logical unit 91 on a storage device.

The PARM= feature in the module specification card is also used to set the maximum number of words given to each functional module for execution. It overrides the default value of each functional module. A few examples of this option are as follows:

Table S4.4.1 Summary of SAS4 input data

	Type of data	Functional modules executed	Data files required from previous SAS4 calculation
1.	Module specification		
	=SAS4	BONAMI,NITAWL-II,(XSDRNPM), XSDRNPM,MORSE-SGC	None
	=SAS4 [a]PARM=AX	XSDRNPM,MORSE-SGC	Cross sections from units 3 and 4 for the LATTICECELL option and from unit 4 for the INFHOMMEDIUM option
	=SAS4 [a]PARM=MO	MORSE-SGC	Cross sections from units 3 and 4 or just 4 as above, and adjoint angular flux from unit 12
2.	Material information processor data		
3.	Adjoint discrete-ordinates data		
4.	Monte Carlo data		
5.	Module termination END		

[a]The "P" starts from column 11 or beyond.

Table S4.4.2 SAS4 input data requirements

Name or keyword	Definitions, comments, and examples
	Module specification and material information processor data
=SAS4[a]	Module specification starting at column 1. Use the PARM= feature for execution from other entry points. The "P" must start from column 11 or beyond
TITLE	An 80-character title
LIB	Name of cross-section library; e.g., 27N-18COUPLE, 22N-18COUPLE, etc. See Sect. M4 and Table S4.2.1 in Sect. S4.2.4 for more details. For neutron dose (ITY = 1), may use a neutron or a neutron-gamma coupled library. For gamma dose (ITY = 2), must use a neutron-gamma coupled library
GE	Type of fuel lattice. Must be LATTICECELL or INFHOMMEDIUM. For spent fuel assemblies LATTICECELL is recommended. For consolidated fuel or other tightly packed fuels, INFHOMMEDIUM is recommended (see Sects. S4.2.3 and S4.4.2 for more details)
Standard compositions specification data. (See Sect. M7.4.4 and Table M7.4.5 for additional detail and information on making arbitrary material mixtures. See Sects. S4.2.3 and S4.4.2 for application of material mixtures.)	
SC	Component name from standard composition library (see Sect. M8)
MX	Mixture number of SC
VF	Volume fraction. Enter 0 if SC is an isotope or element
ADEN	Atom density, atoms/barn-cm. Enter only if VF = 0
TEMP	Temperature, K. May omit if END is next (293)
IZA	SCALE ZA number. Omit if VF = 0 (see Table M8.2.1)
WTP	Wt % for IZA. Omit if VF = 0. Repeat IZA-WTP pairs for 100% sum
END*	End of this SC data. Repeat for all SC of case
	Examples: U02 1 0.94 1000 92235 3.1 92238 96.9 END FE 4 0 4.2-3 END SS304 6 END
END COMP*	Ends entire material data input
Unit cell geometry specification (omit for INFHOMMEDIUM)	
CPT	Type of rod-lattice. Must be SQUAREPITCH
PITCH	Center-to-center spacing between fuel pins, cm For IGO = 3, PITCH must be less than four significant figures (otherwise, SAS4 may have difficulty generating the geometry input for MORSE-SGC because of numerical roundoff)
FUELOD	Outside diam of fuel pin, cm

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Module specification and material information processor data (continued)
MFUEL	Mixture number of fuel
MMOD	Moderator mixture number
CLADOD	Clad outside diam, cm
MCLAD	Clad mixture number
CLADID	Clad inside diameter, cm (omit this and next entry if no gap)
MGAP	Gap mixture number, if gap (always 0)
END	End of unit cell specification
Optional parameter data (omit for INFHOMMEDIUM)	
MORE DATA*	(The following entries may be in any order but must be terminated by END)
SZF=*	Spatial mesh factor. SZF < 1 for finer; >1 for coarser mesh (1)
ISN=*	Order of angular quadrature (8)
IIM=*	Maximum number of inner iterations (20)
ICM=*	Maximum number of outer iterations (25)
EPS=*	Overall convergence criteria (0.0001)
PTC=*	Scalar flux point convergence (0.0001)
IUS=*	IUS = 1, upscatter scaling applied to speed convergence; 0, no scaling applied (0)
END*	End of option Example: MORE DATA ISN=16 SZF=0.9 END
	Adjoint discrete-ordinates input data
Parameter Card (Entries in this card can be in any order, but must be terminated by END)	
IDR=*	Direction of transport calculation. IDR = 0 for radial calculation; IDR > 0 for axial calculation (0). For axial calculation with IDR = 1, next-event point-detector estimation is made from half of the system, with the opposite half ignored. For IDR = 2, estimation is made from the whole system. Estimation probabilities are used for all three IDR options. See Sect. S4.2.4 for discussion on selection of IDR option.
ITY=*	Type of response. ITY = 1 for neutron response; ITY = 2 for gamma-ray response (2).
IZM=*	Number of separate material zones (must be input). IZM≥2 for IDR = 0 and ≥3 for IDR > 0.
ISN=*	Order of quadrature set (8)
IRF=*	Identification number of response function (flux-to-dose-rate factor) in Table S4.2.1. If IRF < 0, response function array RES() must be input by the user. The defaults are ANSI standard response functions: IRF=9029 for neutron and 9504 for gamma ray.
IFS=*	IFS > 0 means no neutron fission in the adjoint XSDRNPM and MORSE-SGC calculations (0). The user should use the default value of 0 unless fission is accounted for by other means.
MHW=*	Mixture number of the fuel hardware material (0). A zero indicates void. The SAS4 shipping cask model assumes a fuel hardware material at both ends of the active fuel (see Fig. S4.2.3 in Sect. S4.2.2). The purpose of this feature is to allow calculations of dose rates contributed by the activated materials in the fuel hardware.

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Adjoint discrete-ordinates input data (continued)
	For the LATTICECELL option, MHW represents the material at both ends of a fuel rod. It is normally a homogeneous mixture of any of the following materials: cladding, plenum spring, end fitting, and expansion spring, etc. The atomic densities of the constituents should be calculated based on the outside diameter of the fuel rod CLADOD and the length of the hardware material HHWR-HFUE. For this option, mixture number MHW should be used only for the fuel hardware material and not for any other materials in the geometry For the INFHOMMEDIUM option, MHW is the mixture at both ends of the fuel zone of height HHWR-HFUE. For this option and IGO = 4, MHW is not used and need not be input
FRD=*	Radius of the fuel zone (must be input). For the LATTICECELL option, (π*FRD*FRD) must be equal to or greater than (NASY*XY*XY), where XY is the outside dimension of a fuel unit (see Fig. S4.2.3) FRD is the radius of the fuel zone (source region) of the Monte Carlo calculation with IGO = 0 For IDR = 0 (radial calculation), FRD = ZB(1) in the zone boundary array FRD < RINS where RINS is the radius of the insert. If the insert is omitted, FRD < (RCAV-0.001), where RCAV is the radius of the cavity
SZF=*	Spatial mesh factor. SZF < L for finer mesh; SZF > L for coarser mesh (1)
END*	End of parameter card
	Fuel assembly card (must be omitted for INFHOMMEDIUM option. Eight entries ended with the keyword END. Refer to Fig. S4.4.2 for an assembly model and Sect. S4.4.2 for more description)
NASY	Number of assemblies in the cask. If IGO = 2 or 3 in Monte Carlo input, NASY must be one of the following: 1, 2, 3, 4, 7, 10, 18, 24, or 52
NCEL	Number of unit cells on each side of an assembly (17 for a 17 × 17 PWR assembly)
NVAC	Number of vacant cells in an assembly (25 for a typical 17 × 17 PWR assembly)
MSPA	Mixture number of the vacant cells and of the spacing between the outermost cells and the fuel channel (typically water or air). A zero may be used to indicate void
MCAN	Mixture number of the fuel channel. A zero may be used to indicate void
MBET	Mixture number of the material between assemblies. A zero may be used to indicate void
TCAN	Thickness of the fuel channel, cm
XY	Outside dimension of a fuel assembly, cm
END*	Terminates the fuel zone card For IGO = 1, the material of MBET must be identical to that of the insert, MINS (or of the cavity MCAV, if the insert is omitted)

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Adjoint discrete-ordinates input data (continued)
Zone boundary array (ZB(I),I=1,IZM), END* - outer boundary of each material zone in cm. Must have IZM entries followed by the keyword END	
ZONE MIXTURE ARRAY (MZ(I),I=1,IZM),END* - Mixture number of zone 1 to IZM. Must have IZM entries followed by the keyword END. A zero mixture number is allowed to indicate a void zone. For the INFHOMMEDIUM option, all MZ(1)'s should not be greater than MXX where MXX is the total number of mixtures input in the material information processor. For the LATTICECELL option, MZ(1) is the fuel zone and is set to MXX2 = MXX+2 regardless of the input value. For the LATTICECELL option and IDR > 0 MZ(2) is the fuel hardware zone and is set to MXX3 = MXX+3. All other MZ(1)'s should not be greater than MXX and not equal to MSPA, MCAN, MBET, MHW, or any mixtures in the unit cell description (MFUL, MMOD, MCLAD, and MGAP). For this option, SAS4 performs cell calculation to create a cell-averaged mixture, MXX1 = MXX+1, for the fuel cell. In the adjoint discrete-ordinates calculation, MZ(1) is composed of mixtures MXX1, MSPA, MCAN, and MBET and is given a mixture number MXX2 = MXX+2. Mixture number MXX3 is composed of mixtures MHW, MSPA, MCAN, and MBET. See Table S4.4.4 for mixture number assignment of the fuel and the fuel hardware zones	
Response function array (enter only if IRF < 0) (RES(I),I=1,IGRESP), END* - Must be IGRESP entries followed by the keyword END, where IGRESP equals to the number of neutron energy groups for ITY = 1 or gamma-ray energy groups for ITY = 2	
XEND*	Termination card for adjoint discrete-ordinates input. Must start from column one.
	Monte Carlo input data
Parameter card	(entries in this card can be in any order, but must be terminated by END)
RAN=*	RANDOM, starting random number in Z12 format for IBM (0000129A7A13)
TIM=*	TMAX, computing time allowed for MORSE run in minutes (1.0)
NST=*	NSTRT, number of source particles per batch (100). 100 is recommended for neutron response, and 500 is recommended for gamma response
NMT=*	NMOST, maximum number of particles allowed (4*NST). NMT should be at least 2*NST
NIT=*	NITS, number of batches for this run (100)
NCO=*	NCOEF, number of Legendre coefficients for each mixture, including $P_o(4)$
IST=*	ISTR, switch to print the cross sections as they are stored if >0 (0). Beware that large amount of output is generated when IST > 0
IPR=*	IPRIN, switch to print the discrete scattering angles and probabilities if >0 (0). Beware that large amount of output is generated when IPR > 0

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Monte Carlo input data (continued)
ISO=*	Source location starting option. If ISO = 0, source starts from the active fuel. If ISO > 0, source starts from the fuel hardware above and below the active fuel (0)
NOD=*	Number of point detectors (0)
SFA=*	Source normalization factor (1.0). This is the total source strength (particles/second) multiplied to the MORSE-SGC results. Refer to the last paragraph of Sect. S4.2.4 for discussion on source normalization
FR1=*	Fraction multiplied to the first surface detector (1.0). Must be greater than zero and not greater than 1.0. The value 1.0 is recommended for either axial or radial detector. See Sect. S4.2.4 and Fig. S4.2.6
FR2=*	Fraction multiplied to the second surface detector (1.0). Must be greater than zero and not greater than 1.0. Recommended value is 1.0 for the axial detector and 0.7 for the radial detector
FR3=*	Fraction multiplied to the third surface detector (1.0). Condition and recommended value are identical to those of FR2
FR4=*	Fraction multiplied to the fourth surface detector (1.0). Condition and recommended value are identical to those of FR2
IGO=*	Flag for geometry input option and source region geometry (0) See Figs. S4.2.3 and S4.2.4 for geometries of the source region for IGO = 0, 1, 2, and 3 For LATTICECELL option, IGO can have a value between 0 to 4 For INFHOMMEDIUM option, IGO can only be 0, 1, or 4 **For IGO = 0,** simplified geometry input option is used, and the fuel is a cylinder of homogenized mixture, which is the same fuel mixture used in the adjoint XSDRNPM calculation. As previously described in the zone mixture array of the adjoint discrete-ordinates input, for the LATTICECELL option the fuel mixture is MXX2 and is composed of MSPA, MCAN, MBET, and MXX1, where MXX1 is the cell-averaged mixture of the unit fuel cell. The hardware zone is given a mixture number MXX3 = MXX+3, and is composed of mixtures MHW, MSPA, MCAN, and MBET. For the INFHOMMEDIUM option, the fuel mixture is MZ(1) in the zone mixture array. The hardware zone is mixture MHW. See Table S4.4.4 **For IGO = 1,** simplified geometry input option is used, and the fuel is two or three concentric cylinders with mixture MINS (or MCAV if the insert is omitted) in between. For the LATTICECELL option, the fuel mixture is MXX2P = MXX+2 and is composed of MSPA, MCAN, and MXX1, where MXX1 is also the cellaveraged mixture of the unit fuel cell. The hardware zone is given a mixture number MXX3P = MXX+3, and is composed of mixtures MHW, MSPA, and MCAN. Furthermore, the volume of each fuel region should be an integer multiple of the fuel assembly volume. For the INFHOMMEDIUM option, the fuel mixture is MFU input by the user and the hardware mixture is MHW **For IGO = 2,** simplified geometry input option is used with each fuel assembly modeled separately. The INFHOMMEDIUM fuel option is not allowed. In each assembly, the mixtures inside the fuel channel are homogenized. For the active fuel section, this homogenized mixture is given a mixture number,

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Monte Carlo input data (continued)
	MXX2Q = MXX+2, and is composed of mixtures MSPA and MXX1, where MXX1 has been previously defined. For the hardware sections, the homogenized mixture is given a mixture number MXX3Q = MXX+3 and is composed of mixtures MHW and MSPA. For this option, NASY in the fuel assembly card of the adjoint discrete-ordinates input must be one of the following: 1, 2, 3, 4, 7, 10, 18, 24, or 52 **For IGO = 3,** simplified geometry input option is used, but unlike the last option, each fuel assembly is modeled in great detail with each fuel rod represented explicitly. The INFHOMMEDIUM fuel option is not allowed. All fuel assemblies are assumed to be identical and contain no vacant cells. If the number of vacant cells, NVAC, in the fuel assembly card of the adjoint discrete-ordinates input, is not zero, the radial dimensions of each fuel rod are reduced in order to conserve the total mass of the fuel material in each assembly. For this option, NASY in the fuel assembly card of the adjoint discrete-ordinates input must be one of the following: 1, 2, 3, 4, 7, 10, 18, 24, or 52. **For IGO = 4,** detailed MARS geometry must be input by the user
MFU=*	Fuel mixture number must be input when the INFHOMMEDIUM option is used and IGO = 1
ISP=*	A flag for source energy spectrum input option (0) **For ISP = 0,** the source energy spectrum is input via the SOE array **For ISP = N,** the source energy spectrum written by ORIGEN-S is read from logical unit 30 and N is the position of the pair of records containing data (including the source energy spectrum) of a time step of ORIGEN-S results. The user must make sure that ORIGEN-S spectrum is in the same multigroup structure as the one used in SAS4
IPF=*	Flag for source axial profile input option in the active fuel (0) For source in the hardware (ISO > 0), IPF is irrelevant because only uniform distribution is allowed in the hardware For IPF = 0, a flat axial profile is used For IPF = 1, default top profiles are used For IPF = -1, default bottom profiles are used The default axial profiles are typical of neutron and gamma sources for PWR with half active fuel length of 182.88 cm (6 ft). The default profiles are shown in Table S4.4.5. **For IPF > 1,** the user must input axial boundary array BUB and the corresponding source strength array BUF. Linear interpolation is assumed between the data points. IPF is the length of BUB and BUF arrays and must be less than 300. The user is reminded that when the axial profile is input, the height of the profile must be equal to HFUE in the fuel geometry card(s) or in the source volume boundary array. HFUE is the height of the active fuel measured from the midplane of the geometry. For PWR, HFUE is equal to 182.88 cm. If the height of the axial profile is not equal to HFUE, execution will be terminated and an error message will be printed.
END*	Terminates the parameter card

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Monte Carlo input data (continued)
Source energy spectrum array (must be skipped if ISP > O)	
SOE*,(FS(I),I=1,NGPFS), END*	– Begins with the keyword SOE and ends with the keyword END. FS(I) is the source for group 1, and NGPFS is the number of entries. FS(I) need not be normalized. NGPFS equals to the number of neutron groups when neutron response is desired; that is, ITY = 1 in the adjoint discrete-ordinates input data. NGPFS equals to the sum of neutron and gamma-ray groups when gamma-ray response is desired (i.e., ITY = 2)
Point detector array (must be skipped if NOD = 0)	
DET*,((XD(I),YD(I),ZD(I)),I=1,NOD), END*	– Begins with the keyword DET and ends with the keyword END. XD, YD, ZD are the detector coordinates with respect to the geometric center of the cask. Must have 3*NOD entries between the keywords
Source volume boundary array (enter only if IGO = 4)	
SXY* MSM XMIN,XMAX,YMIN,YMAX,ZMIN,ZMAX,RCAV,HFUE,RMAX,HMAX END*	Begins with the keyword SXY, ends with the keywords END, and has 11 entries in between. MSM is the mixture number from which source particles start. XMIN, XMAX, YMIN, YMAX, ZMIN, and ZMAX define the boundaries of the upper half of the source volume. Therefore, both ZMIN and ZMAX must be positive, and ZMAX must be greater than ZMIN. ZMIN must equal to zero for source starts from the active fuel (ISO = 0). The mixture number, combined with the source volume boundaries, provide a procedure for random sampling of source particles starting coordinates in a relatively complicated heterogeneous source geometry. Since source points sampled from the specified volume must also be in mixture MSM to be valid source particles, the user must make sure that mixture MSM does exist in the volume specified by the source volume boundary array and the source location starting option ISO is consistent with the source volume boundaries. Otherwise, no source particles will be generated to start the calculation and the calculation is aborted. RCAV is the radius of the cask cavity and is used to determine the radii of the axial surface detectors. HFUE is the height of the active fuel measured from the cask midplane and is used to determine the heights of the radial surface detectors. RMAX is the radius of the outermost radial surface of the cask where the radial surface dose is desired. HMAX is the height of the outermost axial surface of the cask where the axial surface dose is desired. For the SAS4 cask model shown in Fig. S4.4.2, RMAX = RJAC and HMAX = HIM1. See Sects. S4.2.2 and S4.2.4 for more details
Axial source profile boundary array (enter only if ISO = 0 and IPF > 1)	
BUB*, (BB(I),I=1,IPF), END*	– Begins with the keyword BUB and ends with the keyword END. BB(I) is the boundary for the axial source profile measured from the midplane of the cask. Therefore, BB(1) must be zero and BB(IPF) must be equal to HFUE, the height of the active fuel measured from the midplane. IPF is the number of entries and must be greater than one

Table S4.4.2 (continued)

Name or keyword	Definitions, comments, and examples
	Monte Carlo input data (continued)
Axial source profile array (enter only if ISO = 0 and IPF > 1)	
BUF*, (PP(I),I=1,IPF), END*	– Begins with the keyword BUF and ends with the keyword END. PP(I) is the source strength corresponding to boundary BB(I). Linear interpolation is assumed for PP between the boundaries. In principle, PP(IPF) is zero for spent fuel, but SAS4 will run for any reasonable axial source profile
GEND*	Termination card for Monte Carlo nongeometry input data, starting from column one
Monte Carlo geometry input	For IGO = 0, 1, 2, or 3, input simplified geometry data (see Table S4.4.3). For IGO = 4, input detailed MARS geometry. See Sect. S4.2.2 for the conditions that the cask must satisfy, and Sect. M9.A for MARS input
END*	SAS4 module termination card. Must start from column one

* = Keywords that must be part of the input data entry.

Table S4.4.3 Simplified Monte Carlo geometry input

Geometry title card

A 60-character (or less) title for geometry

Fuel geometry cards

For IGO = 0: (one cylindrical fuel zone with radius FRD)

FUE* HFUE HHWR END* - Begins with the keyword FUE and ends with the keyword END. HFUE and HHWR are, respectively, the heights of the fuel zone and fuel hardware, measured from the midplane of the cask geometry. The following conditions must be satisfied

1. HFUE < HHWR
2. HHWR < HINS, where HINS is the height of the fuel insert
3. If the insert is omitted, HHWR < (HCAV - 0.001), where HCAV is the height of the cavity

For IGO = 1: (two or three concentric cylindrical fuel zones)

FU1* RIN(1) ROUT(1) HFUE HHWR END*
FU2* RIN(2) ROUT(2) HFUE HHWR END*
FU3* RIN(3) ROUT(3) HFUE HHWR END*

FU1, FU2, FU3, and END are keywords. HFUE and HHWR are as defined above. RIN(I) is the inner radius of fuel zone I, and ROUT(I) is the outer radius of fuel zone I. The FU3 card may be omitted if there are only two concentric cylindrical fuel zones. The following conditions must be satisfied

1. HFUE < HHWR, and HHWR < HINS
2. RIN(I) < ROUT(I) < RIN(I + 1)
3. ROUT(3) < RINS, where RINS is the radius of the insert
4. If the insert is omitted, ROUT(3) < (RCAV-0.001) and HHWR < (HCAV-0.001)
5. If the FU3 card is omitted when only two fuel zones are present, ROUT(2) < (RINS-0.002)
6. If both the FU3 card and insert are omitted, ROUT(2) < (RCAV-0.003) and HHWR < (HCAV-0.001)

For IGO = 2 or 3: (separate representation of fuel assemblies, homogenized, or explicit fuel pins)

HET* APCH HFUE HHWR END* - HET and END are keywords. APCH is the distance between the centers of assemblies. The following conditions must be satisfied:

1. HFUE < HHWR, and HHWR < HINS
2. If the insert is omitted, HHWR < (HCAV - 0.001)
3. APCH > XY, where XY is the outside dimension of a fuel assembly input by the user in the fuel assembly card of the adjoint discrete-ordinates input. APCH must be less than 4 significant figures. Otherwise, geometry error may occur due to numerical roundoff
4. k*APCH < 2*RINS, where k is a parameter depending on the number of assemblies NASY input in the fuel assembly card of the adjoint discrete-ordinates input. If the insert is omitted, k*APCH < 2*(RCAV - 0.001). The table below gives the value of k as a function of NASY

NASY	1	2	3	4	7	10	18	24	52
k	1.42	2.24	2.59	2.83	3.61	4.25	5.66	6.33	8.95

Termination card for fuel geometry

FEND* Starts from column one

Table S4.4.3 (continued)

Cask geometry cards (input one component per card in any order; see Fig. S4.4.1 for details).

Component	Keyword	Mixture	Radius	Height
Inner shell	INN[a]	MINN	RINN(<RRS1)[b]	HINN(<HAS1)	END[a]
Radial shield 1	RS1[a]	MRS1	RRS1(<RRS2)	HRS1(<HAS3)	END[a]
Radial shield 2[c]	RS2[a]	MRS2	RRS2(<RRS3)[RRS1+0.001][d]	HRS2(=HRS1)[HRS1]	END[a]
Radial shield 3[c]	RS3[a]	MRS3	RRS3(<ROUR)[RRS2+0.001]	HRS3(=HRS1)[HRS1]	END[a]
Outer shell	OUR[a]	MOUR	ROUR(<RWTR)	HOUR(>HAS3)	END[a]
Radial water[c]	WTR[a]	MWTR	RWTR(<RJAC)[ROUR+0.01]	HWTR(<HJAC)[HJAC-0.01]	END[a]
Water jacket[c]	JAC[a]	MJAC	RJAC[ROUR+0.02]	HJAC(<HIM2)[HIM2-0.01]	END[a]
Axial shield 1	AS1[a]	MAS1	RAS1(=RINN)	HAS1(<HAS2)	END[a]
Axial shield 2[c]	AS2[a]	MAS2	RAS2(=RINN)[RINN]	HAS2(<HAS3)[HAS1+0.001]	END[a]
Axial shield 3[c]	AS3[a]	MAS3	RAS3(=RINN)[RINN]	HAS3(<HOUR)[HAS2+0.001]	END[a]
Impact limiter[c]	IMP[a]	MIMP	RIMP[ROUR+0.01]	HIM1(>HOUR)[HOUR+0.01]	
				HIM2(<HIM1) [HOUR-0.01]	END[a]
Corner hole[c]	HOL[a]	MHOL			END[a]
Cavity	CAV[a]	MCAV[e]	RCAV(<RINN)	HCAV(<HINN)	END[a]
Insert[c]	INS[a]	MINST[e]	RINS(<RCAV)[RCAV-0.001]	HINS(<HCAV)[HCAV-0.001]	END[a]

Termination card for cask geometry

CEND[a] Starts from column one.

[a]Keywords that must be part of the data entry.

[b]The condition in the parentheses must be satisfied by the corresponding input value.

[c]Any one of these components can be omitted. The insert mixture MINS is set equal to MCAV if the insert is omitted; the mixture numbers of all other omitted components are set to 1000.

[d]The dimensions of the omitted components are given the values in the brackets.

[e]For the LATTICECELL option and IGO=1, the material of MINS must be identical to the materials of mixture MBET. If the insert is omitted, the material of MCAV must satisfy this condition.

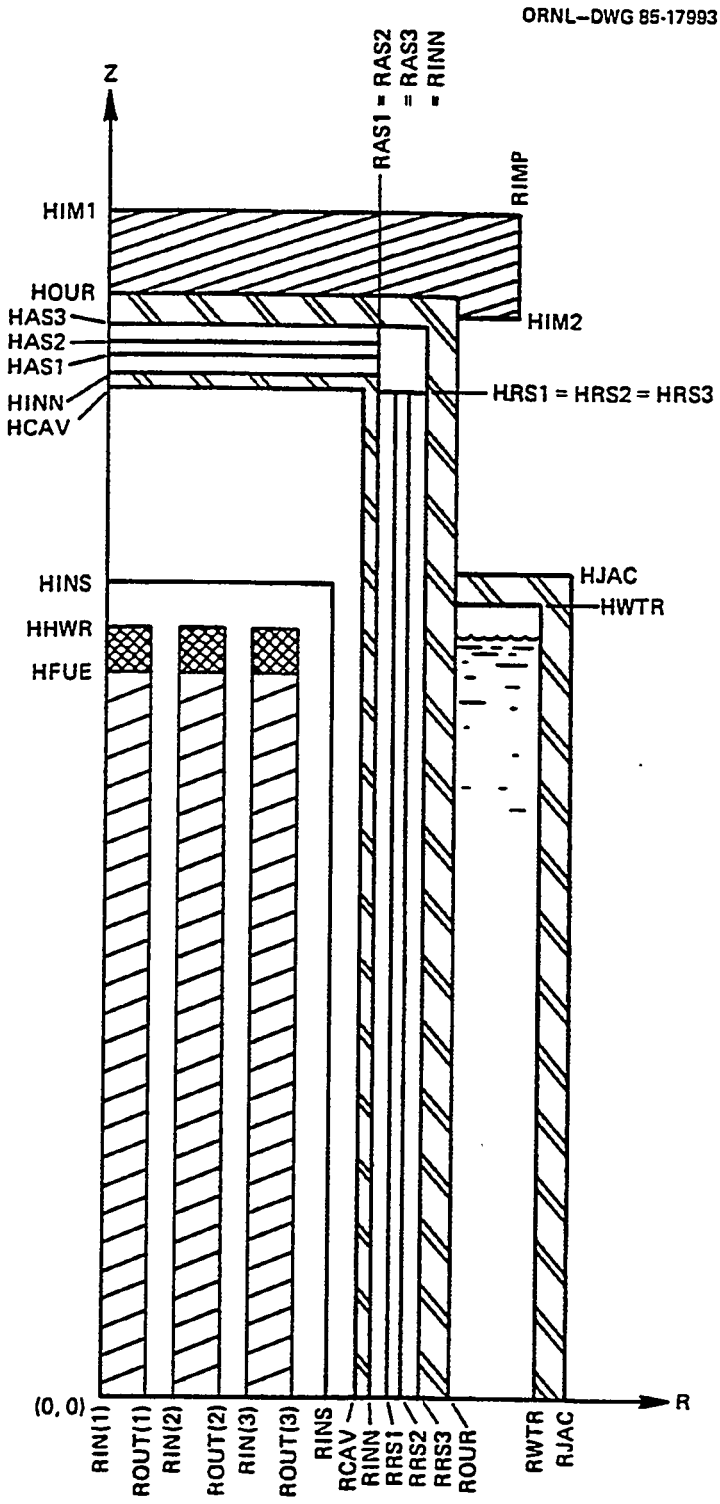


Figure S4.4.1 SAS4 cask model for IGO = 1 (dimensions of each component are shown)

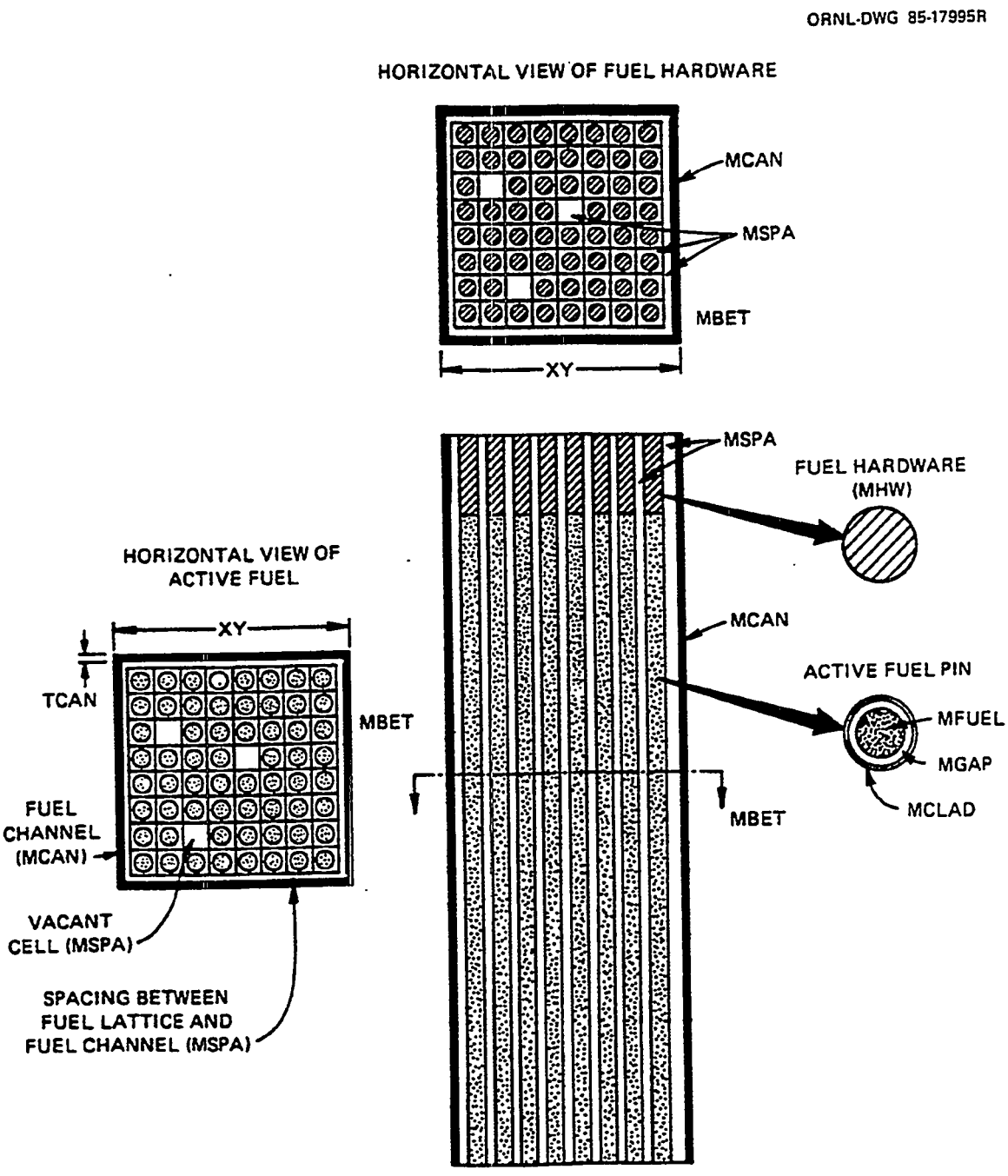


Figure S4.4.2 Fuel assembly model used in LATTICECELL option (only the top half shows)

Table S4.4.4. Mixture numbers of fuel and fuel hardware used in MORSE-SGC/S and adjoint XSDRNPM-S for different IGO options and LATTICECELL and INFHOMMEDIUM options

	IGO Options				
	0	1	2	3	4
LATTICECELL					
Fuel	MXX2(MXX2)[a]	MXX2P(MXX2)	MXX2Q(MXX2)	MFUEL(MXX2)	(MXX2)[b]
Fuel hardware[c]	MXX3(MXX3)	MXX3P(MXX3)	MXX3Q(MXX3)	MHW(MXX3)	(MXX3)[b]
INFHOMMEDIUM					
Fuel	MZ(1)(MZ(1))	MFU[d](MZ(1))	--	--	(MZ(1))[e]
Fuel hardware[c]	MHW(MZ(2))	MHW(MX(2))	--	--	(MX(2))[e]

[a]Quantities in parentheses are mixture numbers used in adjoint XSDRNPM-S.

[b]MORSE-SGC/S mixture numbers specified by the user in MARS input. Should use MFUEL for fuel and MHW for fuel hardware.

[c]Fuel hardware exists in the adjoint XSDRNPM-S calculation only for the axial calculation with IDR>0.

[d]Input via the parameter card of the Monte Carlo input data.

[e]MORSE-SGC/S mixture numbers specified by the user in MARS input.

Table S4.4.5 Axial source profile for a typical PWR

Axial boundaries (measured from midplane)	Source profiles			
	Top		Bottom	
	Neutron	Gamma	Neutron	Gamma
0.0	1.554	1.117	1.554	1.117
11.43	1.537	1.114	1.571	1.120
22.86	1.521	1.111	1.588	1.123
34.29	1.504	1.108	1.605	1.126
45.72	1.486	1.104	1.622	1.129
57.15	1.464	1.100	1.636	1.131
68.58	1.438	1.095	1.648	1.133
80.01	1.401	1.088	1.657	1.135
91.44	1.350	1.078	1.654	1.134
102.87	1.277	1.063	1.625	1.129
114.30	1.165	1.039	1.554	1.117
125.73	0.998	0.9995	1.414	1.091
137.16	0.769	0.9365	1.172	1.041
148.59	0.492	0.8375	0.816	0.951
160.02	0.220	0.6850	0.402	0.797
171.45	0.046	0.4625	0.092	0.551
182.88	0.0	0.0	0.0	0.0

1. PARM=SIZE=200000

2. PARM='SIZE=200000'

3. PARM=(SIZE=200000)

4. PARM ='AX,SIZE = 200000'

5. PARM = (AX,SIZE = 200000)

6. PARM=MO

7. PARM=(MO,SIZE=250000)

Examples 1, 2, and 3 are equivalent and specify that SAS4 is executed from the beginning and that 200,000 words are allowed for each functional module. Examples 4 and 5 are equivalent; SAS4 will execute from adjoint XSDRNPM and 200,000 words are allowed. Examples 6 and 7 are obvious. One important rule to remember is that when both features are used, as in examples 4, 5, and 7, AX or MO must come before SIZE. Finally, note that no blank space is allowed between the parentheses or between the quotation marks.

S4.4.2 FUEL LATTICE TYPES AND USAGE OF FUEL AND CASK MATERIALS

This section describes the details of using input materials under various options in SAS4. This section supplements the description in Sect. S4.2.3.

The input materials of SAS4 are identified as fuel materials and cask materials. SAS4 allows two fuel lattice types (GE=INFHOMMEDIUM or GE=LATTICECELL). For the INFHOMMEDIUM option, SAS4 does not homogenize nor mix the fuel materials. Hence, the usage of the fuel and cask materials in the functional modules is straightforward. Because the mixture numbers and densities given to all the input materials (fuel and cask materials) remain unchanged throughout the control module, the user can use the mixtures in any manner in the adjoint XSDRNPM and the MORSE-SGC functional modules.

For the LATTICECELL option, SAS4 homogenizes the fuel materials based on the unit cell and the fuel assembly geometries input by the user. The unit cell geometry is input in the material information data, whereas the fuel assembly geometry is defined in the adjoint discrete-ordinates input data via the fuel assembly card. In SAS4, a unit cell is composed of a fuel rod and a moderator. A fuel rod may have a clad on the outside and the gap between the fuel and the clad is optional. The fuel assembly geometry used by the LATTICECELL option is shown in Fig. S4.4.2. Axially, the fuel assembly is divided into three sections, a middle active fuel section and two fuel hardware sections at both ends. Horizontally, the assembly has a square cross section with outside dimension XY cm. There are NCEL cells along each side and a total of NCEL*NCEL cells in the assembly. Vacant cells (cells without fuel rods) are allowed in this model, and the number of vacant cells NVAC is input by the user.

As shown in Fig. S4.4.2, for the active fuel section, there are a spacing and a fuel channel surrounding the fuel lattice cells. The material of the spacing is identical to that of the vacant cells and is given a mixture number MSPA. The fuel channel has a thickness of TCAN cm and is given a mixture number MCAN. For assemblies without fuel channels, the user still must define a mixture MCAN with a thickness TCAN outside the spacing. This fuel assembly model allows two material zones (spacing and fuel channel, as they are called here) to be used surrounding the lattice. The material outside the fuel assemblies is given a mixture number MBET. Although MBET is normally void (air) or water, the user can use it to represent any material that separates the assemblies. If any of the materials MCAN, MSPA, and MBET are void, zeroes can be used for their mixture numbers.

For the fuel hardware sections, there are fuel hardware rods and the material in between. The fuel hardware rods have the same diameters as the fuel rods and represent such materials as cladding, plenum spring, end fitting, expansion springs, etc. The mixture number of the fuel hardware (rods) is MHW and is defined by the user in the parameter card of the adjoint discrete-ordinates input. The material between the hardware rods is mixture MSPA, whereas the material outside the assemblies is mixture MBET. For IGO = 1, MSPA must be identical to the material of the insert MINS or the material of the cavity MCAV if the insert is omitted (see Table S4.4.3).

In summary, for the LATTICECELL option, the user must define the fuel materials based on the unit cell geometry and the assembly geometry described herein. Specifically, the user must uniquely define (except for zeroes) the following fuel material mixtures in the input: MFUEL, MMOD, MCLAD, MSPA, MCAN, MHW, and MBET. Except for mixture zero, these mixtures must not be used in the cask geometry. Any other mixtures defined in the material information data can be used in the cask geometry. Moreover, several cask components (see Table S4.4.3) may use the same mixture. More description on the application of the materials is presented in Sect. S4.2.3 and Table S4.4.2.

S4.5 SAMPLE PROBLEMS

Presented in this section are eight sample problems, each of which is described in more detail in subsequent sections. Input listings of each sample problem have been included. However, only a portion of computer output of sample problem 1 is included in the Appendix. Note that the input and output for these problems are for illustrative purposes only. The input and output may not exactly match that actually used for testing and/or distributed with the SCALE system.

S4.5.1 SAMPLE PROBLEM 1

This two-dimensional (2-D) dry cask problem is presented in Ref. 1. Radial neutron doses were calculated in this problem. The geometry of the problem is shown in Fig. S4.5.1. The cask wall is composed of a layer of depleted uranium sandwiched between steel inner and outer liners. The source is made up of seven PWR fuel assemblies, but the source region is modeled as two concentric cylinders. The inner cylinder represents one fuel assembly, and the outer cylinder represents six fuel assemblies. The fuel hardware at the ends of the assemblies has been ignored. Each assembly has 17 × 17 unit cells of which 25 are vacant cells. The pitch dimension between the cells is 1.2598 cm. The diameter of each fuel pin is 0.83566 cm, and the diameter of the clad is 0.94996 cm. There is no gap between the fuel and the clad. The outside dimension of an assembly is 21.4493 cm. The height of the fuel is 365.76 cm (12 ft). Three point detectors are located outside the cask: two radial detectors on the midplane of the cask 91.4 cm (3 ft) and 182.8 cm (6 ft) away from the cask surface, and a corner detector is located 91.4 cm from the rim of the cask on a 45° plane.

The input for this problem is shown in Fig. S4.5.2. The 22N-18COUPLE neutron-gamma coupled library was used, and LATTICECELL was employed for the fuel lattice type. Mixtures 1, 2, and 3 described the unit cell. Mixtures 4 and 5 were, respectively, steel and depleted uranium. Mixtures 6 to 11 were voids, which were needed for the LATTICECELL option (see Sect. S4.4.2). Mixture 12 was also void and was used for the cavity inside the cask. The material information data were followed by 5 lines of discrete-ordinates input data and 17 lines of Monte Carlo input data. Note that mixtures 4, 5, and 12, representing the materials outside the source region, were used in both the adjoint discrete-ordinates calculation and the Monte Carlo calculation. The input values of FR1, FR2, FR3, and FR4 in the parameter card of Monte Carlo input determine the height of the radial surface detectors to be 182.88 cm from the midplane of the cask.

The computer output of MORSE-SGC and SAS4 has been included in the Appendix. Comments and explanations have been added to help the user understand the results of the calculation. The outputs of BONAMI, NITAWL-II, and XSDRNPM for cell-weighting have been left out to limit the size of this document.

The results given in the MORSE-SGC output indicate that very reliable answers were obtained with relatively low computing cost (less than 12 CPU min on IBM-3033) for this problem. Exceptionally low fractional standard deviations (FSD) were obtained for detectors 1 to 6, indicating the results should be accurate for these detectors. The FSD for detector 7 is 12%, and the result is acceptable. Because the source normalization factor, SFA, was omitted in the input, results of this calculation are per-neutron-per-second. To obtain dose rate per assembly, the user must multiply the results by the source strength of each assembly, which is 2.614×10^8 neutrons/s (33 GWd/MTU PWR spent fuel with 120-day cooling time). For the two radial point detectors (detectors 5 and 6), the dose rates are, respectively, 36.51 and 18.152 mrem/h per assembly, which are in excellent agreement with those reported elsehwere. However, for the corner point detector (detector 7), the dose rate is 4.91 mrem/h per assembly compared with 8.73 reported in Ref. 1. After close examination and more comparison in sample problem 2, it was found that in Table 3 of Ref. 1 the results of the corner detector and the axial detectors are a factor of 2 too high because of an error in source normalization.

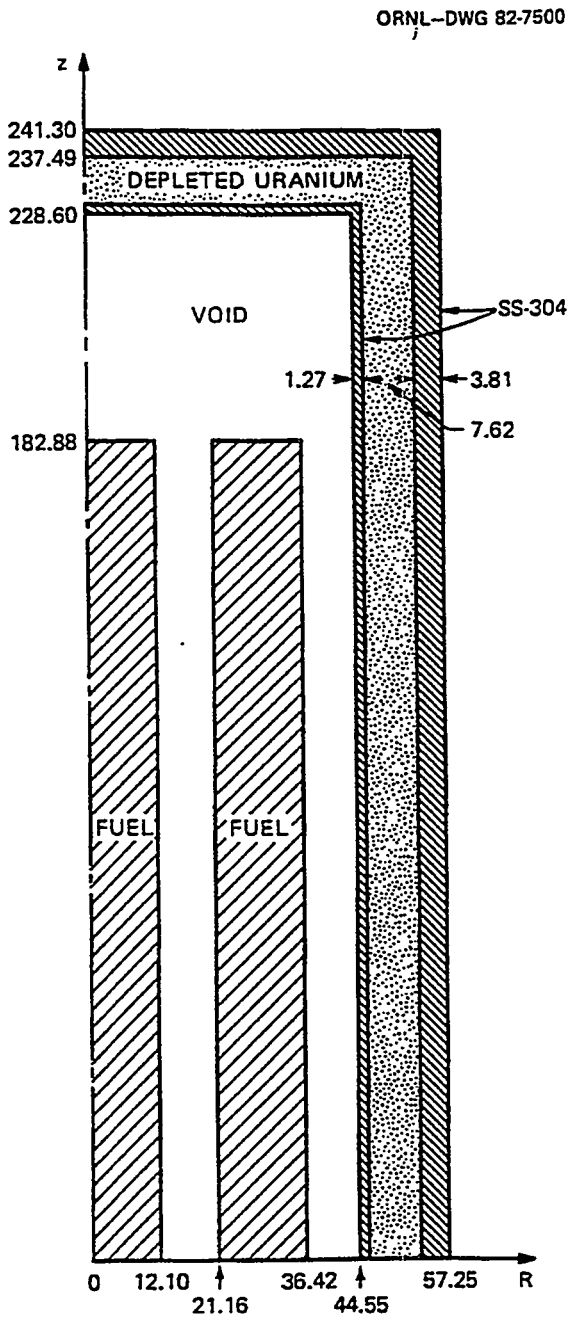


Figure S4.5.1 Upper half of depleted uranium shipping cask of sample problem 1

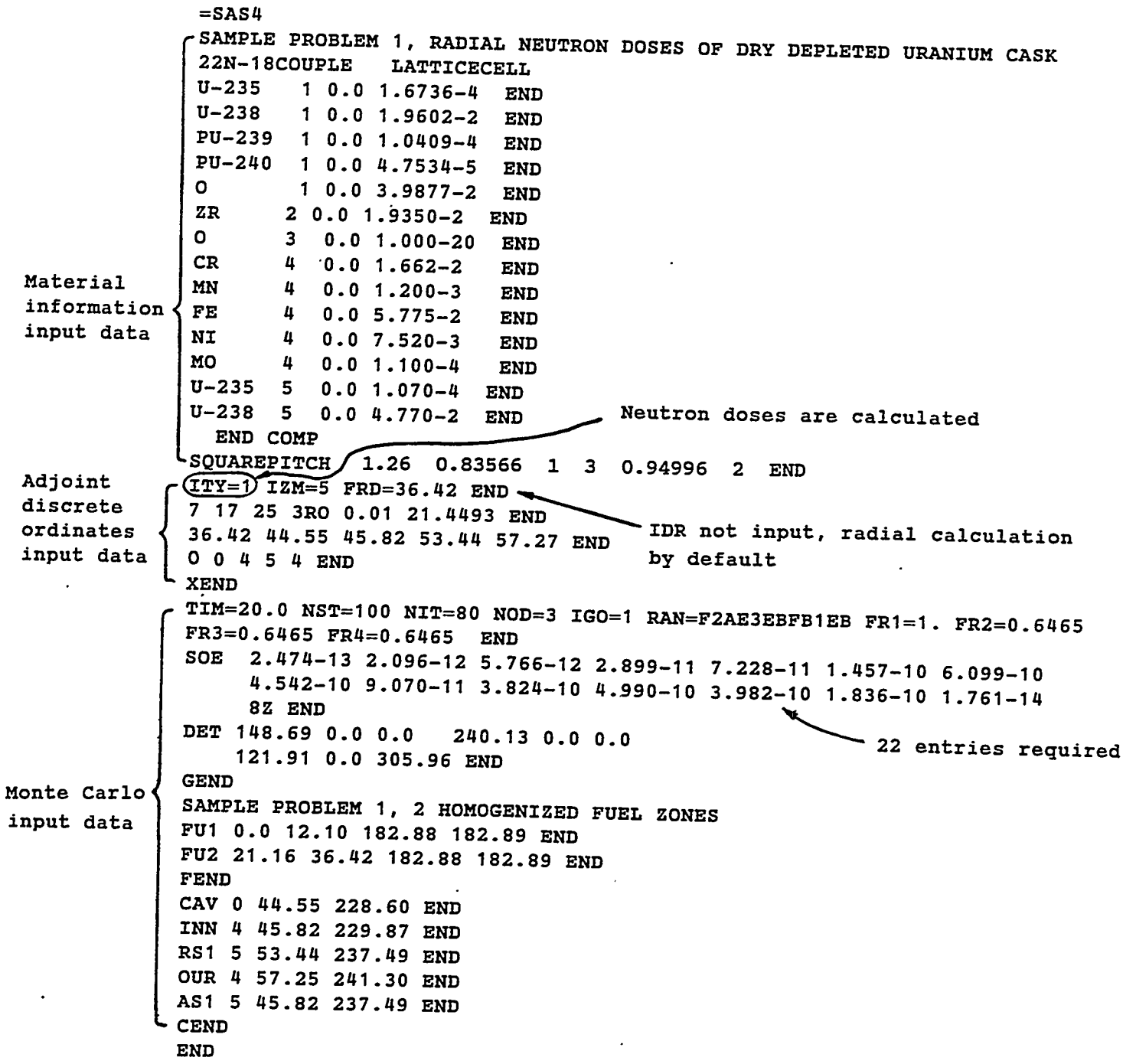


Figure S4.5.2 Input listing of sample problem 1

S4.5.2 SAMPLE PROBLEM 2

This sample problem calculates axial neutron doses of the depleted uranium cask used in sample problem 1. The SAS4 input of this problem is shown in Fig. S4.5.3. As might be expected, the input of this problem is very similar to that of problem 1. The differences between the two inputs are (1) the title cards were changed to differentiate between the two cases, (2) the IDR parameter in the adjoint discrete-ordinates input data had been set to one to indicate an axial calculation, (3) the zone boundary array and the zone mixture array were modified for the axial calculation, and (4) the point detectors array in the Monte Carlo input data was changed to axial locations. The first and second point detectors were on the cask centerline and were, respectively, 91.44 cm and 182.88 cm from the top surface (or 332.74 and 424.18 cm from the origin of the geometry). The third point detector was a corner detector identical to the third point detector of sample problem 1.

The calculation of this problem took about 7 min in CPU time. The fractional standard deviations are quite good (much less than 10%) for detectors 1 to 6, and are acceptable (14%) for detector 7. The calculated neutron dose rates for the two axial point detectors (detectors 5 and 6) are 9.001 and 2.819 mrem/h per assembly. These dose rates are in excellent agreement with the corrected results (9.05 and 2.85) reported earlier in Ref. 1. For the corner point detector, a dose rate of 4.89 mrem/h per assembly was calculated. The corner detector of these two sample problems illustrates the interesting question of selecting the direction of the transport calculation with the IDR parameter discussed in Sect. S4.2.4. It was stated in that section that for point detectors lying within the axial projection of the cask, an axial calculation should be made with IDR > 0. For detectors outside this projection, a radial calculation should be made. For the corner detector in question, the radial calculation is preferable because next-event estimation to the detector is treated correctly, whereas next-event estimation is made only from half of the cask in the axial calculation.

S4.5.3 SAMPLE PROBLEM 3

For this sample problem, the seven fuel assemblies in sample problem 1 were modeled explicitly using the IGO = 3 option. Recall that for IGO = 3, the LATTICECELL option must be used. The fuel material was no longer homogenized, and each fuel rod in the assemblies was modeled separately. Neutron dose rates at radial locations identical to those of sample problem 1 were calculated. Input of this problem is shown in Fig. S4.5.4. Except for the title cards, the IGO value, and the fuel geometry cards in the Monte Carlo input, the input of this problem is identical to that of sample problem 1. Note that PARM = MO was used in the module specification card to indicate execution of the MORSE-SGC functional module only. Cross-section data on logical units 3 and 4 and adjoint angular fluxes on logical unit 12 from sample problem 1 had to be saved and used in this calculation. Also, a source strength of SFA = 1.8298×10^9 neutrons/s was input so that results of this case are expressed per total source strength.

This problem took about 43 min in CPU time to process 5000 histories (vs 12 min to process 8000 histories for sample problem 1). The fractional standard deviations of the results are quite good (much less than 10%) for detectors 1 to 6, and are marginal (23%) for detector 7. The calculated neutron dose rates are comparable with those of sample problem 1, indicating that, for this problem, radial neutron dose rates are not affected by the two fuel geometry models.

S4.5.4 SAMPLE PROBLEM 4

This sample problem illustrates a calculation with IGO = 4, which requires the user to input MARS geometry. This cask is the same as the one used in the previous sample problems. Axial neutron doses were calculated for the heterogeneous fuel identical to sample problem 3. In fact, the MARS geometry input to this case was generated by the last sample problem. Execution of this problem started with the adjoint

```
=SAS4
SAMPLE PROBLEM 2, AXIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK
22N-18COUPLE   LATTICECELL
U-235    1 0.0 1.6736-4  END
U-238    1 0.0 1.9602-2  END
PU-239   1 0.0 1.0409-4  END
PU-240   1 0.0 4.7534-5  END
O        1 0.0 3.9877-2  END
ZR       2 0.0 1.9350-2  END
O        3  0.0 1.000-20  END
CR       4  0.0 1.662-2   END
MN       4  0.0 1.200-3   END
FE       4  0.0 5.775-2   END
NI       4  0.0 7.520-3   END
MO       4  0.0 1.100-4   END
U-235    5  0.0 1.070-4  END
U-238    5  0.0 4.770-2  END
  END COMP
SQUAREPITCH   1.26  0.83566  1  3  0.94996  2  END
IDR=1 ITY=1 IZM=5 FRD=36.42 END          <-- Indicates axial calculation
7 17 25 3RO 0.01 21.4493 END
182.88 228.60 229.87 237.49 241.30 END   <-- Zone boundaries of
7 8 4 5 4 END                                axial calculations
XEND
TIM=50. NST=120 NIT=90 NOD=3 IGO=1 RAN=178E3EBFCB39 END
SOE  2.474-13 2.096-12 5.766-12 2.899-11 7.228-11 1.457-10 6.099-10
     4.542-10 9.070-11 3.824-10 4.990-10 3.982-10 1.836-10 1.761-14
     8Z END
DET  2R0.0 332.74  2R0.0 424.18
    121.91 0.0 305.96 END                <-- Axial detectors
GEND
SAMPLE PROBLEM 2, 2 HOMOGENIZED FUEL ZONES
FU1 0.0 12.10 182.88 182.89 END
FU2 21.16 36.42 182.88 182.89 END
FEND
CAV 0 44.55 228.60 END
INN 4 45.82 229.87 END
RS1 5 53.44 237.49 END
OUR 4 57.25 241.30 END
AS1 5 45.82 237.49 END
CEND
END
```

Figure S4.5.3 Input listing of sample problem 2

```
=SAS4      PARM=MO
SAMPLE PROBLEM 3, RADIAL DOSES OF HETEROGENEOUS FUEL WITH 7
ASSEMBLIES
22N-18COUPLE    LATTICECELL
U-235       1  0.0   1.6736-4  END
U-238       1  0.0   1.9602-2  END
PU-239      1  0.0   1.0409-4  END
PU-240      1  0.0   4.7534-5  END
O           1  0.0   3.9877-2  END
ZR          2  0.0   1.9350-2  END
O           3  0.0   1.000-2   END
CR          4  0.0   1.662-2   END
MN          4  0.0   1.200-3   END
FE          4  0.0   5.775-2   END
NI          4  0.0   7.520-3   END
MO          4  0.0   1.100-4   END
U-235       5  0.0   1.070-4   END
U-238       5  0.0   4.770-2   END
  END COMP
SQUAREPITCH  1.26 0.83566 1 3 0.94996 2 END
ITY=1 IZM=5 FRD=36.42 END
7 17 25 3RO 0.01 21.4493 END
36.42 44.55 45.82 53.44 57.27 END
7 0 4 5 4 END
XEND
TIM=60.0 NST=100 NIT=50 NOD=3 IGO=3 SFA=1.8298+9
FR1=1. FR2=0.6465 FR3=0.6465 FR4=0.6465  RAN=ABC123456789 END
SOE  2.474-13 2.096-12 5.766-12 2.899-11 7.228-11 1.457-10 6.099-10
     4.542-10 9.070-11 3.824-10 4.990-10 3.982-10 1.836-10 1.761-14
     8Z END
DET 148.69 0.0 0.0   240.13 0.0 0.0
    121.91 0.0 305.96 END
GEND
SAMPLE PROBLEM 3, HETEROGENEOUS FUEL WITH 7 ASSEMBLIES
HET  24.7  182.88  182.89  END
FEND
CAV 0 44.55 228.60 END
INN 4 45.82 229.87 END
RS1 5 53.44 237.49 END
OUR 4 57.25 241.30 END
AS1 5 45.82 237.49 END
CEND
END
```

Figure S4.5.4 Input listing of sample problem 3

XSDRNPM functional module, using the PARM=AX option in the module specification card. Again, cross-section data in logical units 3 and 4 from previous problems were input to this problem. Actually, this problem could have started with MORSE-SGC had the adjoint angular fluxes in logical unit 12 of sample problem 2 been saved and input to this calculation. Aside from the IGO parameter and the source volume boundaries array, the input of this problem is identical to that of sample problem 2, up to the geometry input data. Focusing on the source volume boundaries array, we find that mixture 1 is the fuel material from which source particles originate, and the source volume boundaries enclose only the top half of the source. It is imperative that the source volume includes only the top half of the source, whether the source is the active fuel or the fuel hardware, and that the source mixture MSM must be inside the source volume.

Although the geometry input in Fig. S4.5.5 is specifically for this problem, the fact that many features in this geometry are generic to the SAS4 cask model deserves some discussion. In this geometry, there are 36 bodies (25 RCCs and 11 RPPs), 39 input zones, 5 universes (universes 1 to 4 and the absolute universe), and 4 arrays. The first 20 bodies are used to construct input zones 1 to 18 (zones designated as INN to CAV), which make up the cask body. Hence, this portion of geometry data is generic for the SAS4 cask model. The rest of the bodies and input zones are used to describe the fuel geometry.

To discuss modeling of the heterogeneous fuel geometry, we must refer to the fuel assembly model shown in Fig. S4.2.3. Recall that each unit cell in the fuel lattice consists of three sections, an active fuel section and two hardware sections at both ends. In MARS geometry input, the active fuel section of the unit cell is designated as universe 1 and the top and bottom hardware sections are designated as universes 2 and 3, respectively. Hence, the fuel lattice is an array composed of universe 3 at the bottom, universe 1 at the middle, and universe 2 on the top. Thus, for this problem, the fuel lattice is designated as array 1 having 17 $\times$ 17 $\times$ 3 elements of universes 1, 2, and 3. Note that body 29 is the outside boundary (array reference body) of array 1. Outside of array 1 there are a spacing and a fuel channel to make up a fuel assembly. An assembly and the material between assemblies constitute a fuel unit having lateral dimensions of APCH cm, as shown in Fig. S4.2.3. In the MARS geometry model, the fuel unit is designated as universe 4 in the geometry input. Finally, universe 4 is nested inside arrays 2, 3, and 4 to form the packing arrangement of seven fuel units shown in Fig. S4.2.4. For this packing arrangement, arrays 2 and 4 have 2 $\times$ 1 $\times$ 1 elements of universe 4; and array 3 has 3 $\times$ 1 $\times$ 1 elements of universe 4.

Similarly, other packing arrangements in Fig. S4.2.4 were constructed by nesting universe 4 in other array patterns. For example, for the fuel geometry having 52 fuel units, there are six arrays of which arrays 2 to 6 are filled with universe 4. The size of arrays 2 and 6 is 4 $\times$ 1 $\times$ 1, and the size of arrays 3 and 5 is 6 $\times$ 1 $\times$ 1. Finally, array 4 is 8 $\times$ 4 $\times$ 1.

This problem took about 12 min in CPU time to process 5000 histories (vs 6.5 min to process 10,800 histories for sample problem 2). The fractional standard deviations of the results are less than 10% for detectors 1 to 6 and are 15% for detector 7. The calculated dose rates are slightly lower than those of sample problem 2.

S4.5.5 SAMPLE PROBLEM 5

This sample problem demonstrates a calculation using the INFHOMMEDIUM option. Radial neutron doses for the problem identical to sample problem 1 were calculated. Input of this problem is listed in Fig. S4.5.6. Note that mixture 1 is the fuel material used in the Monte Carlo calculation, but mixture 5, having lower atom densities, is the material of the fuel zone in the adjoint XSDRNPM calculation. The fuel assembly card in the adjoint discrete-ordinates input must be omitted for the INFHOMMEDIUM option. The fuel material mixture MFU = 1 was needed in the parameter card of the Monte Carlo input because of the INFHOMMEDIUM option in which IGO = 1.

```
=SAS4      PARM=AX
SAMPLE PROBLEM 4, AXIAL DOSES OF 7 HETER. ASSEMB., USER INPUT GEOMETRY
22N-18COUPLE    LATTICECELL
U-235    1 0.0 1.6736-4   END
U-238    1 0.0 1.9602-2   END
PU-239   1 0.0 1.0409-4   END
PU-240   1 0.0 4.7534-5   END
O        1 0.0 3.9877-2   END
ZR       2 0.0 1.9350-2   END
O        3  0.0 1.000-20   END
CR       4  0.0 1.662-2    END
MN       4  0.0 1.200-3    END
FE       4  0.0 5.775-2    END
NI       4  0.0 7.520-3    END
MO       4  0.0 1.100-4    END
U-235    5  0.0 1.070-4   END
U-238    5  0.0 4.770-2   END
  END COMP
SQUAREPITCH  1.25984 0.83566 1 3 0.94996 2 END
ITY=1 IZM=5 FRD=36.42 IDR=1   END
7 17 25 3RO 0.01 21.4493 END
182.88 228.60 229.87 237.49 241.30   END
14 15 4 5 4 END
XEND
TIM=65.0 NST=100 NIT=50 SFA=1.8298+9 NOD=3 IGO=4 RAN=F2AE3EBFB1EB END
SOE  2.474-13 2.096-12 5.766-12 2.899-11 7.228-11 1.457-10 6.099-10
     4.542-10 9.070-11 3.824-10 4.990-10 3.982-10 1.836-10 1.761-14
     8Z END
DET 2Z 332.74  2Z 424.18  121.91 0. 305.96 END
SXY 1 -37.05 37.05 -37.05 37.05 0.0 182.88 44.55 182.88
    57.27 241.31 END
GEND
SAMPLE PROBLEM 4, HETEROGENEOUS FUEL WITH 7 ASSEMBLIES
    0     0     1    20
RCC     1 0.0   0.0    -2.29870E+02 0.0   0.0     4.59740E+02   4.58200E+01
RCC     2 0.0   0.0    -2.37490E+02 0.0   0.0     4.74980E+02   5.34400E+01
RCC     3 0.0   0.0    -2.37490E+02 0.0   0.0     4.74980E+02   5.34410E+01
RCC     4 0.0   0.0    -2.37490E+02 0.0   0.0     4.74980E+02   5.34420E+01
RCC     5 0.0   0.0    -2.41300E+02 0.0   0.0     4.82600E+02   5.72500E+01
RCC     6 0.0   0.0    -2.41270E+02 0.0   0.0     4.82540E+02   5.72600E+01
RCC     7 0.0   0.0    -2.41280E+02 0.0   0.0     4.82560E+02   5.72700E+01
RCC     8 0.0   0.0    -2.37490E+02 0.0   0.0     4.74980E+02   4.58200E+01
RCC     9 0.0   0.0    -2.37491E+02 0.0   0.0     4.74982E+02   4.58200E+01
RCC    10 0.0   0.0    -2.37492E+02 0.0   0.0     4.74984E+02   4.58200E+01
RCC    11 0.0   0.0    -2.41310E+02 0.0   0.0     4.82620E+02   5.72600E+01
RCC    12 0.0   0.0    -2.41290E+02 0.0   0.0     4.82580E+02   5.72600E+01
RCC    13 0.0   0.0    -2.37492E+02 0.0   0.0     4.74984E+02   5.34420E+01
RCC    14 0.0   0.0    -3.41310E+02 0.0   0.0     6.82620E+02   1.57270E+02
RCC    15 0.0   0.0    -4.41310E+02 0.0   0.0     8.82620E+02   2.57270E+02
RCC    16 0.0   0.0    -5.41310E+02 0.0   0.0     1.08262E+03   3.57270E+02
RCC    17 0.0   0.0    -2.24131E+03 0.0   0.0     4.48262E+03   2.05727E+03
RCC    18 0.0   0.0    -2.34131E+03 0.0   0.0     4.68262E+03   2.15727E+03
```

Figure S4.5.5 Input listing of sample problem 4

```
RCC    19 0.0   0.0    -2.28600E+02 0.0   0.0     4.57200E+02    4.45500E+01
RCC    20 0.0   0.0    -2.28599E+02 0.0   0.0     4.57198E+02    4.45490E+01
RCC    21 0.0   0.0    -1.82880E+02 0.0   0.0     3.65760E+02    3.99349E-01
RCC    22 0.0   0.0    -1.82880E+02 0.0   0.0     3.65760E+02    4.26660E-01
RCC    23 0.0   0.0    -1.82880E+02 0.0   0.0     3.65760E+02    4.53971E-01
RCC    24 0.0   0.0     0.0          0.0   0.0     1.82890E+02    4.53971E-01
RCC    25 0.0   0.0    -1.82890E+02 0.0   0.0     1.82890E+02    4.53971E-01
RPP    26     -0.62991952896      0.62991952896     -0.62991952896
               0.62991952896 -1.8288E+02  1.8288E+02
RPP    27     -0.62991952896      0.62991952896     -0.62991952896
               0.62991952896  1.8288E+02  1.8289E+02
RPP    28     -0.62991952896      0.62991952896     -0.62991952896
               0.62991952896 -1.8289E+02 -1.8288E+02
RPP    29    -10.70863199234     10.70863199234    -10.70863199234
              10.70863199234 -1.8289E+02  1.8289E+02
RPP    30 -1.0715E+01  1.0715E+01 -1.0715E+01  1.0715E+01 -1.8288E+02
          1.8288E+02
RPP    31 -1.0725E+01  1.0725E+01 -1.0725E+01  1.0725E+01 -1.8288E+02
          1.8288E+02
RPP    32 -1.0725E+01  1.0725E+01 -1.0725E+01  1.0725E+01 -1.8289E+02
          1.8289E+02
RPP    33    -12.34999847412     12.34999847412    -12.34999847412
              12.34999847412 -1.8289E+02  1.8289E+02
RPP    34    -24.69999694824     24.69999694824    -37.04999542236
             -12.34999847412 -1.8289E+02  1.8289E+02
RPP    35    -37.04999542236     37.04999542236    -12.34999847412
              12.34999847412 -1.8289E+02  1.8289E+02
RPP    36    -24.69999694824     24.69999694824     12.34999847412
              37.04999542236 -1.8289E+02  1.8289E+02
  END
INN      1   -19
RS1      2   -10
RS2      3    -2
RS3      4    -3
OUR      5   -13
WTR      6    -5
JAC      7    -6    -5
AS1      8    -1
AS2      9    -8
AS3     10    -9
IMP     11    -5   -12
HOL     13    -4   -10
DE2  OR  14    -5    -7   -11 OR     12    -5    -7
DE3     15   -14
DE4     16   -15
INV     17   -16
EXV     18   -17
CAV     19   -20
INS     20   -34   -35   -36
FUE     21
GAP     22   -21
CLA     23   -22
```

Zones 1 to 18 describe the cask body. This portion is generic for the SAS4 cask model

Figure S4.5.5 (continued)

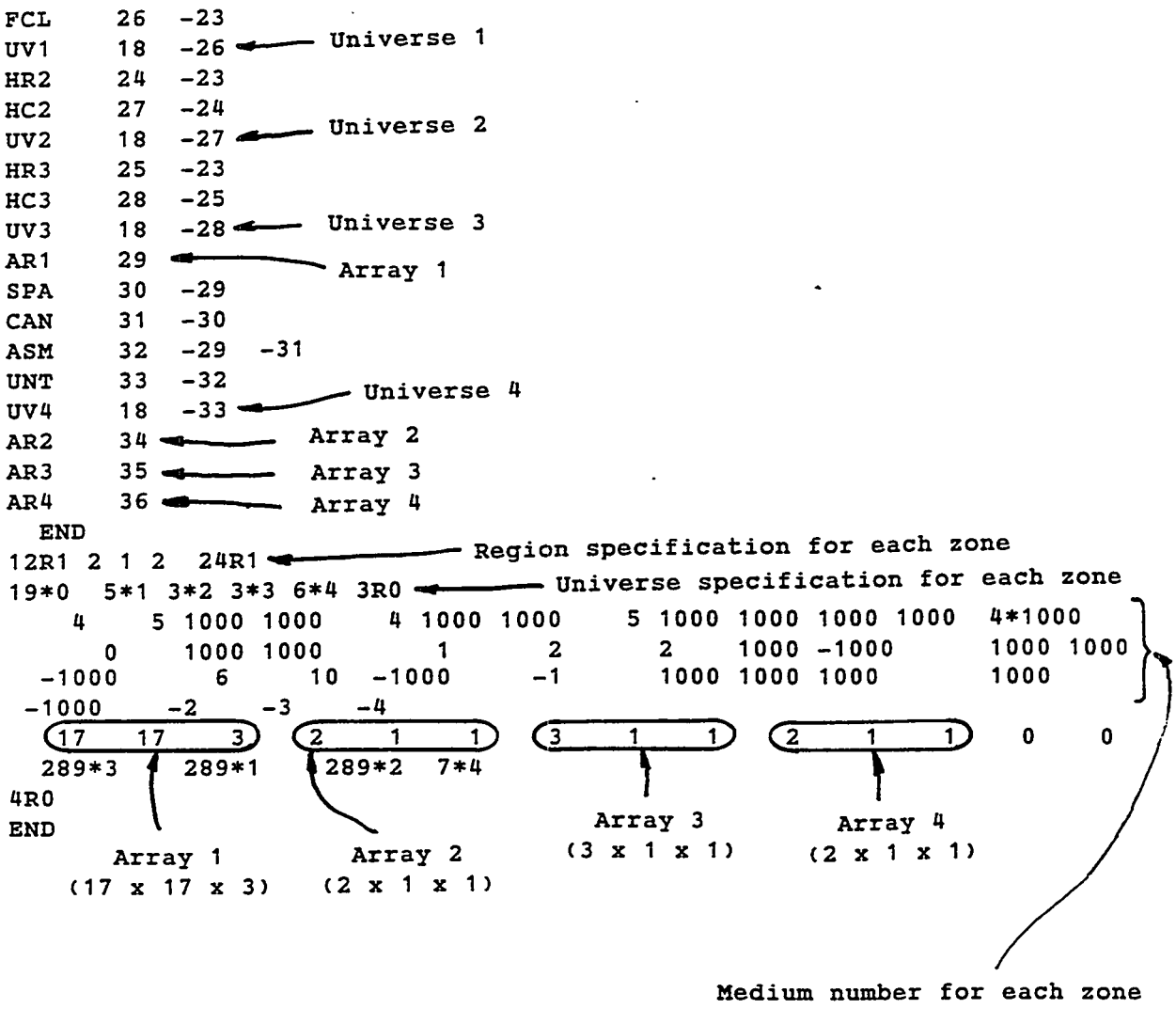


Figure S4.5.5 (continued)

```
=SAS4
SAMPLE PROBLEM 5, RUNS SAMPLE PROBLEM 1 WITH INFHOMMEDIUM OPTION
22N-18COUPLE INFHOMMEDIUM
U-235    1 0.0 5.2672-5  END
U-238    1 0.0 6.1692-3  END
PU-239   1 0.0 3.2759-5  END
PU-240   1 0.0 1.4960-5  END
O        1 0.0 1.2550-2  END
ZR       1 0.0 1.7799-3  END
CR       2  0.0 1.662-2   END
MN       2  0.0 1.200-3   END
FE       2  0.0 5.775-2   END
NI       2  0.0 7.520-3   END
MO       2  0.0 1.100-4   END
U-235    3  0.0 1.070-4  END
U-238    3  0.0 4.770-2  END
O        4 0.0 1.00-20 END
U-235    5 0.  4.07074-5  END
U-238    5 0.  4.76784-3  END
PU-239   5 0.  2.53180-5  END
PU-240   5 0.  1.15618-5  END
O        5 0.  9.69937-3  END
ZR       5 0.  1.37556-3  END
  END COMP
ITY=1 IZM=5 MHW=4 FRD=36.42 END
36.42 44.55 45.82 53.44 57.27 END
5 4 2 3 2 END
XEND
TIM=20.0 NST=100 NIT=80 NOD=3 IGO=1 RAN=F2AE3EBFB1EB
MFU=1 FR1=1. FR2=0.6465 FR3=0.6465 FR4=0.6465 SFA=1.8298+9 END
SOE  2.474-13 2.096-12 5.766-12 2.899-11 7.228-11 1.457-10 6.099-10
     4.542-10 9.070-11 3.824-10 4.990-10 3.982-10 1.836-10 1.761-14
     8Z END
DET 148.69 0.0 0.0   240.13 0.0 0.0
    121.91 0.0 305.96 END
GEND
2 HOMOGENIZED FUEL ZONES
FU1 0.0 12.10 182.88 182.89 END
FU2 21.16 36.42 182.88 182.89 END
FEND
CAV 4 44.55 228.60 END
INN 2 45.82 229.87 END
RS1 3 53.44 237.49 END
OUR 2 57.25 241.30 END
AS1 3 45.82 237.49 END
CEND
END
```

Material of fuel zone in adjoint discrete ordinates calculation

Fuel material mixture used in Monte Carlo calculation

For INFHOMMEDIUM with IGO=1, the fuel mixture number MFU must be input

Could have used zero instead.

Figure S4.5.6 Input listing of sample problem 5

S4.5.6 SAMPLE PROBLEM 6

This sample problem uses the IPF = 1 option to input the top axial gamma profile provided by SAS4 to calculate axial primary gamma-ray doses of the depleted uranium cask. Input of this problem is shown in Fig. S4.5.7. It is very similar to the input of sample problem 2 except for the following items: (1) in the Monte Carlo parameter card, IPF = 1 is input to invoke the top axial profile provided by the code; (2) ITY = 2 in the adjoint discrete-ordinates parameter card to indicate gamma responses to be calculated; (3) in the Monte Carlo parameter card, NST = 600 instead of 100 for neutron calculations, and SFA = 6.3693 + 17 for gamma source strength; and (4) the source spectrum array has 40 entries instead of just 22 entries for neutron responses. Note that the ITY = 2 input can be omitted because the default value of ITY is 2. Finally, for gamma responses, a batch size of NST = 400 or larger is recommended, whereas NST about 100 is normally sufficient for neutron responses.

S4.5.7 SAMPLE PROBLEM 7

This problem computes axial total gamma-ray responses of a large steel cask containing 11.5-GWd/MTU PWR spent fuel that has been cooled for slightly more than 13 years. The geometry of this problem is shown in Fig. S4.5.8. The cask cavity has a radius of 91.1 cm and a height of 436.58 cm, and the cask wall is a solid steel shell of 23.5 cm thick on the side and 22.09 cm thick on both ends. The outside dimensions of the cask are 114.6 cm in radius and 480.76 cm in height. On both ends of the cask are impact limiters. The source region is a cylinder with an active fuel zone at the middle and fuel hardware zones on both ends. The height of the active fuel is 365.76 cm, and the height of the fuel hardware zones is 35.4 cm. The radius of the source region is 72.96 cm. Only the gamma-ray dose from the active fuel zone is evaluated in this problem.

The input for this problem is shown in Fig. S4.5.9. This problem used the 27N-18COUPLE cross-section library with INFHOMMEDIUM option for the fuel lattice type. Six material mixtures were input in the material information input data. Mixture 1 is the spent fuel. Mixture 2 is a borated steel, but is not used in the problem. Mixture 3 is the cask wall material, and mixture 4 is the impact limiter material. Mixture 5 is the fuel hardware material, and mixture 6 is void to represent the cavity. The default value of the source geometry option was used, because IGO was not input in the Monte Carlo parameter card. For the SOE array, both neutron and gamma-ray spectra were input because total gamma-ray doses were desired. Four point detectors were located on the z-axis and were, respectively, 10, 100, 200, and 300 cm above the top impact limiter.

S4.5.8 SAMPLE PROBLEM 8

This sample problem calculates axial gamma-ray doses resulting from the ^{60}Co gamma source in the fuel hardware for the cask described in sample problem 7. Input of this problem is shown in Fig. S4.5.10. Note that execution starts from the MORSE-SGC functional module using the PARM=MO option in the first card. ISO in the parameter card of Monte Carlo input was set to 1 to indicate source would be starting from the fuel hardware. The source normalization factor SFA was not input for this problem. In the source spectrum array SOE, only group 37 has a nonzero value, which indicates that the source is gamma rays of energies between 1.00 and 1.33 MeV. Finally, cross-section data on logical unit 4 and angular fluxes on logical unit 12 from the last sample problem must be saved and used in this problem.

```
=SAS4
SAMPLE PROBLEM 6, AXIAL GAMMA DOSES OF DRY DEPLETED URANIUM CASK
22N-18COUPLE   LATTICECELL
U-235    1 0.0 1.6736-4  END
U-238    1 0.0 1.9602-2  END
PU-239   1 0.0 1.0409-4  END
PU-240   1 0.0 4.7534-5  END
O        1 0.0 3.9877-2  END
ZR       2 0.0 1.9350-2  END
O        3  0.0 1.000-20  END
CR       4  0.0 1.662-2   END
MN       4  0.0 1.200-3   END
FE       4  0.0 5.775-2   END
NI       4  0.0 7.520-3   END
MO       4  0.0 1.100-4   END
U-235    5  0.0 1.070-4  END
U-238    5  0.0 4.770-2  END
  END COMP
SQUAREPITCH  1.26 0.83566 1 3 0.94996 2 END
IDR=1 ITY=2 IZM=5  FRD=36.42 END
7 17 25 3RO 0.01 21.4493 END
182.88 228.60 229.87 237.49 241.30 END
0 0 4 5 4 END
XEND
TIM=50. NST=600 NMT=900 NIT=90 NOD=3 SFA=6.3693+17 IGO=1 IPF=1 END
SOE  22Z 1.108-12  7.217-12  4.421-11  4.181-11  2.604-6  3.893-5
 1.506-3  8.461-4  3.708-3  6.424-3  1.643-1  1.328-1  8.194-2
 1.193-2  2.266-2  6.945-2  8.459-2  4.198-1  END
DET  2R0.0 332.74  2R0.0 424.18
    121.91 0.0 305.96 END
GEND
SAMPLE PROBLEM 6, 2 HOMOGENIZED FUEL ZONES
FU1 0.0 12.10 182.88 182.89 END
FU2 21.16 36.42 182.88 182.89 END
FEND
CAV 0 44.55 228.60 END
INN 4 45.82 229.87 END
RS1 5 53.44 237.49 END
OUR 4 57.25 241.30 END
AS1 5 45.82 237.49 END
CEND
END
```

Gamma doses are calculated

Neutron source spectrum is zero.
Only primary gamma doses are calculated.

40 entries are required

Figure S4.5.7 Input listing of sample problem 6

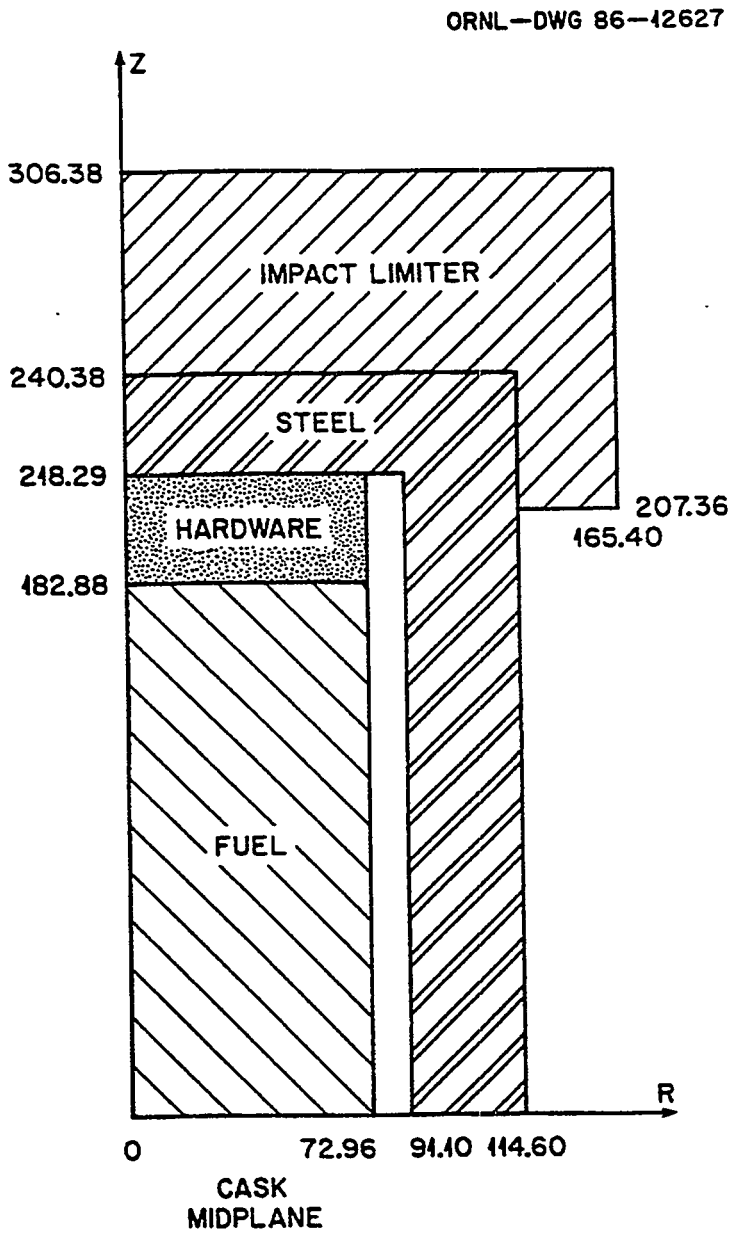


Figure S4.5.8 Upper half of steel cask of sample problem 7

```
=SAS4
SAMPLE PROBLEM 7, AXIAL TOTAL GAMMA RAY DOSES OF A LARGE STEEL CASK
27N-18COUPLE  INFHOMMEDIUM
U-238   1 0 6.104-3 END
U-235   1 0 2.229-4 END
O       1 0 1.265-2 END
ZR      1 0 3.577-3 END
FE      2 0 5.804-2 END
CR      2 0 1.658-2 END
NI      2 0 1.064-2 END
B-10    2 0 1.484-3 END
FE      3 0 8.211-2 END
CR      3 0 1.822-4 END
MN      3 0 1.035-3 END
NI      3 0 1.130-3 END
SI      3 0 3.373-4 END
C       4 0 6.274-3 END
H       4 0 9.035-3 END
O       4 0 4.141-3 END
CR      5 0 1.988-3 END
MN      5 0 1.980-4 END
FE      5 0 6.720-3 END
NI      5 0 8.339-4 END
ZR      5 0 1.307-3 END
END COMP
IDR=1 ITY=2 IZM=4 IRF=9504 MHW=5 FRD=72.96 END
182.88 218.28 240.38 306.38 END
1 5 3 4  END
XEND
TIM=60.0 NST=1200 NMT=2000 NIT=60 NOD=4  SFA=2.6408+16 END
SOE 1.204+4 2.068+5 3.468+5 1.376+5 1.449+5 1.345+5 2.600+4 20Z
    4.1669+2 1.9727+3 1.0131+4 2.5454+4 8.1924+6 6.7708+7 2.3506+9
    2.1830+10 1.9167+12 9.7254+12 4.7619+12 3.1923+14 1.0531+13
    8.2641+12 1.1979+13 3.9054+13 5.7276+13 1.9742+14  END
DET 2R0.0 316.98  2R0.0 406.98  2R0.0 506.98  2R0.0 606.98 END
GEND
LARGE STEEL CASK WITH ONE SOURCE REGION
FUE 182.88 218.28 END
FEND
CAV 0 91.1 218.29 END
INN 3 93.0 220.0  END
RS1 3 110. 233.0  END
AS1 3 93.0 233.0 END
OUR 3 114.6 240.38 END
IMP 4 165.4 306.38  207.36 END
CEND
END
```

Figure S4.5.9 Input listing of sample problem 7

```
=SAS4       PARM=MO
SAMPLE PROBLEM 8, AXIAL GAMMA DOSES DUE TO SOURCE IN HARDWARE
27N-18COUPLE  INFHOMMEDIUM
U-238   1 0 6.104-3 END
U-235   1 0 2.229-4 END
O       1 0 1.265-2 END
ZR      1 0 3.577-3 END
FE      2 0 5.804-2 END
CR      2 0 1.658-2 END
NI      2 0 1.064-2 END
B-10    2 0 1.484-3 END
FE      3 0 8.211-2 END
CR      3 0 1.822-4 END
MN      3 0 1.035-3 END
NI      3 0 1.130-3 END
SI      3 0 3.373-4 END
C       4 0 6.274-3 END
H       4 0 9.035-3 END
O       4 0 4.141-3 END
CR      5 0 1.988-3 END
MN      5 0 1.980-4 END
FE      5 0 6.720-3 END
NI      5 0 8.339-4 END
ZR      5 0 1.307-3 END
END COMP
IDR=1 ITY=2 IZM=4 IRF=9504 MHW=5 FRD=72.96 END
182.88 218.28 240.38 306.38 END
1 5 3 4  END
XEND
TIM=60.0 NST=1200 NMT=2000 NIT=60 NOD=4 ISO=1 END
SOE  36Z 1.0 8Z END
DET 2R0.0 316.98  2R0.0 406.98  2R0.0 506.98  2R0.0 606.98 END
GEND
LARGE STEEL CASK WITH ONE SOURCE REGION
FUE 182.88 218.28 END
FEND
CAV 0 91.1 218.29 END
INN 3 93.0 220.0  END
RS1 3 110. 233.0  END
AS1 3 93.0 233.0 END
OUR 3 114.6 240.38 END
IMP 4 165.4 306.38  207.36 END
CEND
END
```

Source starts from the fuel hardware

Figure S4.5.10 Input listing of sample problem 8

S4.6 REFERENCES

1. J. S. Tang and T. J. Hoffman, "Monte Carlo Shielding Analyses Using an Automated Biasing Procedure," *Nucl. Sci. Eng.* **99**, 329 (1988).

2. M. B. Emmett, *The MORSE Monte Carlo Radiation Transport Code System,* ORNL-4972, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., February 1975.

3. G. Goertzel and M. H. Kalos, *Progress in Nuclear Energy,* Vol. 2, Pergamon Press, Inc., New York, 1958, p. 315.

4. J. E. Hoogenboom, "Optimum Biasing of Integral Equations in Monte Carlo Calculations," *Nucl. Sci. Eng.* 70, 210 (1979).

5. J. S. Tang, P. N. Stevens, and T. J. Hoffman, *Methods of Monte Carlo Biasing Using TwoDimensional Discrete Ordinates Adjoint Flux,* ORNL/TM-5414, Union Carbide Corp., Nuclear Division, Oak Ridge Natl. Lab., June 1976.

6. J. S. Tang, T. J. Hoffman, and P. N. Stevens, "Monte Carlo Shielding Calculations Using EventValue Path-Length Biasing," *Nucl. Sci. Eng.* **62**, 617 (1977).

7. J. E. Stewart, "A General Point-on-a-Ring Detector," *Trans. Am. Nucl. Soc.* **10**, 643 (1978).

APPENDIX S4.A

MM MM OOOOOOOOOO RRRRRRRRRRR SSSSSSSSSS EEEEEEEEEEEE SSSSSSSSSS GGGGGGGGGG SSSSSSSSSS
MMM MMM OOOOOOOOOOOO RRRRRRRRRRRR SSSSSSSSSSS EEEEEEEEEEEE SSSSSSSSSSSS GGGGGGGGGGGG SSSSSSSSSSSS
MMMM MMMM OO OO RR RR SS SS EE SS SS GG GG SS SS
MM MM MM MM MM OO OO RR RR SS EE SS GG SS
MM MM MM MM OO OO RR RR SS EE SS GG SS
MM MMM MM OO OO RRRRRRRRRRRR SSSSSSSSSS EEEEEEEEE SSSSSSSSSSS GG GGGGGG SSSSSSSSSS
MM M MM OO OO RRRRRRRRRRR SSSSSSSSSS EEEEEEEEE SSSSSSSSSSS GG GGGGGG SSSSSSSSSS
MM MM OO OO RR RR SS EE SS GG GG SS
MM MM OO OO RR RR SS EE SS GG GG SS
MM MM OO OO RR RR SS SS EE SS SS GG GG SS SS
MM MM OOOOOOOOOOOO RR RR SSSSSSSSSSS EEEEEEEEEEEE SSSSSSSSSSS GGGGGGGGGGG SSSSSSSSSS
MM MM OOOOOOOOOO RR RR SSSSSSSSSS EEEEEEEEEEEE SSSSSSSSSS GGGGGGGGGG SSSSSSSSSS
JJ SSSSSSSSSS TTTTTTTTTTT 7777777777777 7777777777777 SSSSSSSSSS 11
JJ SSSSSSSSSSS TTTTTTTTTTT 777777777777 777777777777 SSSSSSSSSSS 111
JJ SS SS TT 77 77 77 77 SS SS 1111
JJ SS TT 77 77 SS 11
JJ SS TT 77 77 SS 11
JJ SSSSSSSSSSS TT 77 77 SSSSSSSSSSS 11
JJ SSSSSSSSSSS TT 77 77 SSSSSSSSSSS 11
JJ SS TT 77 77 SS 11
JJ SS TT 77 77 SS 11
JJ JJ SS SS TT 77 77 SS SS 11
JJJJJJJJJJJJ SSSSSSSSSSSS TT 77 77 SSSSSSSSSSSS 11111111
JJJJJJJJJJ SSSSSSSSSS TT 77 77 SSSSSSSSSS 11111111
0000000 11 // 11 11 // 88888888888 88888888888
000000000 111 // 111 111 // 8888888888888 8888888888888
00 00 1111 // 1111 1111 // 88 88 88 88
00 00 11 // 11 11 // 88 88 88 88
00 00 11 // 11 11 // 88 88 88 88
00 00 11 // 11 11 // 88888888888 88888888888
00 00 11 // 11 11 // 88888888888 88888888888
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000000000 11111111 // 11111111 11111111 // 8888888888888 8888888888888
0000000 11111111 // 11111111 11111111 // 88888888888 88888888888
22222222222 22222222222 11 666666666666 5555555555555 5555555555555
2222222222222 2222222222222 111 6666666666666 5555555555555 5555555555555
22 22 22 22 1111 66 55 55
22 22 11 66 55 55
22 22 11 66 55 55
22 22 11 666666666666 555555555555 555555555555
22 22 ..... 11 6666666666666 ..... 5555555555555 5555555555555
22 22 ..... 11 66 66 ..... 55 55
22 22 ..... 11 66 66 ..... 55 55
22 22 ..... 11 66 66 ..... 55 55 55 55
2222222222222 2222222222222 11111111 6666666666666 5555555555555 5555555555555
2222222222222 2222222222222 11111111 66666666666 55555555555 55555555555

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**********************************************************************
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**********************************************************************
*****                                                            *****
*****          PROGRAM VERIFICATION INFORMATION                  *****
*****                                                            *****
**********************************************************************
**********************************************************************
**********************************************************************
*****                                                            *****
*****                                                            *****
*****          PROGRAM:  000106                                  *****
*****                                                            *****
*****     CREATION DATE:  88.011                                 *****
*****                                                            *****
*****          LIBRARY:  SYS88011.T220753.RA000.JST77S1.LIBRARY  *****
*****                                                            *****
*****                                                            *****
*****          JOBNAME:  JST77S1                                 *****
*****                                                            *****
*****  DATE OF EXECUTION:  01/11/88                              *****
*****                                                            *****
*****  TIME OF EXECUTION:  22.16.56                              *****
*****                                                            *****
**********************************************************************
**********************************************************************
**********************************************************************
**********************************************************************
```

```
1Q ARRAY HAS   14 ENTRIES.

2Q ARRAY HAS    5 ENTRIES.

3Q ARRAY HAS   20 ENTRIES.

4Q ARRAY HAS    4 ENTRIES.

5Q ARRAY HAS   28 ENTRIES.
```

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

1 $ ARRAY

IADJM	ADJOINT INDICATOR	0	NSPLT	SPLITTING INDICATOR	1
NSTRT	NUMBER OF PARTICLES PER BATCH	100	NKILL	RUSSIAN ROULETTE INDICATOR	1
NMOST	MAX NUMBER OF PARTICLES ALLOWED	400	NPAST	EXPONENTIAL TRANSFORM INDICATOR	1
NITS	NUMBER OF BATCHES	50	NOLEAK	NON-LEAKAGE INDICATOR	0
NQUIT	NUMBER OF SETS OF BATCHES	1	IEBIAS	ENERGY BIAS INDICATOR	1
NCOLTP	NOT USED	0	NKCALC	BATCH USED IN K-CALCULATION	0
ISTAT	INDICATOR TO STORE LEGRENDRE COEFF	1	NORMF	NORMALIZATION INDICATOR	0

2 $ ARRAY

MEDIA	NUMBER OF CROSS SECTION MEDIA	8	MXREG	NUMBER OF REGIONS	7
NMIX	NUMBER OF MIXING OPERATIONS	19	MFISTP	FISSION INDICATOR	1
MEDALB	ALBEDO INDICATOR	0			

Only neutron is analyzed for neutron dose calculation

3 $ ARRAY

NNGA	NUMBER OF N-GPS TO BE ANALYZED	22	IRDSG	PRINT CROSS SECTIONS AS READ	0
NGGA	NUMBER OF G-GPS TO BE ANALYZED	0	ISTR	PRINT CROSS SECTIONS AS STORED	0
NNGTP	COMPLETELY COUPLED INDICATOR	0	IFMU	PRINT RESULTS OF MU CALCULATION	0
NGOPT	NOT USED	0	IMOM	PRINT MOMENTS OF ANGULAR DISTRIBUTION	0
IGGOPT	NOT USED	0	IPRIN	PRINT ANGLES AND PROBABILITIES	0
NDSN	NUMBER OF ARRAY ANALYSIS COLLISION EDITS	0	IPUN	PRINT BAD LEGENDRE COEF RESULTS	0
NDSG	OPTION OF PATH-LENGTH STRETCHING	9	IXTAPE	LOGICAL UNIT # IF X-S FROM AMPX WORKING LIB	3
NCOEF	NUMBER OF LEGENDRE COEFFICIENTS	4	JXTAPE	LOGICAL UNIT # IF X-S FROM ICE TAPE	0
NSCT	NUMBER OF DISCRETE ANGLES	2	IO6R	NOT USED	0
MAXGP	LAST GP FOR R.R., SPLITTING, OR P.L. STRET	22	MSM	SOURCE PARTICLES MEDIUM NUMBER	0

Not used for homogeneous fuel models (IGO=0 and 1)

Cross section from unit 3 for LATTICECELL option and IGO=0 or 1

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

4 $ ARRAY

ISOUR	SOURCE ENERGY GROUP	0	ISBIAS	SOURCE ENERGY BIAS INDICATOR	1
NGPFS	NUMBER OF SOURCE GROUPS	22	NSOUR	FIXED SOURCE INDICATOR	0

5 $ ARRAY

ND	NUMBER OF DETECTORS	7	NA	NUMBER OF ANGLE BINS	0
NNE	NUMBER OF NEUTRON ENERGY BINS	22	NRESP	NUMBER OF RESPONSE FUNCTIONS	1
NE	NUMBER OF ENERGY BINS	22	NEX	NO OF EXTRA NNGA+NGGA SIZE ARRAYS	6
NT	NUMBER OF TIME BINS	0	NEXND	NUMBER OF EXTRA ND SIZE ARRAYS	4

THE FOLLOWING ANALYSIS SUBROUTINES WILL BE CALLED

SUBROUTINE NRUN VERSION 1
SUBROUTINE NBATCH VERSION 1 } Always called in a MORSE-SGC/S calculation
SUBROUTINE STBTCH VERSION 1
SUBROUTINE SDATA VERSION 1
SUBROUTINE SGAM VERSION 1
SUBROUTINE BDRYX VERSION 1 ← Always called in SAS4
SUBROUTINE RELCOA VERSION -1

SDATA, SGAM, and RELCOA are called when point detectors are input in SAS4

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

6Q ARRAY HAS 10 ENTRIES.

8Q ARRAY HAS 616 ENTRIES.

9Q ARRAY HAS 154 ENTRIES.

10Q ARRAY HAS 183 ENTRIES.

12Q ARRAY HAS 19 ENTRIES.

13Q ARRAY HAS 19 ENTRIES.

14Q ARRAY HAS 19 ENTRIES.

17Q ARRAY HAS 22 ENTRIES.

18Q ARRAY HAS 22 ENTRIES.

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

6 * ARRAY

TMAX	MAXIMUM 91 CPU TIME	0.1500E+02	XMAX	UPPER X LIMIT OF SOURCE VOLUME	0.0000E+00
TCUT	AGE PARTICLES RETIRED	0.0000E+00	YMIN	LOWER Y LIMIT OF SOURCE VOLUME	0.0000E+00
NABP	NEUTR SOURCE ANGUL. BIAS. INDICATOR	0.0000E+00	YMAX	UPPER Y LIMIT OF SOURCE VOLUME	0.0000E+00
NABOG	GAMMA SOURCE ANGUL. BIAS. INDICATOR	0.0000E+00	ZMIN	LOWER Z LIMIT OF SOURCE VOLUME	0.0000E+00
XMIN	LOWER X LIMIT OF SOURCE VOLUME	0.0000E+00	ZMAX	UPPER Z LIMIT OF SOURCE VOLUME	0.0000E+00

7 * ARRAY

GROUP	NEUTRON VELOCITY
1	0.5093E+10
2	0.4608E+10
3	0.4170E+10
4	0.3729E+10
5	0.3290E+10
6	0.2937E+10
7	0.2600E+10
8	0.2287E+10
9	0.2145E+10
10	0.1999E+10
11	0.1677E+10
12	0.1260E+10
13	0.7951E+09
14	0.3307E+09
15	0.6133E+08
16	0.2558E+08
17	0.1115E+08
18	0.6115E+07
19	0.3548E+07
20	0.1999E+07
21	0.1211E+07
22	0.6368E+06

In SAS4, these values are set internally.

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

8 * ARRAY

GROUP	REGION	SPLITTING WT	RR WEIGHT	SURVIVING WT	STRETCH PARAMETERS
1	1	0.4777E+00	0.3908E+00	0.4299E+00	0.2090E+00
2	1	0.5393E+00	0.4412E+00	0.4854E+00	0.1938E+00
3	1	0.5659E+00	0.4630E+00	0.5093E+00	0.1917E+00
4	1	0.6732E+00	0.5508E+00	0.6059E+00	0.1963E+00
5	1	0.8169E+00	0.6684E+00	0.7352E+00	0.1989E+00
6	1	0.8928E+00	0.7305E+00	0.8035E+00	0.1996E+00
7	1	0.9387E+00	0.7621E+00	0.8448E+00	0.1900E+00
8	1	0.9773E+00	0.7917E+00	0.8796E+00	0.2189E+00
9	1	0.9859E+00	0.8029E+00	0.8873E+00	0.2327E+00
10	1	0.1058E+01	0.8302E+00	0.9524E+00	0.2475E+00
11	1	0.1350E+01	0.1018E+01	0.1204E+01	0.2582E+00
12	1	0.1580E+01	0.1113E+01	0.1371E+01	0.2514E+00
13	1	0.2567E+01	0.1794E+01	0.2224E+01	0.1934E+00
14	1	0.1114E+02	0.9113E+01	0.1002E+02	0.2970E-01
15	1	0.1448E+02	0.1145E+02	0.1260E+02	-0.6369E-01
16	1	0.2034E+02	0.1664E+02	0.1831E+02	-0.5992E-01
17	1	0.2546E+02	0.2083E+02	0.2292E+02	-0.4295E-01
18	1	0.1612E+02	0.1319E+02	0.1451E+02	-0.8055E-01
19	1	0.2833E+02	0.2318E+02	0.2549E+02	-0.4646E-01
20	1	0.3874E+01	0.3169E+01	0.3486E+01	-0.1020E-01
21	1	0.5383E+01	0.3765E+01	0.4812E+01	0.1303E+00
22	1	0.8136E+00	0.6574E+00	0.7231E+00	-0.8770E-01
1	2	0.4329E+00	0.3542E+00	0.3896E+00	0.3256E+00
2	2	0.4965E+00	0.4062E+00	0.4469E+00	0.3094E+00
3	2	0.5238E+00	0.4285E+00	0.4714E+00	0.3085E+00
4	2	0.6235E+00	0.5102E+00	0.5612E+00	0.2960E+00
5	2	0.7501E+00	0.6137E+00	0.6751E+00	0.2884E+00
6	2	0.8110E+00	0.6636E+00	0.7299E+00	0.2879E+00
7	2	0.8401E+00	0.6874E+00	0.7561E+00	0.2827E+00
8	2	0.8695E+00	0.7114E+00	0.7825E+00	0.2902E+00
9	2	0.8824E+00	0.7220E+00	0.7941E+00	0.2855E+00
10	2	0.9067E+00	0.7418E+00	0.8160E+00	0.2927E+00
11	2	0.1106E+01	0.9048E+00	0.9953E+00	0.3070E+00
12	2	0.1199E+01	0.9812E+00	0.1079E+01	0.3069E+00
13	2	0.1928E+01	0.1578E+01	0.1736E+01	0.2357E+00
14	2	0.1183E+02	0.9679E+01	0.1065E+02	0.6986E-01
15	2	0.1695E+02	0.1387E+02	0.1526E+02	-0.3641E-01
16	2	0.2391E+02	0.1956E+02	0.2152E+02	-0.4755E-01
17	2	0.2890E+02	0.2364E+02	0.2601E+02	-0.3736E-01
18	2	0.1854E+02	0.1517E+02	0.1668E+02	-0.7572E-01
19	2	0.2565E+02	0.2099E+02	0.2309E+02	-0.6716E-01
20	2	0.3876E+01	0.3171E+01	0.3488E+01	-0.4872E-02
21	2	0.3799E+01	0.3108E+01	0.3419E+01	0.1055E+00
22	2	0.1037E+01	0.8488E+00	0.9337E+00	-0.2455E-01

Russian roulette, splitting, and path length adjustment parameters are generated from the adjoint XSDRNPM-S results

1	3	0.4186E+00	0.3425E+00	0.3768E+00	0.3363E+00	
2	3	0.4848E+00	0.3966E+00	0.4363E+00	0.2896E+00	
3	3	0.5119E+00	0.4189E+00	0.4607E+00	0.2657E+00	
4	3	0.6096E+00	0.4988E+00	0.5487E+00	0.2562E+00	
5	3	0.7341E+00	0.6006E+00	0.6607E+00	0.2501E+00	
6	3	0.7914E+00	0.6475E+00	0.7123E+00	0.2570E+00	
7	3	0.8217E+00	0.6723E+00	0.7396E+00	0.2564E+00	
8	3	0.8447E+00	0.6911E+00	0.7603E+00	0.2567E+00	
9	3	0.8545E+00	0.6991E+00	0.7690E+00	0.2700E+00	
10	3	0.8734E+00	0.7146E+00	0.7860E+00	0.2859E+00	
11	3	0.1068E+01	0.8739E+00	0.9613E+00	0.3190E+00	
12	3	0.1157E+01	0.9468E+00	0.1041E+01	0.3155E+00	

Russian roulette and splitting parameters

Path length adjustment parameters

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

8 * ARRAY

GROUP	REGION	SPLITTING WT	RR WEIGHT	SURVIVING WT	STRETCH PARAMETERS
13	3	0.1854E+01	0.1517E+01	0.1669E+01	0.2362E+00
14	3	0.1222E+02	0.1000E+02	0.1100E+02	0.9028E-01
15	3	0.1977E+02	0.1589E+02	0.1768E+02	-0.2832E-02
16	3	0.3482E+02	0.2298E+02	0.2777E+02	-0.1762E-01
17	3	0.4373E+02	0.2777E+02	0.3394E+02	-0.1889E-01
18	3	0.3206E+02	0.1818E+02	0.2326E+02	-0.4577E-01
19	3	0.3245E+02	0.2316E+02	0.2614E+02	-0.5606E-01
20	3	0.3956E+01	0.3237E+01	0.3561E+01	-0.4847E-02
21	3	0.3222E+01	0.2477E+01	0.2807E+01	0.6914E-01
22	3	0.1386E+01	0.1055E+01	0.1247E+01	0.1027E-01
1	4	0.3510E+00	0.2863E+00	0.3149E+00	0.1090E+00
2	4	0.4083E+00	0.3324E+00	0.3657E+00	0.1122E+00
3	4	0.4320E+00	0.3533E+00	0.3886E+00	0.1244E+00
4	4	0.5237E+00	0.4285E+00	0.4714E+00	0.1643E+00
5	4	0.6505E+00	0.5322E+00	0.5854E+00	0.2104E+00
6	4	0.7000E+00	0.5727E+00	0.6300E+00	0.2163E+00
7	4	0.7354E+00	0.6017E+00	0.6619E+00	0.2237E+00
8	4	0.7608E+00	0.6225E+00	0.6847E+00	0.2459E+00
9	4	0.7636E+00	0.6248E+00	0.6873E+00	0.2558E+00
10	4	0.7689E+00	0.6291E+00	0.6920E+00	0.2650E+00
11	4	0.9556E+00	0.7819E+00	0.8600E+00	0.3249E+00
12	4	0.1033E+01	0.8453E+00	0.9298E+00	0.3263E+00
13	4	0.1643E+01	0.1344E+01	0.1479E+01	0.2483E+00
14	4	0.1278E+02	0.1046E+02	0.1150E+02	0.1433E+00
15	4	0.2628E+02	0.2065E+02	0.2365E+02	0.7849E-01
16	4	0.6715E+02	0.3903E+02	0.5730E+02	0.8383E-01
17	4	0.1073E+03	0.5169E+02	0.9321E+02	0.6137E-01
18	4	0.9095E+02	0.3934E+02	0.7561E+02	0.7957E-01
19	4	0.9641E+02	0.4101E+02	0.8119E+02	0.8997E-01
20	4	0.3864E+01	0.3162E+01	0.3478E+01	-0.3384E-01
21	4	0.2358E+01	0.1913E+01	0.2104E+01	-0.4579E-01
22	4	0.1295E+01	0.1028E+01	0.1130E+01	-0.8788E-01

1	5	0.2863E+00	0.2341E+00	0.2576E+00	0.9525E-02
2	5	0.3318E+00	0.2702E+00	0.2977E+00	0.9043E-02
3	5	0.3532E+00	0.2871E+00	0.3167E+00	0.3847E-01
4	5	0.4295E+00	0.3437E+00	0.3827E+00	0.1141E+00
5	5	0.5356E+00	0.4177E+00	0.4723E+00	0.1897E+00
6	5	0.5751E+00	0.4444E+00	0.5048E+00	0.2036E+00
7	5	0.6059E+00	0.4676E+00	0.5318E+00	0.2169E+00
8	5	0.6273E+00	0.4814E+00	0.5492E+00	0.2479E+00
9	5	0.6279E+00	0.4808E+00	0.5490E+00	0.2596E+00
10	5	0.6286E+00	0.4789E+00	0.5478E+00	0.2678E+00
11	5	0.7809E+00	0.5783E+00	0.6719E+00	0.3505E+00
12	5	0.8405E+00	0.6146E+00	0.7184E+00	0.3640E+00
13	5	0.1332E+01	0.9746E+00	0.1138E+01	0.2782E+00
14	5	0.1128E+02	0.8891E+01	0.1014E+02	0.1992E+00
15	5	0.2768E+02	0.2265E+02	0.2491E+02	0.1512E+00
16	5	0.6716E+02	0.5219E+02	0.6018E+02	0.1557E+00
17	5	0.1026E+03	0.7771E+02	0.8930E+02	0.1090E+00
18	5	0.8869E+02	0.6745E+02	0.7754E+02	0.1359E+00
19	5	0.9379E+02	0.7206E+02	0.8240E+02	0.1520E+00
20	5	0.3732E+01	0.3054E+01	0.3359E+01	-0.8787E-01
21	5	0.1970E+01	0.1612E+01	0.1773E+01	-0.1833E+00
22	5	0.1019E+01	0.8337E+00	0.9171E+00	-0.2601E+00
1	6	0.2430E+00	0.1988E+00	0.2187E+00	-0.3286E+00
2	6	0.2807E+00	0.2296E+00	0.2526E+00	-0.3319E+00

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

8 * ARRAY

GROUP	REGION	SPLITTING WT	RR WEIGHT	SURVIVING WT	STRETCH PARAMETERS
3	6	0.2974E+00	0.2433E+00	0.2676E+00	-0.2259E+00
4	6	0.3477E+00	0.2845E+00	0.3129E+00	-0.3062E-01
5	6	0.4075E+00	0.3322E+00	0.3667E+00	0.1273E+00
6	6	0.4312E+00	0.3476E+00	0.3870E+00	0.1667E+00
7	6	0.4535E+00	0.3621E+00	0.4055E+00	0.1971E+00
8	6	0.4664E+00	0.3658E+00	0.4143E+00	0.2522E+00
9	6	0.4658E+00	0.3652E+00	0.4137E+00	0.2697E+00
10	6	0.4639E+00	0.3650E+00	0.4123E+00	0.2718E+00
11	6	0.5571E+00	0.4101E+00	0.4812E+00	0.4087E+00
12	6	0.5913E+00	0.4295E+00	0.5075E+00	0.4645E+00
13	6	0.9388E+00	0.6954E+00	0.8129E+00	0.3559E+00
14	6	0.8556E+01	0.6013E+01	0.7287E+01	0.2452E+00
15	6	0.2207E+02	0.1585E+02	0.1908E+02	0.2123E+00
16	6	0.4995E+02	0.2362E+02	0.3740E+02	0.2975E+00
17	6	0.7489E+02	0.2872E+02	0.5624E+02	0.3312E+00
18	6	0.6504E+02	0.2828E+02	0.5002E+02	0.3720E+00
19	6	0.6957E+02	0.2517E+02	0.5110E+02	0.4247E+00
20	6	0.3830E+01	0.3133E+01	0.3447E+01	-0.1622E+00
21	6	0.2021E+01	0.1632E+01	0.1796E+01	-0.3620E+00
22	6	0.1170E+01	0.8178E+00	0.8995E+00	-0.6275E+00
1	7	0.2190E+00	0.1256E+00	0.1796E+00	-0.3785E-01
2	7	0.2568E+00	0.1506E+00	0.2131E+00	-0.1063E+00
3	7	0.2698E+00	0.1595E+00	0.2239E+00	-0.2368E-01
4	7	0.2968E+00	0.1613E+00	0.2340E+00	0.6800E-01
5	7	0.3204E+00	0.1589E+00	0.2388E+00	0.1238E+00
6	7	0.3332E+00	0.1621E+00	0.2454E+00	0.2083E+00
7	7	0.3461E+00	0.1728E+00	0.2581E+00	0.2780E+00
8	7	0.3470E+00	0.1798E+00	0.2625E+00	0.3238E+00
9	7	0.3463E+00	0.1820E+00	0.2637E+00	0.3583E+00
10	7	0.3468E+00	0.1817E+00	0.2641E+00	0.3901E+00
11	7	0.3807E+00	0.1850E+00	0.2780E+00	0.5325E+00
12	7	0.4001E+00	0.2015E+00	0.2980E+00	0.6030E+00
13	7	0.6558E+00	0.3457E+00	0.4993E+00	0.5191E+00
14	7	0.5588E+01	0.2487E+01	0.3835E+01	0.2367E+00
15	7	0.1478E+02	0.6251E+01	0.9872E+01	0.2226E+00
16	7	0.1861E+02	0.5884E+01	0.1009E+02	0.2316E+00
17	7	0.1932E+02	0.5535E+01	0.9737E+01	0.3101E+00
18	7	0.1914E+02	0.5350E+01	0.9484E+01	0.3126E+00
19	7	0.1584E+02	0.5141E+01	0.8612E+01	0.2472E+00
20	7	0.5446E+01	0.4067E+01	0.4619E+01	-0.4027E-01
21	7	0.4737E+01	0.2494E+01	0.3565E+01	-0.1631E+00
22	7	0.7942E+01	0.1847E+01	0.3852E+01	-0.2635E+00

9 * ARRAY

GROUP	REGION	RELATIVE IMPORTANCE
1	1	0.1123E-05
2	1	0.9950E-06
3	1	0.9483E-06
4	1	0.7971E-06
5	1	0.6569E-06
6	1	0.6010E-06
7	1	0.5717E-06
8	1	0.5491E-06
9	1	0.5443E-06
10	1	0.5071E-06
11	1	0.4010E-06
12	1	0.3522E-06
13	1	0.2172E-06
14	1	0.4818E-07
15	1	0.3834E-07
16	1	0.2638E-07
17	1	0.2107E-07
18	1	0.3329E-07
19	1	0.1894E-07
20	1	0.1385E-06
21	1	0.1004E-06
22	1	0.6679E-06
1	2	0.1240E-05
2	2	0.1081E-05
3	2	0.1025E-05
4	2	0.8606E-06
5	2	0.7154E-06
6	2	0.6617E-06
7	2	0.6387E-06
8	2	0.6172E-06
9	2	0.6081E-06
10	2	0.5918E-06
11	2	0.4852E-06
12	2	0.4474E-06
13	2	0.2783E-06
14	2	0.4536E-07
15	2	0.3166E-07
16	2	0.2244E-07
17	2	0.1857E-07
18	2	0.2895E-07
19	2	0.2092E-07
20	2	0.1384E-06
21	2	0.1413E-06
22	2	0.5173E-06

Collision energy biasing parameters calculated from the adjoint XSDRNPM-S results. They are input as function of energy group and importance region.

1	3	0.1282E-05
2	3	0.1107E-05
3	3	0.1048E-05
4	3	0.8802E-06
5	3	0.7310E-06
6	3	0.6781E-06
7	3	0.6530E-06
8	3	0.6352E-06
9	3	0.6280E-06
10	3	0.6144E-06
11	3	0.5024E-06
12	3	0.4637E-06

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

9 * ARRAY

GROUP	REGION	RELATIVE IMPORTANCE
13	3	0.2894E-06
14	3	0.4390E-07
15	3	0.2732E-07
16	3	0.1739E-07
17	3	0.1423E-07
18	3	0.2076E-07
19	3	0.1848E-07
20	3	0.1356E-06
21	3	0.1721E-06
22	3	0.3872E-06
1	4	0.1533E-05
2	4	0.1321E-05
3	4	0.1243E-05
4	4	0.1025E-05
5	4	0.8249E-06
6	4	0.7666E-06
7	4	0.7297E-06
8	4	0.7053E-06
9	4	0.7027E-06
10	4	0.6979E-06
11	4	0.5615E-06
12	4	0.5194E-06
13	4	0.3266E-06
14	4	0.4199E-07
15	4	0.2042E-07
16	4	0.8429E-08
17	4	0.5181E-08
18	4	0.6387E-08
19	4	0.5949E-08
20	4	0.1389E-06
21	4	0.2296E-06
22	4	0.4272E-06
1	5	0.1875E-05
2	5	0.1622E-05
3	5	0.1525E-05
4	5	0.1262E-05
5	5	0.1023E-05
6	5	0.9568E-06
7	5	0.9082E-06
8	5	0.8794E-06
9	5	0.8798E-06
10	5	0.8817E-06
11	5	0.7187E-06
12	5	0.6722E-06
13	5	0.4245E-06

14	5	0.4761E-07
15	5	0.1938E-07
16	5	0.8026E-08
17	5	0.5408E-08
18	5	0.6229E-08
19	5	0.5861E-08
20	5	0.1438E-06
21	5	0.2724E-06
22	5	0.5266E-06
1	6	0.2208E-05
2	6	0.1912E-05

9 * ARRAY

GROUP	REGION	RELATIVE IMPORTANCE
3	6	0.1805E-05
4	6	0.1543E-05
5	6	0.1317E-05
6	6	0.1248E-05
7	6	0.1191E-05
8	6	0.1166E-05
9	6	0.1167E-05
10	6	0.1171E-05
11	6	0.1004E-05
12	6	0.9516E-06
13	6	0.5941E-06
14	6	0.6627E-07
15	6	0.2532E-07
16	6	0.1291E-07
17	6	0.8588E-08
18	6	0.9654E-08
19	6	0.9451E-08
20	6	0.1401E-06
21	6	0.2690E-06
22	6	0.5369E-06
1	7	0.2689E-05
2	7	0.2266E-05
3	7	0.2157E-05
4	7	0.2064E-05
5	7	0.2022E-05
6	7	0.1968E-05
7	7	0.1871E-05
8	7	0.1840E-05
9	7	0.1831E-05
10	7	0.1829E-05
11	7	0.1737E-05
12	7	0.1620E-05
13	7	0.9673E-06
14	7	0.1259E-06
15	7	0.4892E-07
16	7	0.4786E-07
17	7	0.4960E-07
18	7	0.5092E-07
19	7	0.5608E-07
20	7	0.1046E-06
21	7	0.1355E-06
22	7	0.1254E-06

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

10 * ARRAY, FISSION NEUTRON WEIGHTS

REGION	NEUTRON WEIGHT
1	0.1353E+01
2	0.1149E+01
3	0.1121E+01
4	0.1022E+01
5	0.8165E+00
6	0.5937E+00
7	0.3541E+00

Weights given to fission neutrons as a function of importance region.

12$, 13$, AND 14* ARRAYS

MEDIUM	ELEMENT	DENSITY
7	92235	5.2672E-05
5	592235	1.0700E-04
7	92238	6.1692E-03
5	592238	4.7700E-02
7	94239	3.2759E-05
7	94240	1.4960E-05
7	8016	1.2550E-02
7	308016	5.0406E-21
7	40000	1.7799E-03
4	24000	1.6620E-02
4	25055	1.2000E-03
4	26000	5.7750E-02
4	28000	7.5200E-03
4	42000	1.1000E-04
1	42000	1.0000E-10
2	42000	1.0000E-10
3	42000	1.0000E-10
6	42000	1.0000E-10
8	42000	1.0000E-10

Cross-section mixing table

17* AND 18* ARRAYS

GROUP	FS(IG)	BFS(IG)
1	2.4740E-13	1.1234E-06
2	2.0960E-12	9.9504E-07
3	5.7660E-12	9.4826E-07
4	2.8990E-11	7.9711E-07
5	7.2280E-11	6.5689E-07
6	1.4570E-10	6.0103E-07
7	6.0990E-10	5.7168E-07
8	4.5420E-10	5.4908E-07
9	9.0700E-11	5.4430E-07
10	3.8240E-10	5.0709E-07
11	4.9900E-10	4.0105E-07
12	3.9820E-10	3.5219E-07
13	1.8360E-10	2.1718E-07
14	1.7610E-14	4.8179E-08
15	0.0000E+00	3.8339E-08
16	0.0000E+00	2.6382E-08
17	0.0000E+00	2.1075E-08
18	0.0000E+00	3.3293E-08
19	0.0000E+00	1.8944E-08
20	0.0000E+00	1.3853E-07
21	0.0000E+00	1.0036E-07
22	0.0000E+00	6.6789E-07

Source energy biasing parameters

Source energy spectrum

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

19Q ARRAY HAS 21 ENTRIES.

20Q ARRAY HAS 22 ENTRIES.

21Q ARRAY HAS 22 ENTRIES.

CORE AVAILABLE FOR MIXING = 185409
CORE NEEDED FOR MIXING = 1154

TOTAL STORAGE SPACE = 187904
LENGTH OF NON CROSS SECTION DATA = 15939
SPACE FOR XSEC DATA AND SUPERGROUP DATA = 171965
MINIMUM SPACE NEEDED FOR CROSS SECTIONS = 968
TOTAL STORAGE NEEDED FOR CROSS SECTIONS = 9614

NUMBER OF SUPERGROUPS = 1
SPACE FOR CROSS SECTIONS = 171826

FISSION SPECTRUM

IGM	MEDI 1	MEDI 2	MEDI 3	MEDI 4	MEDI 5	MEDI 6	MEDI 7	MEDI 8
1	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.36070E-04	0.00000E+00	3.36070E-04	0.00000E+00
2	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.79267E-03	0.00000E+00	1.79267E-03	0.00000E+00
3	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.50127E-03	0.00000E+00	6.50127E-03	0.00000E+00
4	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.31053E-02	0.00000E+00	2.31053E-02	0.00000E+00
5	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	5.92003E-02	0.00000E+00	5.92003E-02	0.00000E+00
6	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.07389E-01	0.00000E+00	1.07389E-01	0.00000E+00
7	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.12259E-01	0.00000E+00	2.12259E-01	0.00000E+00
8	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	2.98587E-01	0.00000E+00	2.98587E-01	0.00000E+00
9	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	3.19251E-01	0.00000E+00	3.19251E-01	0.00000E+00
10	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	4.34711E-01	0.00000E+00	4.34711E-01	0.00000E+00
11	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	6.47302E-01	0.00000E+00	6.47302E-01	0.00000E+00
12	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	8.46322E-01	0.00000E+00	8.46322E-01	0.00000E+00
13	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	9.85752E-01	0.00000E+00	9.85752E-01	0.00000E+00
14	0.00000E+00	0.00000E+00	0.00000E+00	0.00000E+00	1.00000E+00	0.00000E+00	1.00000E+00	0.00000E+00

IGM 15 THRU IGM 22 SAME AS ABOVE

Fission spectrum by medium (mixture) number

GROUP	FS	BFS
1	4.29918E-01	2.00292E-04
2	4.85359E-01	1.70336E-03
3	5.09302E-01	5.64383E-03
4	6.05879E-01	2.22976E-02
5	7.35214E-01	5.65155E-02
6	8.03546E-01	1.19626E-01
7	8.44793E-01	3.70906E-01
8	8.79572E-01	5.50638E-01
9	8.87296E-01	5.86216E-01
10	9.52389E-01	7.25967E-01
11	1.20422E+00	8.70192E-01
12	1.37128E+00	9.71263E-01
13	2.22374E+00	1.00000E+00
14	1.00240E+01	1.00000E+00
15	0.00000E+00	1.00000E+00
16	0.00000E+00	1.00000E+00
17	0.00000E+00	1.00000E+00
18	0.00000E+00	1.00000E+00
19	0.00000E+00	1.00000E+00
20	0.00000E+00	1.00000E+00
21	0.00000E+00	1.00000E+00
22	0.00000E+00	1.00000E+00

Biased source energy spectrum in CDF

Weight correction factors due to source energy biasing

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

DETECTOR		Y	Z	RAD	TO
1	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
2	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
3	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
4	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00
5	1.4869E+02	0.0000E+00	0.0000E+00	1.4869E+02	2.9196E-08
6	2.4013E+02	0.0000E+00	0.0000E+00	2.4013E+02	4.7151E-08
7	1.2191E+02	0.0000E+00	3.0596E+02	3.2935E+02	6.4671E-08

Detectors 1 to 4 are surface detectors and detectors 5, 6, and 7 are point detectors.

Coordinates of the point detectors input by the user in SAS4

RESPONSE FUNCTIONS

GROUP	RESP(1)
1	1.9448E-04
2	1.5971E-04
3	1.4706E-04
4	1.4772E-04
5	1.5339E-04
6	1.5062E-04
7	1.3892E-04
8	1.2843E-04
9	1.2527E-04
10	1.2632E-04
11	1.2894E-04
12	1.1687E-04
13	6.5278E-05
14	9.1897E-06
15	3.7134E-06
16	4.0086E-06
17	4.2946E-06
18	4.4761E-06
19	4.5673E-06
20	4.5355E-06
21	4.3701E-06
22	3.7147E-06

SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK MONDAY, JANUARY 11,1988

PRIMARY ENERGY BINS

BIN NO	LOWER GROUP NO	LOWER ENERGY LIMIT
1	1	1.2200E+07
2	2	1.0000E+07
3	3	8.1800E+06
4	4	6.3600E+06
5	5	4.9600E+06
6	6	4.0600E+06
7	7	3.0100E+06
8	8	2.4600E+06
9	9	2.3500E+06
10	10	1.8300E+06
11	11	1.1100E+06
12	12	5.5000E+05
13	13	1.1100E+05
14	14	3.3500E+03
15	15	5.8300E+02
16	16	1.0100E+02
17	17	2.9000E+01
18	18	1.0100E+01
19	19	3.0600E+00
20	20	1.1200E+00
21	21	4.1400E-01
22	22	1.0000E-02

TIME REQUIRED FOR INPUT WAS 1 SECOND.
***START BATCH 1 RANDOM=F2AE3EBFB1EB

SOURCE DATA

WTAVE	IAVE	UAVE	VAVE	WAVE	XAVE	YAVE	ZAVE	AGEAVE
9.827E+01	9.16	-0.1388	-0.0647	0.0373	-3.033E+00	4,522E+00	9.790E+00	0.000E+00

UNCOL RESPONSES BY RESP. FUNCTION & DETECTOR:

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	3.9503E-13	3.4656E-13	9.9898E-15

TOTAL RESPONSES BY RESP. FUNCTION & DETECTOR:

5.6340E-10	1.3804E-10	7.2226E-11	4.3355E-11	1.4432E-10	7.1694E-11	8.3341E-12

For point detectors, source neutrons, and fission neutrons make uncollided contributions to the results. For surface detectors, contributions are stored in total response array.

NUMBER OF COLLISIONS OF TYPE NCOLL

SOURCE SPLIT(D)	FISHN	GAMGEN	REALCOLL	ALBEDO	BDRYX	ESCAPE	E-CUT	TIMEKILL	R R KILL	R R SURV	GAMLOST
100	478	2390	41	3053	0	3083	187	0	0	432	998	0

TIME REQUIRED FOR THE PRECEDING BATCH WAS 10 SECONDS.
***START BATCH 2 RANDOM=0B83E5794FF7

SOURCE DATA

WTAVE	IAVE	UAVE	VAVE	WAVE	XAVE	YAVE	ZAVE	AGEAVE
9.871E+01	9.06	0.0138	0.0568	-0.0516	-4.656E-01	1.450E-01	-2.268E+01	0.000E+00

UNCOL RESPONSES BY RESP. FUNCTION & DETECTOR:

0.0000E+00	0.0000E+00	0.0000E+00	0.0000E+00	9.5948E-14	5.6369E-14	1.3359E-18

TOTAL RESPONSES BY RESP. FUNCTION & DETECTOR:

4.3583E-10	1.0152E-10	4.6807E-11	2.7848E-11	1.1187E-10	5.5596E-11	8.9683E-12

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NUMBER OF COLLISIONS OF TYPE NCOLL
  SOURCE SPLIT(D)    FISHN   GAMGEN REALCOLL   ALBEDO    BDRYX   ESCAPE    E-CUT TIMEKILL R R KILL R R SURV  GAMLOST
     100      375     2076       44     2681        0     2477      139        0        0      380      792        0

TIME REQUIRED FOR THE PRECEDING BATCH WAS 8 SECONDS.
***START BATCH    3                          RANDOM=F1C3541E83A3

SOURCE DATA
  WTAVE        IAVE    UAVE    VAVE    WAVE       XAVE       YAVE       ZAVE       AGEAVE
 9.980E+01     9.22  -0.0196  0.0091  0.0548   1.149E+00  2.703E+00 -1.333E+01   0.000E+00
UNCOL RESPONSES BY RESP. FUNCTION & DETECTOR:
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  3.3289E-14  3.2205E-14  7.4125E-18
TOTAL RESPONSES BY RESP. FUNCTION & DETECTOR:
  4.4651E-10  1.1872E-10  5.7442E-11  3.3465E-11  1.8170E-10  9.0558E-11  1.8970E-11

NUMBER OF COLLISIONS OF TYPE NCOLL
  SOURCE SPLIT(D)    FISHN   GAMGEN REALCOLL   ALBEDO    BDRYX   ESCAPE    E-CUT TIMEKILL R R KILL R R SURV  GAMLOST
     100      442     2269       49     2906        0     2624      160        0        0      431      937        0

TIME REQUIRED FOR THE PRECEDING BATCH WAS 10 SECONDS.
```



```
***START BATCH   49                          RANDOM=CEB25AFC987F

SOURCE DATA
  WTAVE        IAVE    UAVE    VAVE    WAVE       XAVE       YAVE       ZAVE       AGEAVE
 9.940E+01     9.22   0.0565  0.0795 -0.0941   4.556E+00 -5.433E+00  1.273E+01   0.000E+00
UNCOL RESPONSES BY RESP. FUNCTION & DETECTOR:
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.8894E-13  2.7244E-13  1.4115E-15
TOTAL RESPONSES BY RESP. FUNCTION & DETECTOR:
  4.4884E-10  9.1462E-11  4.4420E-11  2.6730E-11  1.0237E-10  5.1473E-11  1.0288E-11

NUMBER OF COLLISIONS OF TYPE NCOLL
  SOURCE SPLIT(D)    FISHN   GAMGEN REALCOLL   ALBEDO    BDRYX   ESCAPE    E-CUT TIMEKILL R R KILL R R SURV  GAMLOST
     100      423     2517       41     3086        0     2545      152        0        0      412      955        0

TIME REQUIRED FOR THE PRECEDING BATCH WAS 9 SECONDS.
***START BATCH   50                          RANDOM=EC3CB3E2585F

SOURCE DATA
  WTAVE        IAVE    UAVE    VAVE    WAVE       XAVE       YAVE       ZAVE       AGEAVE
 1.004E+02     9.30  -0.0233 -0.0050  0.0397   1.083E+00 -3.815E+00  1.904E+01   0.000E+00
UNCOL RESPONSES BY RESP. FUNCTION & DETECTOR:
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.0647E-13  1.7823E-13  1.1021E-15
TOTAL RESPONSES BY RESP. FUNCTION & DETECTOR:
  5.8814E-10  1.2744E-10  5.6455E-11  2.8596E-11  1.4878E-10  8.1065E-11  1.1325E-11

NUMBER OF COLLISIONS OF TYPE NCOLL
  SOURCE SPLIT(D)    FISHN   GAMGEN REALCOLL   ALBEDO    BDRYX   ESCAPE    E-CUT TIMEKILL R R KILL R R SURV  GAMLOST
     100      472     2547       59     3250        0     3059      199        0        0      432     1046        0

TIME REQUIRED FOR THE PRECEDING BATCH WAS 11 SECONDS.
```

Tallies of source particles in each batch:

WTAVE	- total weight of source particles
IAVE	- mean energy group number of source particles
UAVE	- mean direction cosine with respect to the X axis
VAVE	- mean direction cosine with respect to the Y axis
WAVE	- mean direction cosine with respect to the Z axis
XAVE	- mean X-coordinate
YAVE	- mean Y-coordinate
ZAVE	- mean Z-coordinate
AGEAVE	- mean age (used for time-dependent problems)

Tallies of different events in each batch:

SOURCE	- number of source particles
SPLIT	- number of split particles
FISHN	- number of collisions in fissile materials
GAMGEN	- number of secondary particles generated (fission neutrons in this case)
REALCOLL	- number of collisions
ALBEDO	- number of particles crossing albedo boundaries
BDRYX	- number of particles crossing zone boundaries
ESCAPE	- number of particles escape from the system
E-CUT	- number of particles terminated by energy cutoff
TIMEKILL	- number of particles terminated by time cutoff
R R KILL	- number of particles
R R SURV	- number of particles survive Russian roulette
GAMLOST	- number of secondary particles lost due to lack of storage space

Note: SOURCE + SPLIT + GAMGEN = ESCAPE + E-CUT + TIMEKILL + R R KILL

For batch 1, 100 + 478 + 41 = 187 + 0 + 0 + 432 = 619

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO. OF ENTRIES	LOC. FOR NEXT ZONE
1	1				
		228	2	48230	645
		645	8	1371	0
1	-19				
		233	19	39525	0
2	2				
		239	3	80114	633
		633	4	2511	648
		648	12	595	0
2	-10				
		244	1	39877	666
		666	8	141	0
3	3				
		250	4	80115	696
		696	5	1	0
3	-2				
		255	2	30867	0
4	4				
		261	5	82627	0
4	-3				
		266	3	30869	0
5	5				
		272	6	119068	651
		651	11	1570	678
		678	7	3	690
		690	14	2	0
5	-13				
		277	4	30870	657
		657	12	62	663
		663	10	61	0
6	6				
		283	7	119068	0
6	-5				
		288	0	0	0
7	7				
		294	13	119067	681
		681	14	4	0
7	-6				
		299	0	0	0
7	-5				
		304	0	0	0
8	8				
		310	9	928	654
		654	2	424	672
		672	5	1	0
8	-1				

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO. OF ENTRIES	LOC. FOR NEXT ZONE
8	-1	315	1	362	0
9	9	321	10	928	0
9	-8	326	8	61	0
10	10	332	5	928	0
10	-9	337	9	61	0
11	11	343	13	1572	0
11	-5	348	0	0	0
11	-12	353	0	0	0
12	13	359	5	595	0
12	-4	364	2	62	0
12	-10	369	0	0	0
13	14	375	15	45797	0
13	-5	380	0	0	0
13	-7	385	0	0	0
13	-11	390	0	0	0
14	12	396	13	4	693
		693	11	2	0
14	-5	401	0	0	0
14	-7	406	0	0	0
15	15	412	16	8374	0
15	-14	417	0	0	0
16	16	423	17	8374	0
16	-15	428	0	0	0
17	17				

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO. OF ENTRIES	LOC. FOR NEXT ZONE
17	17	434	18	8374	0
17	-16	439	0	0	0
18	18	445	0	0	0
18	-17	450	0	0	0
19	19	456	1	46756	0
19	-20	461	20	39523	0
20	20	467	19	46754	669
		669	1	9	0
20	-32	472	29	27406	630
		630	31	843	636
		636	22	244	660
		660	30	100	675
		675	32	3	0
21	31	478	20	1	0
21	-30	483	31	1	0
21	-25	488	28	1	0
22	29	494	20	497	687
		687	31	1	0
22	-28	499	0	0	0
22	-23	504	25	243	0
23	27	510	0	0	0
23	-21	515	0	0	0
24	25	521	29	33423	0
24	-30	526	28	27405	0
25	23	532	28	17768	642
		642	22	497	0
25	-28				

COMBINATORIAL GEOMETRY ZONE TRANSFER SUMMARY TABLES

EXIT ZONE	EXIT BODY	LOC. IN MA ARRAY	ENTERING ZONE	NO. OF ENTRIES	LOC. FOR NEXT ZONE
25	-28	537	27	9423	0
26	21	543	27	28	0
27	22	549	25	10559	639
		639	30	241	0
27	-21	554	26	28	0
28	24	560	24	33423	627
		627	31	1673	0
28	-23	565	25	16886	0
29	26	571	20	33424	0
29	-25	576	24	27405	0
30	28	582	20	241	0
30	-27	587	0	0	0
30	-22	592	27	100	0
31	30	598	20	1672	684
		684	21	1	0
31	-29	603	0	0	0
31	-24	608	28	845	0
32	32	614	20	1	0
32	-31	619	21	2	0
32	-26	624	0	0	0

THIS CASE WAS RUN ON MONDAY, JANUARY 11,1988

ANSI STANDARD NEUTRON DOSE RATE (REM PER HOUR)

	RESPONSES(DETECTOR)			
DETECTOR	UNCOLL RESPONSE	FSD UNCOLL	TOTAL RESPONSE	FSD TOTAL
1	0.0000E+00	0.00000	5.0626E-10	0.02740
2	0.0000E+00	0.00000	1.1447E-10	0.02337
3	0.0000E+00	0.00000	5.5269E-11	0.02376
4	0.0000E+00	0.00000	3.2709E-11	0.02537
5	6.8480E-13	0.23264	1.4098E-10	0.03296
6	3.7414E-13	0.16422	7.1925E-11	0.03020
7	2.4311E-14	0.45406	3.0920E-11	0.31118

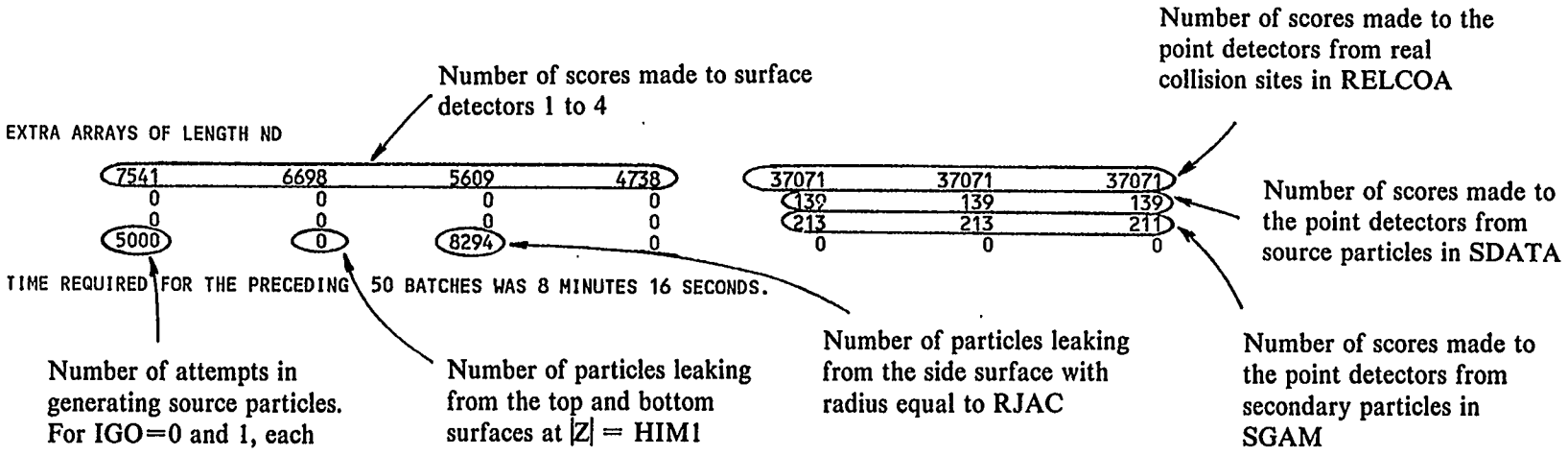
Detectors 1 to 4 are radial surface detectors, respectively, at radii 57.27, 157.27, 257.27, and 357.27 cm (see surface detector information in SAS4 output). Detectors 5, 6,and 7 are the point detectors input by the user. The results are presented in dose rate (rem per hour) per source strength input by the user. For this problem, a unity source strength was input. Since there are 7 PWR assemblies each emitting 2.614×10^8 neutrons per second, the total source strength is 1.8298×10^9 neutrons per second. Hence, the total responses must be multiplied by 1.8298×10^9 to obtain the correct dose rates.

FLUENCE(ENERGY,DETECTOR) PARTICLES/SEC/CM**2/EV

DETECTOR NO. ENERGIES	1	2	3	4	5	6	7
1.492E+07	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
	0.000	0.000	0.000	0.000	0.000	0.000	0.000
1.220E+07	4.244E-16	1.160E-16	6.955E-17	2.163E-17	3.976E-16	1.120E-17	1.086E-20
	0.700	0.705	0.706	1.000	0.880	3.846	1.256
1.000E+07	9.997E-16	3.468E-16	1.776E-16	1.277E-16	4.438E-16	2.151E-16	2.693E-20
	0.462	0.461	0.522	0.522	0.643	0.603	7.785
8.180E+06	4.604E-15	1.362E-15	7.700E-16	5.021E-16	2.277E-15	5.432E-16	3.019E-17
	0.377	0.364	0.355	0.384	0.482	0.410	0.709
6.360E+06	9.273E-15	1.889E-15	8.935E-16	4.938E-16	3.175E-15	2.065E-15	1.723E-16
	0.290	0.284	0.282	0.297	0.401	0.293	0.560
4.960E+06	3.159E-14	9.130E-15	5.138E-15	3.264E-15	9.888E-15	5.573E-15	1.989E-14
	0.168	0.181	0.186	0.189	0.286	0.232	0.981
4.060E+06	8.736E-14	2.278E-14	1.112E-14	6.923E-15	2.231E-14	1.119E-14	2.150E-15
	0.103	0.108	0.101	0.108	0.161	0.107	0.606
3.010E+06	1.281E-13	3.443E-14	1.775E-14	1.048E-14	3.637E-14	2.427E-14	4.043E-15
	0.117	0.103	0.107	0.117	0.133	0.104	0.410
2.460E+06	1.954E-13	5.586E-14	3.051E-14	1.845E-14	6.766E-14	2.732E-14	8.520E-15
	0.159	0.162	0.170	0.173	0.265	0.218	0.572
2.350E+06	1.892E-13	4.320E-14	2.227E-14	1.392E-14	5.714E-14	3.210E-14	4.600E-15
	0.094	0.087	0.090	0.097	0.116	0.096	0.288
1.830E+06	3.149E-13	6.927E-14	3.261E-14	1.944E-14	9.674E-14	5.266E-14	9.060E-14
	0.079	0.063	0.071	0.083	0.084	0.073	0.894
1.110E+06	2.329E-12	5.422E-13	2.606E-13	1.523E-13	6.394E-13	3.423E-13	1.007E-13
	0.049	0.047	0.051	0.054	0.045	0.039	0.238
5.500E+05	9.445E-12	2.071E-12	9.948E-13	5.886E-13	2.607E-12	1.270E-12	4.165E-13
	0.036	0.032	0.033	0.036	0.044	0.038	0.217
1.110E+05	8.695E-12	1.577E-12	7.158E-13	4.105E-13	1.884E-12	9.436E-13	2.192E-13
	0.201	0.163	0.149	0.160	0.152	0.137	0.229
3.350E+03	2.953E-11	9.923E-12	4.181E-12	1.779E-12	1.813E-11	7.852E-12	6.816E-13
	0.440	0.444	0.574	0.703	0.515	0.438	0.898
5.830E+02	1.123E-10	1.882E-11	0.000E+00	0.000E+00	1.255E-12	5.282E-13	2.577E-14
	1.000	1.000	0.000	0.000	0.544	0.438	0.924

FLUENCE(ENERGY,DETECTOR) PARTICLES/SEC/CM**2/EV

DETECTOR NO. ENERGIES	1	2	3	4	5	6	7
1.010E+02	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	1.830E-15 0.043	9.139E-16 0.034	3.578E-16 0.299
2.900E+01	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	1.687E-15 0.042	8.414E-16 0.035	3.270E-16 0.292
1.010E+01	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	1.826E-15 0.042	9.111E-16 0.035	3.441E-16 0.298
3.060E+00	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	1.654E-15 0.042	8.273E-16 0.035	3.098E-16 0.298
1.120E+00	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	1.620E-15 0.043	8.103E-16 0.035	3.037E-16 0.299
4.140E-01	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	0.000E+00 0.000	2.566E-24 0.443	1.125E-24 0.371	6.708E-28 1.004
1.000E-02							


Number of scores made to surface detectors 1 to 4
Number of scores made to the point detectors from real collision sites in RELCOA
EXTRA ARRAYS OF LENGTH ND
7541 6698 5609 4738
0 0 0 0
0 0 0 0
5000 0 8294 0
37071 37071 37071
139 139 139
213 213 211
0 0 0
Number of scores made to the point detectors from source particles in SDATA
TIME REQUIRED FOR THE PRECEDING 50 BATCHES WAS 8 MINUTES 16 SECONDS.
Number of attempts in generating source particles. For IGO=0 and 1, each attempt generates a source particle.
Number of particles leaking from the top and bottom surfaces at |Z| = HIM1
Number of particles leaking from the side surface with radius equal to RJAC
Number of scores made to the point detectors from secondary particles in SGAM

NEUTRON DEATHS	NUMBER	WEIGHT
KILLED BY RUSSIAN ROULETTE	20764	0.17917E+05
ESCAPED	8374	0.31097E+04
REACHED ENERGY CUTOFF	0	0.00000E+00
REACHED TIME CUTOFF	0	0.00000E+00

NUMBER OF SCATTERINGS

MEDIUM	NUMBER
1	0
2	0
3	0
4	32036
5	80998
6	0
7	36536
8	0

Scattering occurs only in medium with finite total cross sections. For this case, media 1, 2, 3, 6, and 8 either have extremely small total cross sections to represent a void or they were not used in the geometry.

REAL SCATTERING COUNTERS

ENERGY GROUP	REGION 1 NUMBER	REGION 1 WEIGHT	REGION 2 NUMBER	REGION 2 WEIGHT	REGION 3 NUMBER	REGION 3 WEIGHT	REGION 4 NUMBER	REGION 4 WEIGHT	REGION 5 NUMBER	REGION 5 WEIGHT	REGION 6 NUMBER	REGION 6 WEIGHT
1	10	3.69E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	1	3.74E-01	0	0.00E+00
2	12	5.06E+00	0	0.00E+00	6	2.95E+00	6	2.64E+00	8	2.63E+00	5	1.19E+00
3	46	2.22E+01	0	0.00E+00	17	7.37E+00	17	6.45E+00	19	6.28E+00	12	3.26E+00
4	184	1.05E+02	3	1.61E+00	45	2.50E+01	65	3.38E+01	76	3.20E+01	31	1.11E+01
5	311	2.27E+02	2	1.29E+00	78	5.32E+01	134	8.11E+01	157	8.19E+01	92	3.67E+01
6	559	4.50E+02	5	3.98E+00	140	1.07E+02	206	1.39E+02	241	1.37E+02	129	5.59E+01
7	2524	2.12E+03	16	1.24E+01	436	3.46E+02	653	4.67E+02	818	4.78E+02	455	1.99E+02
8	1738	1.52E+03	22	1.72E+01	402	3.29E+02	603	4.45E+02	683	4.06E+02	355	1.60E+02
9	364	3.22E+02	2	1.49E+00	94	7.54E+01	136	1.04E+02	172	1.04E+02	99	4.41E+01
10	1560	1.45E+03	9	7.19E+00	446	3.59E+02	657	4.95E+02	727	4.34E+02	370	1.57E+02
11	2993	3.40E+03	58	5.58E+01	715	6.95E+02	1069	9.43E+02	1205	8.42E+02	850	4.16E+02
12	8916	1.14E+04	170	1.80E+02	1931	1.96E+03	4497	4.13E+03	7127	5.12E+03	5177	2.58E+03
13	16807	3.46E+04	451	7.58E+02	5184	8.33E+03	12361	1.74E+04	20840	2.30E+04	16159	1.26E+04
14	1820	1.78E+04	23	2.38E+02	792	8.45E+03	786	8.54E+03	1264	1.21E+04	952	6.46E+03
15	79	9.95E+02	0	0.00E+00	67	1.08E+03	43	9.30E+02	51	1.20E+03	47	7.78E+02
16	8	1.45E+02	0	0.00E+00	0	0.00E+00	4	1.75E+02	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	1	6.54E+01	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7 NUMBER	REGION 7 WEIGHT
1	0	0.00E+00
2	3	6.83E-01
3	3	8.91E-01
4	26	7.91E+00
5	80	2.19E+01
6	106	3.17E+01
7	358	1.10E+02
8	291	8.94E+01
9	102	3.02E+01
10	413	1.20E+02
11	813	2.73E+02
12	4451	1.56E+03
13	13062	6.94E+03
14	1340	5.23E+03
15	117	1.07E+03
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

FISSION PRODUCTION COUNTERS

ENERGY GROUP	REGION 1		REGION 2		REGION 3		REGION 4		REGION 5		REGION 6	
	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT
1	1	1.35E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
2	0	0.00E+00	0	0.00E+00	0	0.00E+00	1	1.02E+00	0	0.00E+00	2	1.19E+00
3	6	8.12E+00	0	0.00E+00	0	0.00E+00	1	1.02E+00	5	4.08E+00	5	2.97E+00
4	29	3.92E+01	0	0.00E+00	0	0.00E+00	20	2.04E+01	13	1.06E+01	12	7.12E+00
5	27	3.65E+01	0	0.00E+00	0	0.00E+00	21	2.15E+01	29	2.37E+01	18	1.07E+01
6	33	4.47E+01	0	0.00E+00	0	0.00E+00	25	2.56E+01	34	2.78E+01	25	1.48E+01
7	191	2.58E+02	1	1.15E+00	0	0.00E+00	83	8.49E+01	115	9.39E+01	57	3.38E+01
8	140	1.89E+02	3	3.45E+00	0	0.00E+00	67	6.85E+01	89	7.27E+01	39	2.32E+01
9	29	3.92E+01	0	0.00E+00	0	0.00E+00	28	2.86E+01	28	2.29E+01	14	8.31E+00
10	156	2.11E+02	0	0.00E+00	0	0.00E+00	94	9.61E+01	114	9.31E+01	42	2.49E+01
11	128	1.73E+02	1	1.15E+00	0	0.00E+00	76	7.77E+01	79	6.45E+01	59	3.50E+01
12	41	5.55E+01	0	0.00E+00	0	0.00E+00	12	1.23E+01	14	1.14E+01	11	6.53E+00
13	61	8.25E+01	0	0.00E+00	0	0.00E+00	11	1.12E+01	29	2.37E+01	19	1.13E+01
14	39	5.28E+01	0	0.00E+00	0	0.00E+00	9	9.20E+00	11	8.98E+00	10	5.94E+00
15	6	8.12E+00	0	0.00E+00	0	0.00E+00	2	2.04E+00	7	5.72E+00	3	1.78E+00
16	1	1.35E+00	0	0.00E+00	0	0.00E+00	1	1.02E+00	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	1	1.02E+00	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7	
	NUMBER	WEIGHT
1	0	0.00E+00
2	0	0.00E+00
3	0	0.00E+00
4	0	0.00E+00
5	0	0.00E+00
6	0	0.00E+00
7	0	0.00E+00
8	0	0.00E+00
9	0	0.00E+00
10	0	0.00E+00
11	0	0.00E+00
12	0	0.00E+00
13	0	0.00E+00
14	0	0.00E+00
15	0	0.00E+00
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

NUMBER OF SPLITTINGS

ENERGY GROUP	REGION 1		REGION 2		REGION 3		REGION 4		REGION 5		REGION 6	
	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT
1	6	2.71E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
2	6	2.71E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	3	8.16E-01	3	5.94E-01
3	12	5.41E+00	0	0.00E+00	0	0.00E+00	6	2.04E+00	12	3.27E+00	2	5.94E-01
4	55	2.47E+01	0	0.00E+00	1	3.16E-01	11	5.62E+00	9	3.67E+00	9	2.33E+00
5	29	1.94E+01	0	0.00E+00	1	4.03E-01	28	1.41E+01	21	8.52E+00	23	6.42E+00
6	43	2.91E+01	0	0.00E+00	8	3.41E+00	27	1.33E+01	37	1.44E+01	33	9.20E+00
7	127	8.23E+01	0	0.00E+00	46	2.01E+01	75	3.66E+01	115	4.48E+01	71	1.90E+01
8	78	5.14E+01	1	5.75E-01	83	3.79E+01	61	3.00E+01	86	3.42E+01	74	2.04E+01
9	13	8.80E+00	0	0.00E+00	14	6.35E+00	17	7.92E+00	27	1.09E+01	10	2.62E+00
10	108	7.26E+01	1	5.75E-01	116	5.54E+01	107	5.19E+01	127	4.88E+01	69	1.94E+01
11	269	1.86E+02	5	3.01E+00	195	1.17E+02	207	1.10E+02	220	9.49E+01	174	5.45E+01
12	383	3.37E+02	25	1.68E+01	445	3.00E+02	889	5.32E+02	1181	5.80E+02	1149	4.02E+02
13	552	7.72E+02	57	6.02E+01	987	1.06E+03	2109	1.96E+03	2860	2.14E+03	3067	1.68E+03
14	77	4.86E+02	0	0.00E+00	46	3.01E+02	22	1.52E+02	63	3.76E+02	95	4.50E+02
15	8	6.81E+01	0	0.00E+00	6	6.90E+01	0	0.00E+00	0	0.00E+00	1	1.11E+01
16	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7	
	NUMBER	WEIGHT
1	0	0.00E+00
2	0	0.00E+00
3	0	0.00E+00
4	2	3.35E-01
5	13	2.29E+00
6	23	4.48E+00
7	97	2.12E+01
8	72	1.47E+01
9	29	6.18E+00
10	107	2.20E+01
11	231	6.09E+01
12	1324	3.42E+02
13	2991	1.19E+03
14	112	3.82E+02
15	6	4.93E+01
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

NUMBER OF SPLITTINGS PREVENTED BY LACK OF ROOM

ENERGY GROUP	REGION 1		REGION 2		REGION 3		REGION 4		REGION 5		REGION 6	
	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT
1	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
2	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
3	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
4	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
5	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
6	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
7	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
8	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
9	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
10	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
11	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
12	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
13	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
14	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
15	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
16	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7	
	NUMBER	WEIGHT
1	0	0.00E+00
2	0	0.00E+00
3	0	0.00E+00
4	0	0.00E+00
5	0	0.00E+00
6	0	0.00E+00
7	0	0.00E+00
8	0	0.00E+00
9	0	0.00E+00
10	0	0.00E+00
11	0	0.00E+00
12	0	0.00E+00
13	0	0.00E+00
14	0	0.00E+00
15	0	0.00E+00
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

NUMBER OF RUSSIAN ROULETTE KILLS

ENERGY GROUP	REGION 1		REGION 2		REGION 3		REGION 4		REGION 5		REGION 6	
	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT
1	2	5.40E-01	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
2	7	2.04E+00	0	0.00E+00	0	0.00E+00	1	2.57E-01	2	3.64E-01	1	1.48E-01
3	10	3.25E+00	0	0.00E+00	2	5.19E-01	5	1.22E+00	8	1.58E+00	1	1.58E-01
4	36	1.39E+01	1	4.45E-01	11	3.83E+00	8	2.67E+00	8	2.12E+00	5	9.59E-01
5	44	2.48E+01	1	4.54E-01	3	1.56E+00	20	8.70E+00	13	4.75E+00	14	3.49E+00
6	59	3.83E+01	0	0.00E+00	8	4.02E+00	27	1.24E+01	38	1.40E+01	21	5.27E+00
7	240	1.62E+02	4	2.19E+00	46	2.25E+01	79	3.73E+01	99	3.68E+01	71	1.84E+01
8	258	1.77E+02	2	9.57E-01	58	2.78E+01	80	3.79E+01	107	3.93E+01	56	1.39E+01
9	81	5.52E+01	0	0.00E+00	7	3.31E+00	19	8.32E+00	26	9.59E+00	18	4.06E+00
10	249	1.73E+02	3	1.70E+00	93	4.59E+01	127	5.82E+01	123	4.42E+01	77	1.86E+01
11	447	3.55E+02	6	4.86E+00	160	9.72E+01	240	1.30E+02	257	1.09E+02	199	5.45E+01
12	894	8.17E+02	29	2.04E+01	396	2.71E+02	930	5.64E+02	1275	5.96E+02	1124	3.40E+02
13	1468	2.14E+03	67	7.51E+01	884	9.74E+02	2217	2.13E+03	3104	2.30E+03	3109	1.57E+03
14	115	7.97E+02	0	0.00E+00	63	4.66E+02	81	6.36E+02	127	8.11E+02	165	7.00E+02
15	8	7.31E+01	0	0.00E+00	11	1.21E+02	5	8.57E+01	5	9.10E+01	7	6.49E+01
16	1	1.46E+01	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	1	3.51E+01	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7	
	NUMBER	WEIGHT
1	0	0.00E+00
2	1	1.28E-01
3	0	0.00E+00
4	0	0.00E+00
5	2	3.03E-01
6	0	0.00E+00
7	8	1.29E+00
8	16	2.73E+00
9	1	1.45E-01
10	19	3.16E+00
11	39	6.26E+00
12	225	3.99E+01
13	758	2.38E+02
14	19	4.38E+01
15	2	1.14E+01
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

NUMBER OF RUSSIAN ROULETTE SURVIVALS

ENERGY GROUP	REGION 1		REGION 2		REGION 3		REGION 4		REGION 5		REGION 6	
	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT	NUMBER	WEIGHT
1	7	2.19E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
2	7	2.30E+00	0	0.00E+00	3	1.11E+00	2	5.92E-01	4	8.26E-01	3	5.43E-01
3	31	1.13E+01	0	0.00E+00	7	2.24E+00	10	2.50E+00	11	2.53E+00	5	1.13E+00
4	123	5.18E+01	1	4.08E-01	9	4.07E+00	28	9.72E+00	33	9.55E+00	7	1.61E+00
5	159	9.45E+01	0	0.00E+00	25	1.34E+01	91	4.16E+01	76	2.80E+01	44	1.25E+01
6	344	2.30E+02	1	5.94E-01	31	1.72E+01	91	4.43E+01	87	3.37E+01	57	1.61E+01
7	1225	8.65E+02	3	1.88E+00	111	6.23E+01	276	1.38E+02	312	1.24E+02	148	4.37E+01
8	1017	7.27E+02	11	6.86E+00	111	5.93E+01	226	1.16E+02	264	1.05E+02	130	3.76E+01
9	248	1.75E+02	1	6.07E-01	26	1.37E+01	53	2.77E+01	66	2.62E+01	29	8.33E+00
10	864	6.39E+02	3	1.80E+00	193	1.07E+02	283	1.44E+02	317	1.26E+02	148	4.14E+01
11	1141	9.92E+02	33	2.36E+01	332	2.26E+02	476	2.89E+02	457	2.11E+02	327	1.04E+02
12	2051	2.00E+03	83	6.86E+01	1022	7.87E+02	2250	1.52E+03	2636	1.33E+03	2118	7.16E+02
13	3185	4.96E+03	156	2.08E+02	2326	2.90E+03	5544	5.94E+03	6613	5.28E+03	6107	3.39E+03
14	408	3.34E+03	5	4.61E+01	165	1.41E+03	304	2.86E+03	373	2.85E+03	242	1.15E+03
15	45	4.64E+02	0	0.00E+00	18	2.26E+02	25	4.44E+02	41	8.45E+02	21	2.74E+02
16	7	9.75E+01	0	0.00E+00	0	0.00E+00	2	4.39E+01	0	0.00E+00	0	0.00E+00
17	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
18	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
19	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
20	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
21	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00
22	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00	0	0.00E+00

ENERGY GROUP	REGION 7	
	NUMBER	WEIGHT
1	0	0.00E+00
2	0	0.00E+00
3	0	0.00E+00
4	0	0.00E+00
5	4	5.98E-01
6	4	6.02E-01
7	16	2.61E+00
8	14	2.42E+00
9	10	1.69E+00
10	38	6.42E+00
11	57	9.55E+00
12	327	5.98E+01
13	1375	4.38E+02
14	30	7.05E+01
15	6	3.60E+01
16	0	0.00E+00
17	0	0.00E+00
18	0	0.00E+00
19	0	0.00E+00
20	0	0.00E+00
21	0	0.00E+00
22	0	0.00E+00

**NEXT RANDOM NUMBER IS 21BD17AC756B

TOTAL CPU TIME FOR THIS PROBLEM WAS 8.27 MINUTES. This is the CPU time for MORSE-SGC/S.

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SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK


**** PROBLEM PARAMETERS ****

LIB 22N-18COUPLE LIBRARY
MXX            5 MIXTURES
MSC           14 COMPOSITION SPECIFICATIONS
IZM            3 MATERIAL ZONES
GE  LATTICECELL  GEOMETRY
MORE           0 0/1 DO NOT READ/READ OPTIONAL PARAMETER DATA
MSLN           0 FUEL SOLUTIONS


**** PROBLEM COMPOSITION DESCRIPTION ****

SC  U-235        STANDARD COMPOSITION
MX             1 MIXTURE NO.
DEN   1.6736E-04 ATOMIC DENSITY
END

SC  U-238        STANDARD COMPOSITION
MX             1 MIXTURE NO.
DEN   1.9602E-02 ATOMIC DENSITY
END

SC  PU-239       STANDARD COMPOSITION
MX             1 MIXTURE NO.
DEN   1.0409E-04 ATOMIC DENSITY
END

SC  PU-240       STANDARD COMPOSITION
MX             1 MIXTURE NO.
DEN   4.7534E-05 ATOMIC DENSITY
END

SC  O            STANDARD COMPOSITION
MX             1 MIXTURE NO.
DEN   3.9877E-02 ATOMIC DENSITY
END

SC  ZR           STANDARD COMPOSITION
MX             2 MIXTURE NO.
DEN   1.9350E-02 ATOMIC DENSITY
END

SC  O            STANDARD COMPOSITION
MX             3 MIXTURE NO.
DEN   1.0000E-20 ATOMIC DENSITY
END

SC  CR           STANDARD COMPOSITION
MX             4 MIXTURE NO.
DEN   1.6620E-02 ATOMIC DENSITY
END
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SC  MN            STANDARD COMPOSITION
MX              4 MIXTURE NO.
DEN   1.2000E-03 ATOMIC DENSITY
END

SC  FE            STANDARD COMPOSITION
MX              4 MIXTURE NO.
DEN   5.7750E-02 ATOMIC DENSITY
END

SC  NI            STANDARD COMPOSITION
MX              4 MIXTURE NO.
DEN   7.5200E-03 ATOMIC DENSITY
END

SC  MO            STANDARD COMPOSITION
MX              4 MIXTURE NO.
DEN   1.1000E-04 ATOMIC DENSITY
END

SC  U-235         STANDARD COMPOSITION
MX              5 MIXTURE NO.
DEN   1.0700E-04 ATOMIC DENSITY
END

SC  U-238         STANDARD COMPOSITION
MX              5 MIXTURE NO.
DEN   4.7700E-02 ATOMIC DENSITY
END
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**** PROBLEM GEOMETRY ****

CTP SQUAREPITCH  CELL TYPE
PITCH     1.2598 CM CENTER TO CENTER SPACING
FUELOD    0.8357 CM FUEL DIAMETER OR SLAB THICKNESS
MFUEL          1 MIXTURE NO. OF FUEL
MMOD           3 MIXTURE NO. OF MODERATOR
CLADOD    0.9500 CM CLAD OUTER DIAMETER
MCLAD          2 MIXTURE NO. OF CLAD


ZONE SPECIFICATIONS FOR LATTICECELL GEOMETRY

              ZONE  1 IS FUEL
              ZONE  2 IS CLAD
              ZONE  3 IS MOD

**** XSDRN MESH INTERVALS ****

   4 MESH INTERVALS IN ZONE  1
   4 MESH INTERVALS IN ZONE  2
   4 MESH INTERVALS IN ZONE  3
```

Output from cell-weighting calculation

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**** NEUTRON RESPONSE FUNCTION OF IRF= 9029 ****

1.9448E-04  1.5971E-04  1.4706E-04  1.4772E-04  1.5339E-04  1.5062E-04  1.3892E-04  1.2843E-04  1.2527E-04  1.2632E-04
1.2894E-04  1.1687E-04  6.5278E-05  9.1897E-06  3.7134E-06  4.0086E-06  4.2946E-06  4.4761E-06  4.5673E-06  4.5355E-06
4.3701E-06  3.7147E-06

**** ADJOINT XSDRN MESH INTERVALS ****

   8 MESH INTERVALS IN ZONE  1
   4 MESH INTERVALS IN ZONE  2
   4 MESH INTERVALS IN ZONE  3
  39 MESH INTERVALS IN ZONE  4
   5 MESH INTERVALS IN ZONE  5

**** SOURCE SPECTRUM FROM CARD ****

2.4740E-13  2.0960E-12  5.7660E-12  2.8990E-11  7.2280E-11  1.4570E-10  6.0990E-10  4.5420E-10  9.0700E-11  3.8240E-10
4.9900E-10  3.9820E-10  1.8360E-10  1.7610E-14  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00
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**** MORSE IMPORTANCE REGION INFORMATIONS ****

REGION	# OF XSDRN INT.	REGION BOUNDRY	ESTIMATION PROB
1	8	3.6420E+01	2.7207E-02
2	4	4.4550E+01	4.2455E-02
3	4	4.5820E+01	5.5240E-02
4	20	4.7725E+01	7.3143E-02
5	10	5.0900E+01	1.3721E-01
6	9	5.3440E+01	3.2471E-01
7	4	5.7270E+01	1.0000E+00

Estimation probability to point detectors from each importance region

Boundaries of importance regions in Monte Carlo calculation

**** SURFACE DETECTORS INFORMATIONS ****

DETECTORS LOCATIONS: RADIAL

DET #	RADIUS(CM)	HEIGHT(CM)
1	5.7270E+01	1.8288E+02
2	1.5727E+02	1.8288E+02
3	2.5727E+02	1.8288E+02
4	3.5727E+02	1.8288E+02

Radial locations of the surface detectors

Height of the radial surface detectors

SAMPLE PROBLEM 1, 2 HOMOGENIZED FUEL ZONES

IVOPT = 0 IDBG = 0

BODY DATA

RCC	1	0.0000000E+00	0.0000000E+00	-0.2298700E+03	0.0000000E+00	0.0000000E+00	0.4597400E+03
		0.4582000E+02					
RCC	2	0.0000000E+00	0.0000000E+00	-0.2374900E+03	0.0000000E+00	0.0000000E+00	0.4749800E+03
		0.5344000E+02					
RCC	3	0.0000000E+00	0.0000000E+00	-0.2374900E+03	0.0000000E+00	0.0000000E+00	0.4749800E+03
		0.5344100E+02					
RCC	4	0.0000000E+00	0.0000000E+00	-0.2374900E+03	0.0000000E+00	0.0000000E+00	0.4749800E+03
		0.5344200E+02					
RCC	5	0.0000000E+00	0.0000000E+00	-0.2413000E+03	0.0000000E+00	0.0000000E+00	0.4826000E+03
		0.5725000E+02					
RCC	6	0.0000000E+00	0.0000000E+00	-0.2412700E+03	0.0000000E+00	0.0000000E+00	0.4825400E+03
		0.5726000E+02					
RCC	7	0.0000000E+00	0.0000000E+00	-0.2412800E+03	0.0000000E+00	0.0000000E+00	0.4825600E+03
		0.5727000E+02					
RCC	8	0.0000000E+00	0.0000000E+00	-0.2374900E+03	0.0000000E+00	0.0000000E+00	0.4749800E+03
		0.4582000E+02					
RCC	9	0.0000000E+00	0.0000000E+00	-0.2374910E+03	0.0000000E+00	0.0000000E+00	0.4749820E+03
		0.4582000E+02					
RCC	10	0.0000000E+00	0.0000000E+00	-0.2374920E+03	0.0000000E+00	0.0000000E+00	0.4749840E+03
		0.4582000E+02					
RCC	11	0.0000000E+00	0.0000000E+00	-0.2413100E+03	0.0000000E+00	0.0000000E+00	0.4826200E+03
		0.5726000E+02					
RCC	12	0.0000000E+00	0.0000000E+00	-0.2412900E+03	0.0000000E+00	0.0000000E+00	0.4825800E+03
		0.5726000E+02					
RCC	13	0.0000000E+00	0.0000000E+00	-0.2374920E+03	0.0000000E+00	0.0000000E+00	0.4749840E+03
		0.5344200E+02					
RCC	14	0.0000000E+00	0.0000000E+00	-0.3413100E+03	0.0000000E+00	0.0000000E+00	0.6826200E+03
		0.1572700E+03					
RCC	15	0.0000000E+00	0.0000000E+00	-0.4413100E+03	0.0000000E+00	0.0000000E+00	0.8826200E+03
		0.2572700E+03					
RCC	16	0.0000000E+00	0.0000000E+00	-0.5413100E+03	0.0000000E+00	0.0000000E+00	0.1082620E+04
		0.3572700E+03					
RCC	17	0.0000000E+00	0.0000000E+00	-0.2241310E+04	0.0000000E+00	0.0000000E+00	0.4482620E+04
		0.2057270E+04					
RCC	18	0.0000000E+00	0.0000000E+00	-0.2341310E+04	0.0000000E+00	0.0000000E+00	0.4682620E+04
		0.2157270E+04					
RCC	19	0.0000000E+00	0.0000000E+00	-0.2286000E+03	0.0000000E+00	0.0000000E+00	0.4572000E+03
		0.4455000E+02					
RCC	20	0.0000000E+00	0.0000000E+00	-0.2285990E+03	0.0000000E+00	0.0000000E+00	0.4571980E+03
		0.4454900E+02					
RCC	21	0.0000000E+00	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
		0.1000000E-02					
RCC	22	0.0000000E+00	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
		0.1210000E+02					
RCC	23	0.0000000E+00	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
		0.2116000E+02					

RCC	24	0.0000000E+00 0.3642000E+02	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
RCC	25	0.0000000E+00 0.3642100E+02	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
RCC	26	0.0000000E+00 0.3642200E+02	0.0000000E+00	-0.1828800E+03	0.0000000E+00	0.0000000E+00	0.3657600E+03
RCC	27	0.0000000E+00 0.1000000E-02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03
RCC	28	0.0000000E+00 0.1210000E+02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03
RCC	29	0.0000000E+00 0.2116000E+02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03
RCC	30	0.0000000E+00 0.3642000E+02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03
RCC	31	0.0000000E+00 0.3642100E+02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03
RCC	32	0.0000000E+00 0.3642200E+02	0.0000000E+00	-0.1828900E+03	0.0000000E+00	0.0000000E+00	0.3657800E+03

NUMBER OF BODIES 32
LENGTH OF FPD-ARRAY 288

INPUT ZONE DATA

	INPUT ZONE	CODE ZONE		BODY NUMBERS			
INN	1	1		1	-19		
RS1	2	2		2	-10		
RS2	3	3		3	-2		
RS3	4	4		4	-3		
OUR	5	5		5	-13		
WTR	6	6		6	-5		
JAC	7	7		7	-6	-5	
AS1	8	8		8	-1		
AS2	9	9		9	-8		
AS3	10	10		10	-9		
IMP	11	11		11	-5	-12	
HOL	12	12		13	-4	-10	
DE2	13	13		14	-5	-7	-11
		14	OR	12	-5	-7	
DE3	14	15		15	-14		
DE4	15	16		16	-15		
INV	16	17		17	-16		
EXV	17	18		18	-17		
CAV	18	19		19	-20		
INS	19	20		20	-32		
		21	OR	31	-30	-25	
		22	OR	29	-28	-23	
		23	OR	27	-21		
		24	OR	25	-30		
		25	OR	23	-28		
		26	OR	21			

FU1	20	27	22	-21	
FU2	21	28	24	-23	
FU3	22	29	26	-25	
HW1	23	30	28	-27	-22
HW2	24	31	30	-29	-24
HW3	25	32	32	-31	-26

NUMBER OF INPUT ZONES 25
NUMBER OF CODE ZONES 32
LENGTH OF INTEGER ARRAY 1061

CODE ZONE	INPUT ZONE	ZONE DATA LOC.	NO. OF BODIES	REGION NO.	MEDIA NO.	BOX INPUT ZONE	BOX CODE ZONE
1	1	225	2	1	4	0	0
2	2	236	2	1	5	0	0
3	3	247	2	1	1000	0	0
4	4	258	2	1	1000	0	0
5	5	269	2	1	4	0	0
6	6	280	2	1	1000	0	0
7	7	291	3	1	1000	0	0
8	8	307	2	1	5	0	0
9	9	318	2	1	1000	0	0
10	10	329	2	1	1000	0	0
11	11	340	3	1	1000	0	0
12	12	356	3	1	1000	0	0
13	13	372	4	2	1000	0	0
14	13	393	3	2	1000	0	0
15	14	409	2	1	1000	0	0
16	15	420	2	2	1000	0	0
17	16	431	2	1	1000	0	0
18	17	442	2	1	0	0	0
19	18	453	2	1	1000	0	0
20	19	464	2	1	1000	0	0
21	19	475	3	1	1000	0	0
22	19	491	3	1	1000	0	0
23	19	507	2	1	1000	0	0
24	19	518	2	1	1000	0	0
25	19	529	2	1	1000	0	0
26	19	540	1	1	1000	0	0
27	20	546	2	1	7	0	0
28	21	557	2	1	7	0	0
29	22	568	2	1	7	0	0
30	23	579	3	1	8	0	0
31	24	595	3	1	8	0	0
32	25	611	3	1	8	0	0

```
                                                
```

```
MORSE REGION IN INPUT ZONE(I) ARRAY  (MRIZ(I),I=1,25)
    1    1    1    1    1    1    1    1    1    1    1    1    2    1    2    1    1    1    1    1    1    1
    1    1    1

MORSE MEDIA IN INPUT ZONE(I) ARRAY (MMIZ(I),I=1,25)
    4    5 1000 1000    4 1000 1000    5 1000 1000 1000 1000 1000 1000 1000 1000    0 1000 1000    7    7    7
    8    8    8

MORSE UNIVERSE IN INPUT ZONE(I) ARRAY (NBIZ(I),I=1,25)
    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
    0    0    0

 OPTION 0 WAS USED IN CALCULATING VOLUMES, FOR  2 REGIONS
0-SET VOLUMES = 1, 1-CONCENTRIC SPHERES, 2-SLABS, 3-INPUTVOLUMES.

          VOLUMES ( CC ) USED IN COLLISIONS DENSITY AND TRACK LENGTH ESTIMATORS.
   REG        1          2
VOLUME  1.000E+00   1.000E+00

ARRAY DATA REQUIRES         8 LOCATIONS, LEAVING    332335 LOCATIONS

 CONTROL MODULE SAS4      IS COMPLETE.
```

```
MODULE SAS4     WILL BE CALLED  TIME OF DAY 22.13.27  DATE 88.011

  SAMPLE PROBLEM 1, RADIAL NEUTRON DOSES OF DRY DEPLETED URANIUM CASK
  22N-18COUPLE   LATTICECELL
  U-235    1 0.0 1.6736-4  END
  U-238    1 0.0 1.9602-2  END
  PU-239   1 0.0 1.0409-4  END
  PU-240   1 0.0 4.7534-5  END
  O        1 0.0 3.9877-2  END
  ZR       2 0.0 1.9350-2  END
  O        3  0.0 1.000-20  END
  CR       4  0.0 1.662-2   END
  MN       4  0.0 1.200-3   END
  FE       4  0.0 5.775-2   END
  NI       4  0.0 7.520-3   END
  MO       4  0.0 1.100-4   END
  U-235    5  0.0 1.070-4  END
  U-238    5  0.0 4.770-2  END
    END COMP
  SQUAREPITCH  1.25984 0.83566 1 3 0.94996 2 END
  ITY=1 IZM=5 FRD=36.42 END
  7 17 25 0 0 0  0.01 21.4493 END
  36.42 44.55 45.82 53.44 57.27 END
  0 0 4 5 4 END
  XEND
  TIM=15.0 NST=100 NIT=50 NOD=3 IGO=1 RAN=F2AE3EBFB1EB FR1=1. FR2=0.6465
  FR3=0.6465 FR4=0.6465  END
  SOE  2.474-13 2.096-12 5.766-12 2.899-11 7.228-11 1.457-10 6.099-10
       4.542-10 9.070-11 3.824-10 4.990-10 3.982-10 1.836-10 1.761-14
       8Z END
  DET 148.69 0.0 0.0   240.13 0.0 0.0
      121.91 0.0 305.96 END
  GEND
  SAMPLE PROBLEM 1, 2 HOMOGENIZED FUEL ZONES
  FU1 0.0 12.10 182.88 182.89 END
  FU2 21.16 36.42 182.88 182.89 END
  FEND
  CAV 0 44.55 228.60 END
  INN 4 45.82 229.87 END
  RS1 5 53.44 237.49 END
  OUR 4 57.25 241.30 END
  AS1 5 45.82 237.49 END
  CEND
  END
```

```
SECONDARY MODULE 000008   HAS BEEN CALLED
MODULE 000008   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED     2.02 (SECONDS). I/O'S USED     357.
SECONDARY MODULE 000002   HAS BEEN CALLED
MODULE 000002   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED     2.17 (SECONDS). I/O'S USED     826.
SECONDARY MODULE 000001   HAS BEEN CALLED
MODULE 000001   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED     9.29 (SECONDS). I/O'S USED    1199.
SECONDARY MODULE 000001   HAS BEEN CALLED
MODULE 000001   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED    32.17 (SECONDS). I/O'S USED     969.
SECONDARY MODULE 000106   HAS BEEN CALLED
MODULE 000106   IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED   498.57 (SECONDS). I/O'S USED    4703.
MODULE SAS4     IS FINISHED.  COMPLETION CODE - SYSTEM 000 USER  0000. CPU TIME USED   556.38 (SECONDS). I/O'S USED    9013.
```

```
        PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - 10/26/87 - 11.50)
*****************************************************************************************************************
*  MESSAGES OF CURRENT INTEREST TO SCALE USERS WILL APPEAR HERE                                                 *
*                                                                                                               *
*    CURRENTLY FORTRAN 77 SCALE AND FORTRAN Q SCALE SHARE THE SAME MESSAGES.  IN THE FUTURE THESE WILL BE       *
*   SEPARATED INTO DIFFERENT SETS FOR EACH PROCEDURE.                                                           *
*                                                                                                               *
*    FOR FORTRAN Q SCALE USERS WHO ARE UNAWARE OF THE FORTRAN 77 SCALE THE FOLLOWING CONTROL PROGRAMS ARE       *
*   AVAILABLE BY EXECUTING SCALE77:                                                                             *
*                                                                                                               *
*       CSASN,CSAS1X,CSASI,CSASIX,CSAS25,CSAS2X,CSAS4,CSAS4X                                                    *
*       SAS1,SAS1X,SAS1T                                                                                        *
*       SAS3,SAS3X                                                                                              *
*                                                                                                               *
*    THE FOLLOWING FUNCTIONAL MODULES ARE ALSO AVAILABLE:                                                       *
*       AIM                                                                                                     *
*       BONAMI                                                                                                  *
*       NITAWL                                                                                                  *
*       NITAWL2                                                                                                 *
*       ICE                                                                                                     *
*       XSDRN                                                                                                   *
*       KENO5,KENO5A,KENOVA,KENOV                                                                               *
*       MORSE                                                                                                   *
*       ORIGEN                                                                                                  *
*       COUPLE                                                                                                  *
*       PLORIGEN                                                                                                *
*       XSDOSE                                                                                                  *
*                                                                                                               *
*                                        SCALE77                                                                *
*     10/15/87                                                                                                  *
*                                                                                                               *
*        PROGRAMS BONAMI, NITAWL, ICE, XSDRN, KENOV.A, XSDOSE, CSAS25, SAS1, AND SAS3 HAVE ALL BEEN RELINKED    *
*        TO ELIMINATE A PROBLEM THAT OCCURED WHEN A MODULE ABENDED WITH AN 822.  RATHER THAN TERMINATING, THE   *
*        MODULE CONTINUED TO LOOP UNTIL THE SPECIFIED TIME LIMIT EXPIRED.  THE FORTRAN LIBRARY HAD TO BE        *
*        MODIFIED TO CORRECT THIS PROBLEM.                                                                      *
*                                                                                                               *
*     11/25/87                                                                                                  *
*                                                                                                               *
*        AN ERROR WAS CORRECTED IN XSDRN THAT EFFECTED THE CREATION OF AN ISOTXS FILE.                          *
*                                                                                                               *
*     11/30/87                                                                                                  *
*                                                                                                               *
*        THE CSAS4 SEQUENCES WERE UPDATED WITH A CHANGE THAT ALLOWS SPECIFYING THE MIXTURE NUMBER TO BE USED AS *
*        THE CELL MIXTURE IN AN INFINITE HOMOGENEOUS MEDIUM CALCULATION.                                        *
*                                                                                                               *
*                                                                                                               *
*                                     SCALE (Q VERSION)                                                         *
*                                                                                                               *
*    11/25/87                                                                                                   *
*                                                                                                               *
*        THE SCALE DRIVER WAS UPDATED TO PRINT THIS MESSAGE.                                                    *
*     THE PROGRAM LIBRARY WAS RELOADED FROM BACKUP TO TRY TO CORRECT AN ERROR IN SAS1.                           *
*        SAS1 WAS RELINKED TO GET A CORRECTED LOAD MODULE.                                                      *
*                                                                                                               *
*    12/03/87                                                                                                   *
*                                                                                                               *
*        THE PROGRAM LIBRARY WAS MOVE FROM A MASS STORE VOLUME TO AN ONLINE VOLUME. THE FUNCTIONAL MODULE       *
*      REGPLOT WAS RELINKED TO GET A VERSION THAT COULD BE LOADED.                                              *
*                                                                                                               *
*                                                                                                               *
*  FURTHER INFORMATION ABOUT THESE AND OTHER UPDATES MAY BE FOUND IN NEDO.PBF10287.SCALE77.QAFORMS IN THE MEMBER *
*  WITH THE SAME NAME AS THE MODULE.                                                                            *
*                                                                                                               *
*****************************************************************************************************************
```

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Computing Applications Division

HTAS1: A TWO-DIMENSIONAL HEAT TRANSFER ANALYSIS OF FUEL CASKS, VERSION 4.0

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ABSTRACT

The Heat Transfer Analysis Sequence Number One (HTAS1) control module was developed for the U.S. Nuclear Regulatory Commission to perform standardized thermal analyses on a class of nuclear fuel shipping containers. HTAS1 uses the HEATING and OCULAR functional modules to perform the prescribed thermal analysis. The nuclear fuel shipping container must be composed of acceptable combinations of zones consisting of a cavity, an inner shell, shielding, an outer shell, a neutron shield, a water jacket, and impact limiters. Thermal properties for the material in each zone may be extracted from a material property library or may be supplied by the user. The desired thermal analysis of the nuclear fuel shipping container is defined by an analytical sequence composed of one or more of the following calculations chosen in an acceptable order: an initial steady state; a prefire steady state; a fire transient; a postfire transient; and a final steady state. Each calculation in an analytical sequence specifies the type (steady-state or transient), the ambient temperature, the duration of any transient, and the heat transfer mechanisms at the surface of the model. Selected portions of the model may be deleted at certain points in an analytical sequence to simulate changes in the nuclear fuel shipping container during an analysis. The model and analytical sequence are described to HTAS1 using free-form, keyword-oriented data making extensive use of defaults. HTAS1 generates the HEATING input data necessary to model each calculation in an analytical sequence. In addition, if the neutron shield has been deleted but the water jacket remains, HTAS1 adds OCULAR input to the HEATING data for representation of two-dimensional radiative exchange in the annular region within the water jacket. HTAS1 then transfers control to the SCALE driver, which accesses OCULAR (if required) and HEATING to perform the desired analysis.

The HTAS1 control module has recently been revised to allow data for various geometry and output plots to be generated and to update default values to match those specified by Part 71 of Title 10 in the Code of Federal Regulations-Energy, U.S. States Nuclear Regulatory Commission.

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H1.1 INTRODUCTION

The Heat Transfer Analysis Sequence Number One (HTAS1) control module was developed for the U.S. Nuclear Regulatory Commission (NRC) as part of their efforts to develop standardized methods for performing safety analyses of nuclear fuel shipping containers. Frequently, it is desired to perform a thermal analysis on a class of nuclear fuel transport packages that can be modeled by a combination of homogeneous, right, circular cylinders (see Fig. H1.1.1). During the thermal analysis of such a model, it is usually of interest to determine its steady-state temperature distribution under normal operating conditions, its transient temperature distribution during exposure to a fire of specified duration at a specified temperature, and its transient temperature distribution for a specified period of time following exposure to the fire. At times, it is also of interest to determine the final steady-state temperature distribution following exposure to the fire. HTAS1 was designed to perform standardized thermal analyses on this class of problems.

HTAS1 is a control module in the SCALE system. HTAS1 uses the HEATING functional module (see Sect. F10) to perform the desired thermal analysis on the model. The input data to HTAS1 define the physical model and the analytical sequence to be performed. HTAS1 reads these input data, checks them for errors, and determines each thermal analysis to be performed. The HEATING input data set is then generated by HTAS1 which subsequently directs the SCALE driver to call HEATING to perform each thermal analysis in the prescribed analytical sequence. The final temperature distribution from the previous HEATING thermal analysis is used as the initial temperature distribution for the current HEATING thermal analysis.

Some analyses may start with a neutron shield in place inside of a water jacket, but at some later time lose the neutron shield leaving either a cavity or air inside the water jacket. For these analyses, in order to represent the radiation exchange within the water jacket with a full two-dimensional (2-D) model HTAS1 uses another SCALE functional module, OCULAR. OCULAR generates exchange factors between the nodes in the model in the form of node-to-node connectors for the HEATING calculation. HTAS1 adds the additional data required to run OCULAR to the HEATING input. For each portion of the analysis after the neutron shield has been deleted from the model, HTAS1 directs the SCALE driver to call the OCULAR module immediately before calling the HEATING module. OCULAR reads the same input that is read by HEATING and writes the resulting node-to-node connecters out in binary form for subsequent use by HEATING.

The input data to HTAS1, which use SCALE's free-form routines, are quite simple and are keyword-oriented. HTAS1 makes extensive use of default values for most of the thermal parameters used to define a physical model and analytical sequence. Of course, these values can be overridden easily by entering the appropriate keyword and data at specified locations in the input data stream. HTAS1 has a built-in material property library, with thermal parameters for materials frequently used in nuclear fuel transport packages.

Section H1.2 contains a detailed description of the capabilities of the control module. Included is a discussion of its modeling capabilities, a description of each thermal analysis available in defining particular analytical sequences and a description of the boundary conditions used for the various model configurations and analytical sequences. Default conditions and values are also presented, along with a number of suggestions concerning the use of special features of the control module.

The general structure of HTAS1 is outlined in Sect. H1.3. A brief description of each subroutine in the control module and the identification of each logical unit used by HTAS1 are included.

Section H1.4 contains a detailed description of the input data available to describe a set of calculations to HTAS1.

Sample problems are presented in Sect. H1.5. A description of the problems, listings of the input data, and selected portions of the computer output generated by the runs are included.

The English units of density, heat flux, temperature, etc., that are used in the description of HTAS1 are those specifically requested by the NRC during the initial development of HTAS1 in the early 1980s. Constants for conversion to SI units can be found in most standard engineering references.

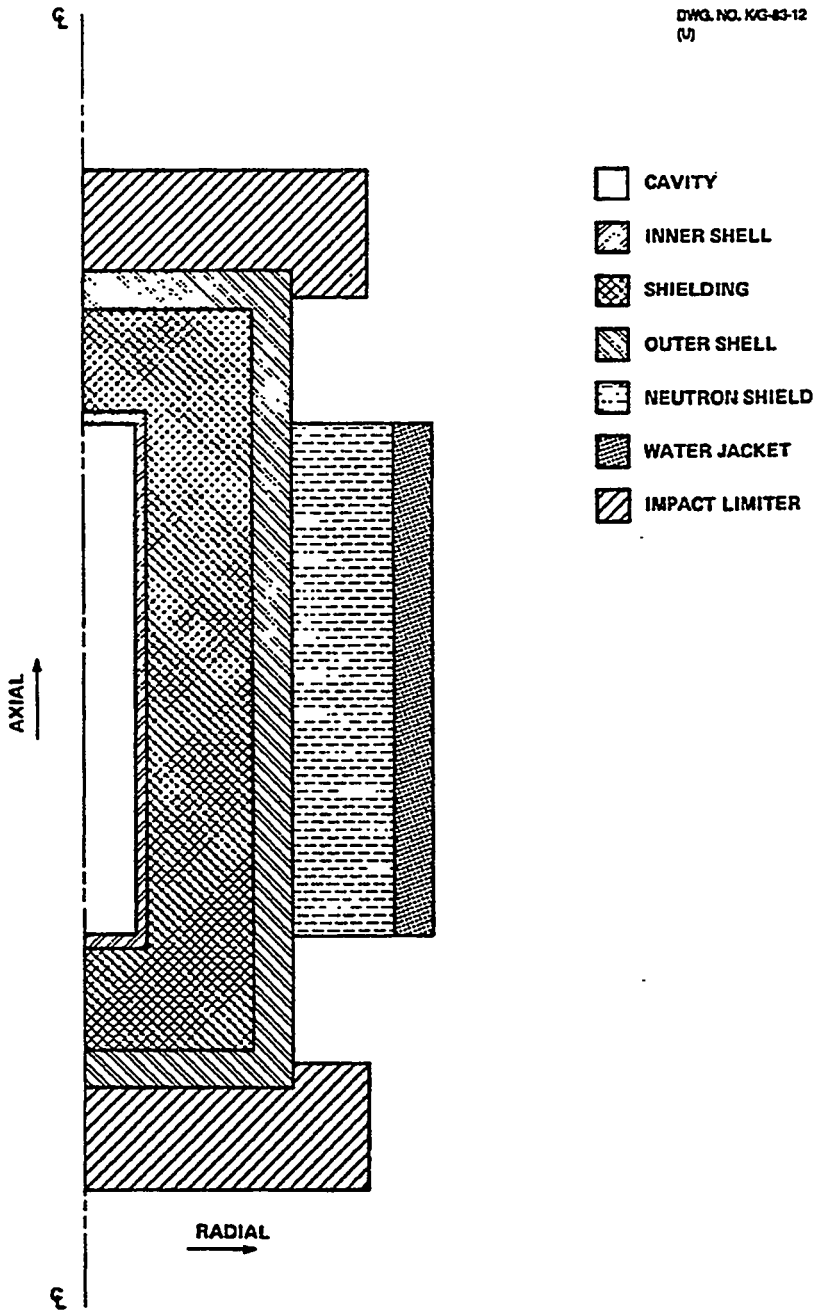


Figure H1.1.1 Zone configuration in HTAS1 general model

H1.2 USE OF HTAS1

This section presents a detailed description of the various options available to HTAS1 for modeling nuclear fuel transport packages. It contains a description of each zone, a discussion of acceptable combinations of zones, definitions of boundary conditions associated with each zone and thermal analysis, and default values for most parameters. It discusses the various thermal analyses available for defining analytical sequences. Assumptions HTAS1 makes in modeling problems are discussed. These assumptions should be considered in interpreting results of analysis generated by the control module.

H1.2.1 DESCRIPTION OF THE PHYSICAL MODEL

HTAS1 can be used in the steady-state and transient thermal analysis of a group of nuclear fuel shipping packages which can be modeled by acceptable combinations of homogeneous, right, circular cylinders (denoted as zones) as depicted in Fig. H1.2.1. The model must be composed of a minimum of the cavity, inner shell and outer shell. The water jacket and neutron shield must appear as a pair. The user defines the physical model to be used in the thermal analysis by entering the appropriate keywords, along with the physical dimensions necessary to define the zones comprising the model. Default values exist for most parameters associated with each zone, such as the material, thermal properties and boundary conditions. However, the user may override most of these default values by supplying a keyword to identify the parameters to be defined along with parameter data. HTAS1 generates up to ten HEATING boundary conditions and applies each condition to one or more specific surfaces of the model. The location of each boundary condition is depicted in Figs. H1.2.2, H1.2.3, H1.2.4, and H1.2.5.

The cavity must be present in the model, and both its radius and its axial height as measured from its axial midplane must be positive. The total heat load within the package must be defined with the cavity data. HTAS1 assumes this heat is located within the cavity. It calculates the surface area of the cavity as

$$A_c = 2\pi r_c h_c + 2\pi r_c^2 , \qquad \text{(H1.2.1)}$$

where

- A_c is the total surface area of the cavity,
- r_c is the radius of the cavity,
- h_c is the height of the cavity,

and computes the average surface heat flux as

$$q_c = \frac{Q_c}{A_c} , \qquad \text{(H1.2.2)}$$

where

- q_c is the average surface heat flux,
- Q_c is the heat load in the cavity.

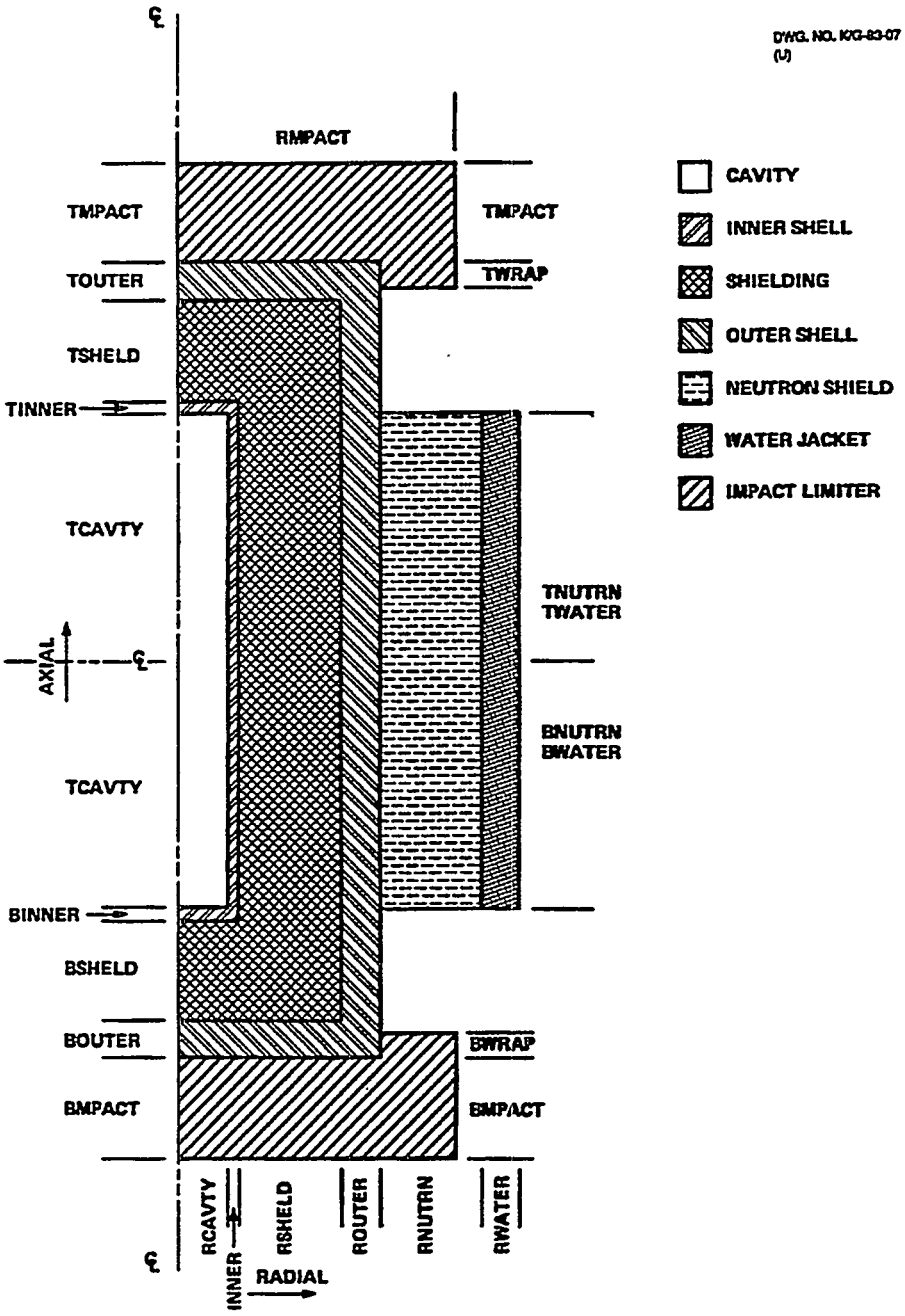


Figure H1.2.1 Zone configuration in HTAS1 general model with physical dimensional labels

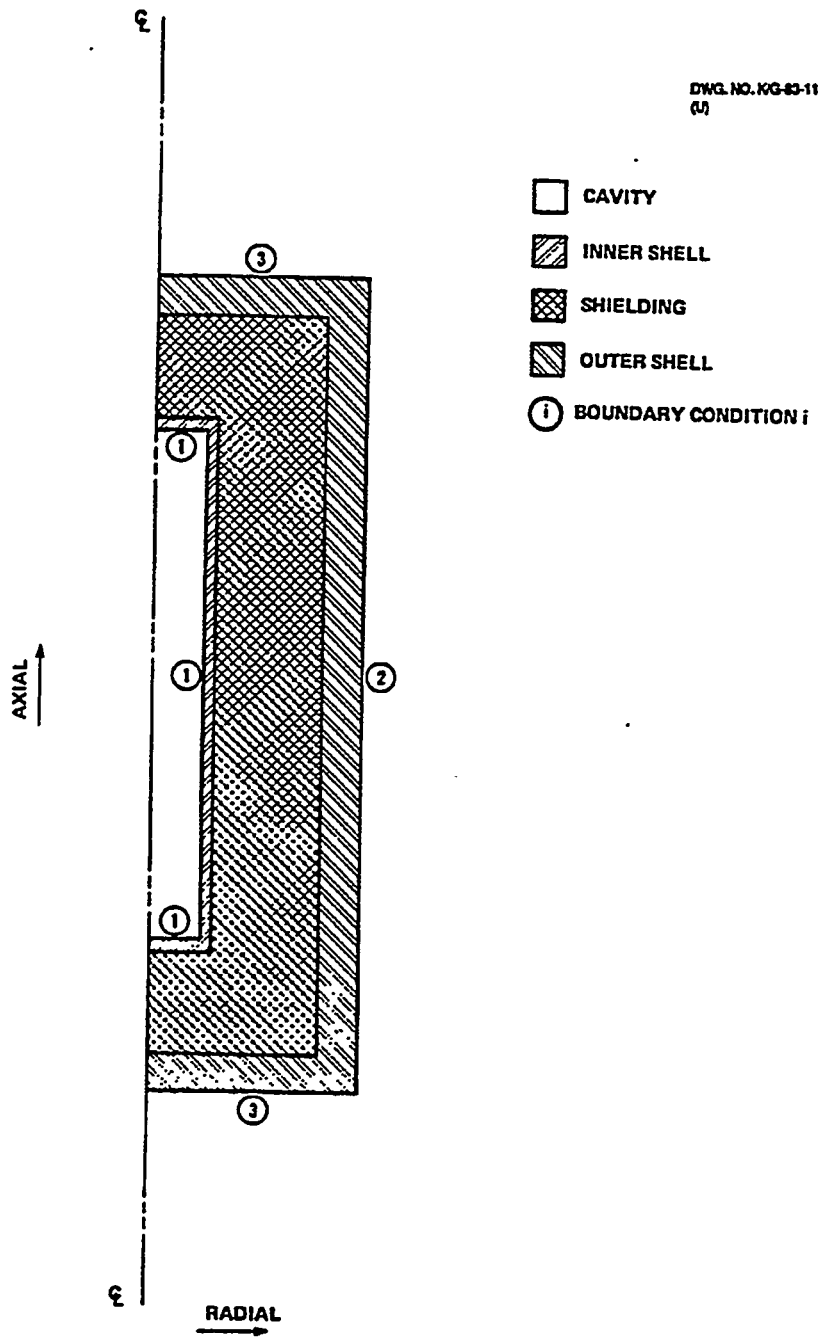


Figure H1.2.2 Location of boundary conditions in HTAS1 basic model (cavity, inner shell, shielding, outer shell)

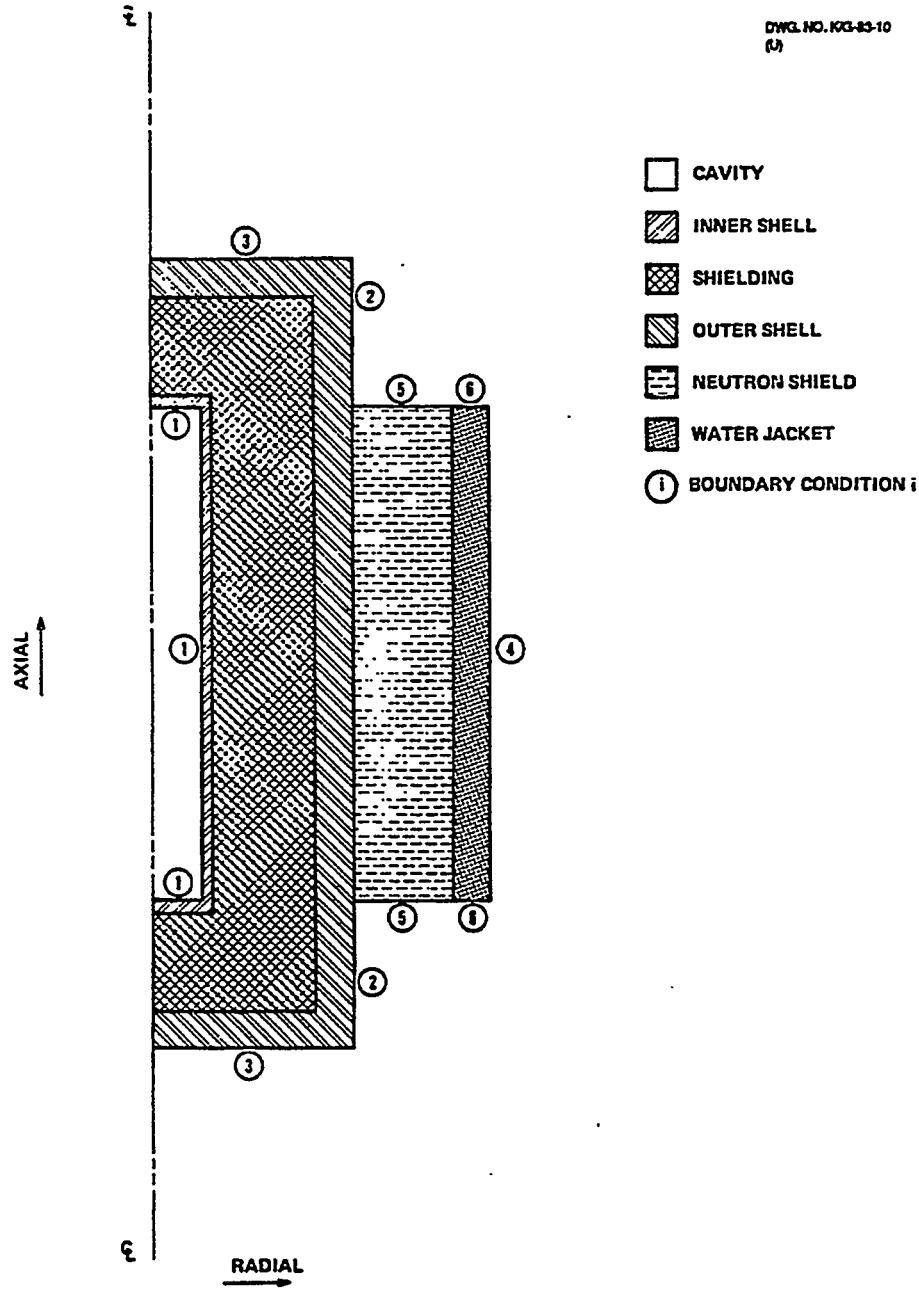


Figure H1.2.3 Location of boundary conditions in HTAS1 basic model with addition of neutron shield and water jacket

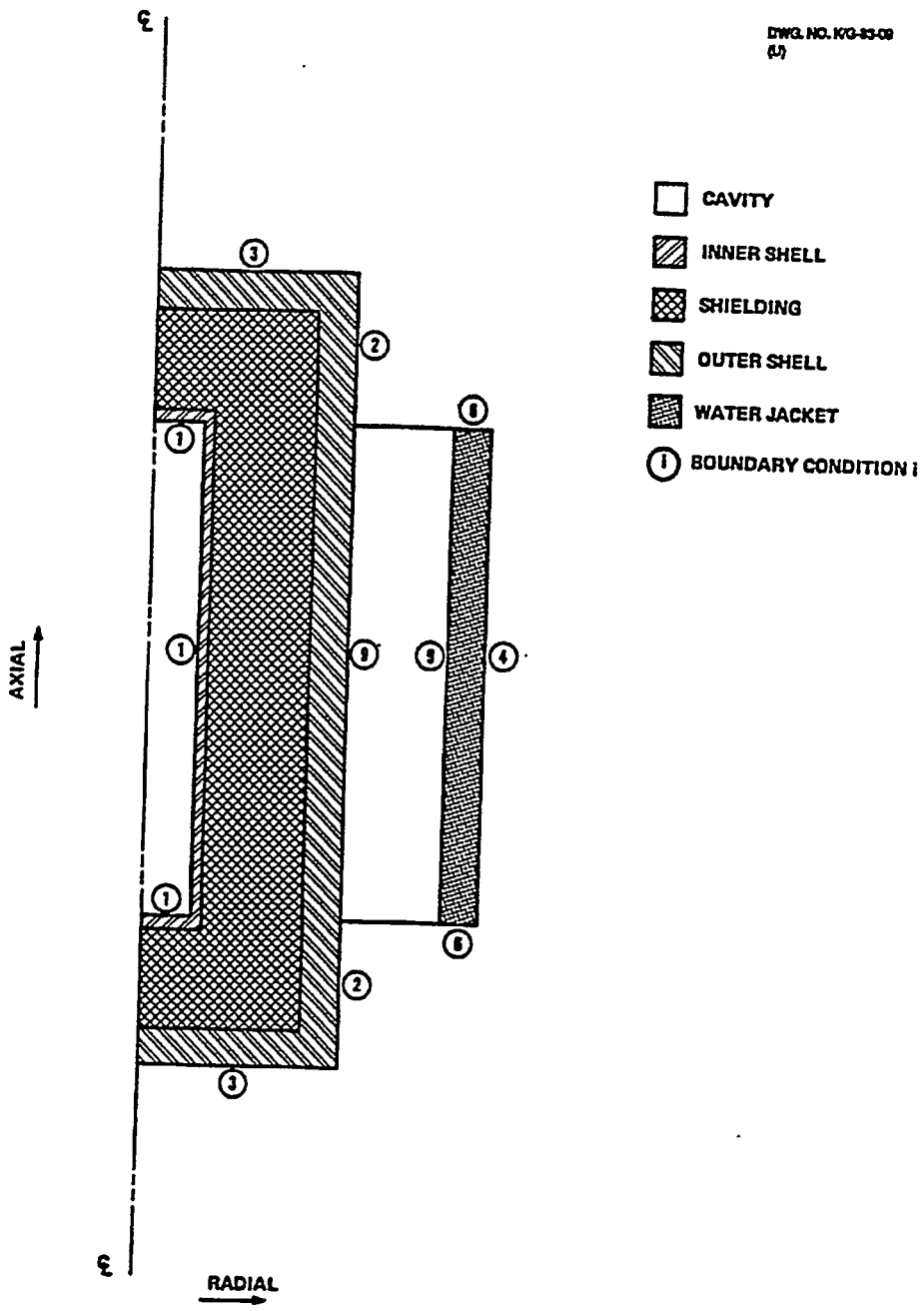


Figure H1.2.4 Location of boundary conditions in HTAS1 basic model with addition of neutron shield and water jacket after neutron shield has been deleted

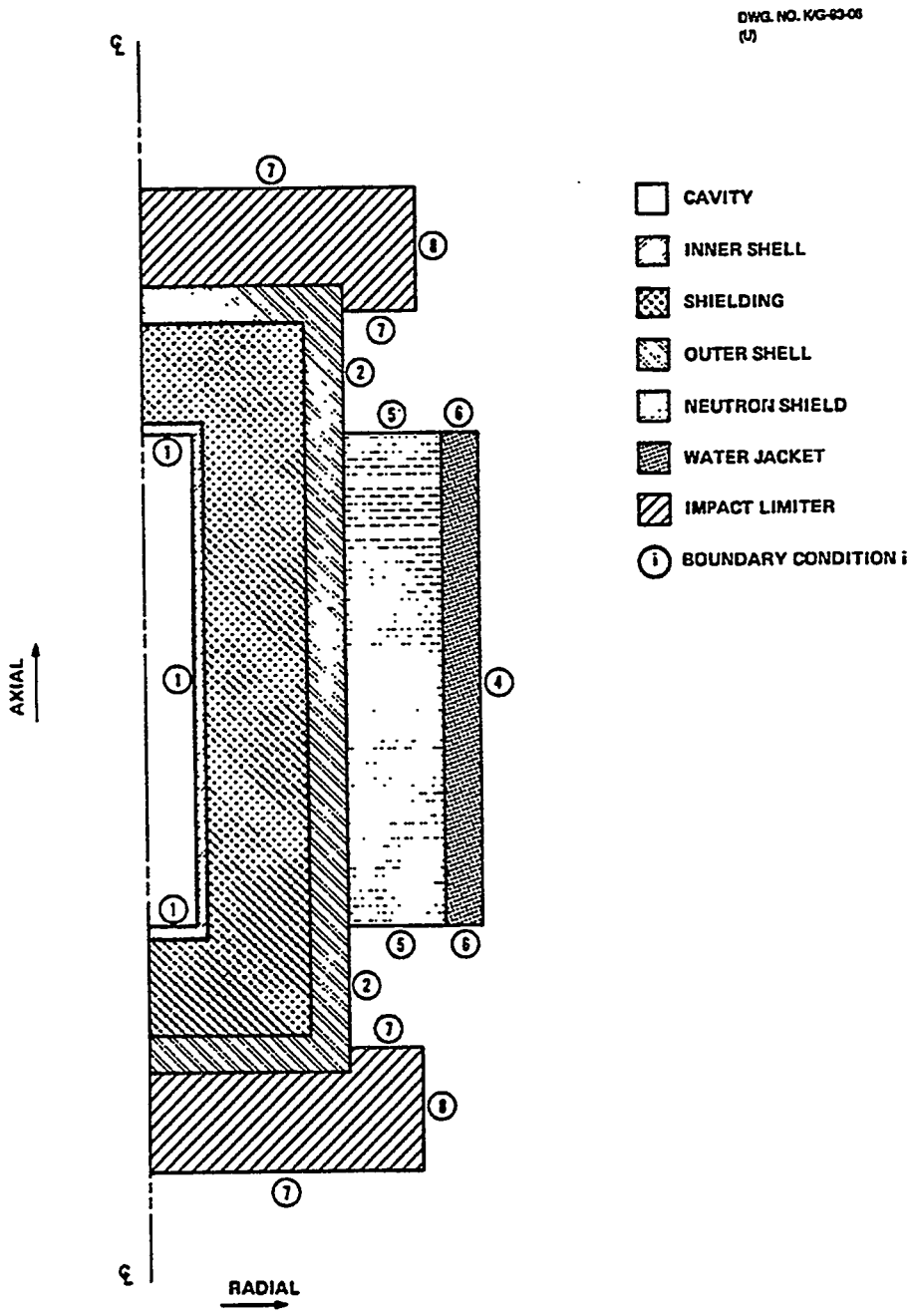


Figure H1.2.5 Location of boundary conditions in HTAS1 general model

HTAS1 then generates boundary condition number 1 with this heat flux and applies it along the inner surfaces of the inner shell (see Fig. H1.2.2).

The inner shell must be present in the model, and its radial thickness and its axial thickness at both the top and bottom must be positive. The top and bottom axial thicknesses may be different. Thus, the inner shell completely encloses the cavity, as shown in Fig. H1.2.1.

The shielding zone is optional. If it is present in the model, its axial extent must at least be equal to that of the inner shell. If it extends axially beyond both the top and bottom of the inner shell, the shielding completely encloses the inner shell, as depicted in Fig. H1.2.1.

The outer shell must be present in the model, and it completely encloses the cavity, inner shell and shielding. Thus, the radial thickness, as well as the axial thicknesses at both the top and bottom of the outer shell, must be positive. HTAS1 generates boundary conditions for any surfaces of the outer shell that are outer surfaces of the model. In particular, HTAS1 generates boundary conditions 2 and 3 and applies them along the radial and axial outer surfaces, respectively, of the outer shell (see Figs. H1.2.2, H1.2.3, H1.2.4, and H1.2.5).

The neutron shield and water jacket zones are optional for the model. However, if they are present, they must appear as a pair, and their axial extent must be the same. The radial thickness of each zone must be positive. As the default, the axial extent of each zone is equal to that of the cavity. However, the default may be overridden as long as the zones do not extend beyond the top and bottom of the outer shell. When the neutron shield and water jacket are present in the model, HTAS1 generates boundary conditions 4, 5, and 6 and applies boundary condition 4 along the outer radial surface of the water jacket and boundary conditions 5 and 6 along the outer axial surfaces of the neutron shield and water jacket, respectively (see Fig. H1.2.3).

The material in the neutron shield can be replaced by air or deleted following any thermal analysis in a prescribed analytical sequence. If this option is invoked, HTAS1 will generate boundary condition 9 which will be a surface-to-boundary connection with the magnitude of the Stefan-Boltzmann constant. This boundary condition will be referred to by the node-to-node connectors generated by OCULAR for 2-D radiative heat transfer within the water jacket.

The neutron shield and water jacket may be deleted following any thermal analysis in a prescribed analytical sequence. If this option is invoked, HTAS1 will generate a boundary condition and apply it along the portion of the outer radial surface of the outer shell that was previously covered by the neutron shield and water jacket (see Figs. H1.2.3 and H1.2.2). The boundary condition will be 2 if the outer radial surface of the outer shell is unfinned and 10 if it is finned. Thus, if the outer shell is finned, boundary condition 2 will model the finned, radial surface of the outer shell and boundary condition 10 will model the unfinned portion.

The impact limiter zone is optional for the model. If the impact limiter zone is defined, the impact limiters may appear independently at the top and/or bottom of the transport package. If they both appear, the radius of each impact limiter must be the same. However, the axial thickness of the top and bottom impact limiters may be different. Although there is no upper limit on the radius of the impact limiter, it must be at least equal to the radius of the outer shell. The default radius of the impact limiter is equal to the radius of the outer shell. Each impact limiter may be a disk at the top or bottom of the outer shell, or it may wrap around the top and/or bottom of the outer shell. If one of the impact limiters extends around the outer shell, it may extend axially to the neutron shield and water jacket if they are defined or it may extend to the axial midplane of the cavity if they are not defined. Boundary conditions 7 and 8 are generated by HTAS1 and applied along the axial and radial outer surfaces, respectively, of the impact limiters (see Fig. H1.2.5).

One or both of the impact limiters may be deleted after any thermal analysis in an analytical sequence. If both impact limiters are deleted, they must be deleted at the same time. If either of the impact limiters are deleted, HTAS1 will apply boundary condition 3 along the axial surface or surfaces of the outer shell that were previously covered by the impact limiter or limiters (see Figs. H1.2.5 and H1.2.3). HTAS1 will also generate a boundary condition and apply it along the portion of the outer radial surface of the outer shell that was previously covered by one or both of the impact limiters. As in the case of deleting the neutron shield and water jacket, the boundary condition will be 2 if the outer radial surface of the outer shell is unfinned and 10 if it is finned.

H1.2.2 DISCUSSION OF THE THERMAL PROPERTIES ASSOCIATED WITH EACH ZONE

A default material is associated with each of the seven zones available to HTAS1 in modeling a problem (see Table H1.2.1). A material property library is included in HTAS1 (see Table H1.2.2). This library contains the thermal conductivity, density, specific heat, emissivity, latent heat and transition temperature for each material in the library. In addition to the default materials for each zone, a number of additional materials associated with nuclear fuel transport packages are included in the library. These materials may be used to replace some or all of the default materials for a particular analysis. Since some materials of interest may not be included in the material property library, a material and values for its thermal parameters may be defined with the data for a specific zone to override the HTAS1 defaults. The HTAS1 material property library is located in subroutine MATLIB, and it is a straightforward task to add additional materials to it or to modify the thermal properties of materials in it.

As the default, HTAS1 does not allow any material to undergo a change of phase. The user may override this default condition for each specific zone and cause HTAS1 either to obtain the latent heat and accompanying transition temperature for the material from HTAS1's material property library or to read it with the other data defining the zone. When the model specifies the change-of-phase option, the transient calculations must be performed by HEATING with either the classical explicit procedure which is stability-limited or Levy's modified explicit procedure. Under the default conditions HTAS1 will generate data enabling HEATING to perform the calculations using Levy's modified explicit procedure with a time step factor of 10. This default condition may be overridden as long as an attempt is not made to use one of the implicit procedures. Since radiative heat transfer may be considered across outer surfaces of a shipping container, an emissivity is associated with each zone which can be on an outer surface of the model. These emissivities may vary during an analytical sequence to model changing conditions on a surface. Default emissivities for each thermal analysis are presented in Table H1.2.3 for each zone that can be on an outer surface.

H1.2.3 DESCRIPTION OF THERMAL ANALYSES AVAILABLE FOR ANALYTICAL SEQUENCES

After the user has defined the physical model to HTAS1 by providing all appropriate data for each zone, the actual sequence of thermal calculations to be performed by HEATING must be defined. HTAS1 is designed to generate data for HEATING to perform the following five independent thermal analyses:

1. to obtain the steady-state normal operating thermal conditions for the transport package for the operating conditions specified in Part 71 of Title 10, Chapter 1, Code of Federal Regulations—Energy, U.S. Nuclear Regulatory Commission,

2. to obtain the steady-state normal operating thermal conditions for the transport package for a realistic ambient boundary temperature (default, 100°F),

3. to obtain the transient thermal conditions during a specified accident in which the transport package is subjected to a fire at a stated temperature (default, 1475°F) for a stated period of time (default, 30 min),

4. to obtain the transient thermal conditions of the transport package for a specified period of time (default, 180 min) in an environment at a specified temperature (default, 100°F) following exposure to the fire, and

5. to obtain the steady-state operating thermal conditions for the transport package for a realistic ambient boundary temperature (default, 100°F) following the accident and exposure to the fire.

Table H1.2.1 Keywords for zones in HTAS1 model

Zone keyword	Default material index	Default material name	Default material description
CAVITY			Void
INNER SHELL	13	SST304	Stainless Steel 304
SHIELDING	11	LEAD	Lead
OUTER SHELL	13	SST304	Stainless Steel 304
NEUTRON SHIELD	17	H2OCON	Water, effective conductivity simulating natural convection
WATER JACKET	13	SST304	Stainless Steel 304
IMPACT LIMITERS	19	BALSA	Balsa wood, thermal conductivity across grain

Table H1.2.2 HTAS1 material property library

Material Index	Material Name	Temp. (°F)	Conductivity (btu/hr-ft°F)	Density (lb/ft)	Temp. (°F)	Specific Heat (Btu/lb°F)	Transition Temperature (°F)	Latent Heat of Fusion (Btu/lb)	Reference
11	LEAD	32	20.3	710	32.0	0.0305	621.3	10.6	1,2
		212	19.3		212.0	0.0315			
		392	18.2		621.5	0.0338			
		572	17.2		621.7	0.0340			
		630	12.1		1832.0	0.0328			
		717	9.7						
		800	9.0						
		980	8.7						
		1276	8.66						
12	DURANIUM[a]	32	15.0	1190	32	0.0275	2069.6	22.7	2
		752	20.1		662	0.035			
		1472	27.6		1225	0.048			
		1652	30.2		1234	0.830			
					1243	0.045			
					1418	0.045			
					1427	0.930			
					1436	0.0384			
13	SST304	32	8.1	491	32	0.12	2552	117.0	1,2
		212	8.7		752	0.135			
		392	8.7						
		572	9.4						
		752	10.0						
		1112	11.0						
		1472	13.0						
14	CARSTEEL	32	25	487	68	0.113	2796.8	117.0	1,2
		212	25						
		392	24						
		572	23						
		752	21						
		1112	19						
		1472	17						
		1832	16						
17	H2OCONV[b]	150	14.75	60	32	1.00720			3,4,5
		200	17.33		68	0.99861			
		250	19.15		104	0.99780			
		300	20.83		140	0.99921			
		400	23.35		176	1.0021			
					212	1.0068			
					248	1.0149			
					284	1.0228			
					320	1.0369			
					356	1.0548			
					392	1.0758			
					428	1.1009			
					464	1.1357			
					500	1.1818			
					537	1.2437			
					572	1.3678			
18	AIRCONV[c]		0.1	0.059	-6.67	0.24007			3
					83.33	0.24016			
					173.33	0.24095			
					263.33	0.24214			
					353.33	0.24374			
					443.33	0.24584			
					533.33	0.24816			

Table H1.2.2 (continued)

Material Index	Material Name	Temp. (°F)	Conductivity (btu/hr-ft°F)	Density (lb/ft)	Temp. (°F)	Specific Heat (Btu/lb°F)	Transition Temperature (°F)	Latent Heat of Fusion (Btu/lb)	Reference
					623.33	0.25196			
					713.33	0.25396			
					803.33	0.25676			
					893.33	0.25924			
					983.33	0.26215			
					1073.33	0.26495			
					1163.33	0.26774			
					1253.33	0.27035			
					1343.33	0.27264			
					1523.33	0.27701			
19	BALSA[d]		0.0484	20.0		0.55			2
20	REDWOOD[d]		0.0636	26.0		0.69			6
21	PURETHAN[e]		0.0242	3.7		0.42			2

[a]Depleted uranium.
[b]Water with effective thermal conductivity simulating natural convection.
[c]Air with effective thermal conductivity simulating natural convection.
[d]Thermal conductivity across grain.
[e]Flexible polyurethane foam.

Table H1.2.3 Default emissivities on outer surfaces of zones modeled by HTAS1

Zone keyword	Default emissivities[a]				
	INITIAL	PREFIRE	FIRE	POSTFIRE	FINAL
OUTER SHELL	0.5	0.5	0.8	0.8	0.8
NEUTRON SHIELD	0.5	0.5	0.8	0.8	0.8
WATER JACKET	0.5	0.5	0.8	0.8	0.8
IMPACT LIMITERS	0.5	0.5	0.8	0.8	0.8

[a]Data taken from Refs. 7 and 8.

Fifteen different analytical sequences may be performed by using various acceptable combinations of these five thermal analyses.

Under the default conditions, HTAS1 uses HEATING's direct-solution technique to calculate the steady-state temperature distribution and the Crank-Nicolson implicit procedure to calculate the transient temperature distribution. For transient problems, it allows HEATING to determine the initial time step size by setting it equal to the stability criterion for the classical explicit procedure. It then allows HEATING to vary the size of the time step to keep the maximum relative change in temperature at any node equal to 2%. When the model contains a material that is allowed to undergo a change of phase, HTAS1's default conditions will use Levy's modified explicit procedure with a time-step factor of 10. The initial time-step size will be determined by HEATING by setting it equal to the stability criterion for the classical explicit procedure. The user may override these default conditions and use any numerical technique available in HEATING as long as it is compatible with the thermal analysis to be performed.

H1.2.4 DEFINITION OF BOUNDARY CONDITIONS

HTAS1 generates appropriate boundary conditions for the outer surfaces of the model based on the thermal analysis being performed, the boundary parameters associated with the thermal analysis, and the emissivities of the materials on the outer surfaces. In generating boundary conditions on external surfaces of the model, HTAS1 allows for the following heat transfer mechanisms: natural convection to or from the surrounding medium, radiation to or from the surrounding medium, and a prescribed heat flux to simulate the solar heat load.

The film coefficient correlation to simulate the natural convective heat transfer effects across a surface has the form

$$h_c = h_n \, |T_s - T_n|^{h_e}, \tag{H1.2.3}$$

where

T_s is the surface temperature,

T_a is the ambient temperature for the thermal analysis involved,

h_n is the natural convective coefficient,

h_e is the natural convective exponent.

For a radial surface, the default values of h_n and h_e are 0.18 Btu/(hr-ft^2-°F$^{4/3}$) and 1/3, respectively, to simulate the turbulent natural convective heat transfer in air on the radial surface of a long, horizontal cylinder.[9] For an axial surface, the default values of h_n and h_e are 0.19 Btu/(hr-ft^2-°F$^{4/3}$) and 1/3, respectively, to simulate the turbulent natural convective heat transfer in air on the end of a horizontal cylinder.[9]

The heat transfer coefficient to simulate the radiative heat transfer at the surfaces of the model before and after the fire has the form (Ref. 9)

$$h_r = \sigma \epsilon_s \, , \tag{H1.2.4}$$

where

σ is the Stefan-Boltzmann constant or 0.173×10^{-8} Btu/(hr-ft^2-°R^4),

ϵ_s is the emissivity of the material on the surface of the model.

The emissivity for each material will be extracted from HTAS1's material property library (see Table H1.2.2) unless it is provided by the user when a particular zone is defined. The emissivity is defined independently for each thermal analysis to be performed on the model. During the fire, the radiative heat transfer coefficient used by HTAS1 has the form (Ref. 9)

$$h_r = \sigma \left[\frac{1}{\frac{1}{\epsilon_s} + \frac{1}{\epsilon_f} - 1} \right], \qquad \text{(H1.2.5)}$$

where

ϵ_f is the emissivity of the fire.

In keeping with the specifications in Part 71 of Title 10, Chapter 1, Code of Federal Regulations-Energy, U.S. Nuclear Regulatory Commission, the default values for the emissivity of the fire is 0.9 and for the emissivity on the surfaces of the package during the fire is 0.8. Also, the default temperature of the fire is 1475°F. However, the default value of each of these parameters may be overridden.

The default value for the solar heat load is 122.92 Btu/(hr-ft^2) (Ref. 8), except the solar heat load, is not applied to the surface of the package during the fire analysis. The user may override these defaults and specify a heat flux across the surface of the package for any thermal analysis.

When the material in the neutron shield is deleted or replaced, HTAS1 uses the OCULAR program to simulate 2-D radiative heat exchange within the water jacket. HTAS1 generates boundary condition 9 which has a connectance equal to the Stefan-Boltzmann constant. Before the HEATING execution, OCULAR then calculates exchange factors between all of the nodes in the model which lie on the surface of the annular region between the water jacket and outer shell. The node-to-node connector generated by OCULAR between any two of these surface nodes has a connector value equal to the product of the exchange factor, F, and the area, A, of the emitting surface associated with the emitting node. These connectors all reference boundary condition 9, so that the effective heat transfer between any two of these surface nodes, Q, is

$$Q = \sigma AF[T_i^4 - T_j^4], \qquad \text{(H1.2.6)}$$

where

T_i is the emitting node, and

T_j is the receiving node.

H1.2.4.1 Finned Surface Option

Under the default conditions, HTAS1 assumes all surfaces are smooth (unfinned). However, this default can be overridden by defining one of eight fin effectiveness techniques on the outer radial and/or axial surfaces of any zone that is part of the outer surface of the model.

This technique is based on simple geometric descriptions and well-known fin effectiveness relations [Refs. 1 (pp. 3-115–3-119), 11, and 12] and has been implemented for the eight types of enhanced heat transfer surfaces shown in Table H1.2.4 and Fig. H1.2.6. These analytical techniques assume that the thermal conductivity and heat transfer coefficients are uniform for the fin. The technique implemented in HTAS1 requires the boundary temperature remain constant during each HEATING analysis. Although these

Table H1.2.4 Fin effectiveness models, analytical

(See Fig. H1.2.6 for geometry variable not defined in this table)

Fin type	Description

1 STRAIGHT FIN WITH RECTANGULAR CROSS SECTION

$$\psi = \frac{\tanh(\ell m)}{\ell m} \qquad m = \sqrt{\frac{h}{k\delta_B}}$$

$$R_{Sf} = (\ell + \delta_B)/\frac{S_1}{2}$$

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

h = convective heat transfer coefficient

k = thermal conductivity

R_{VA} = fin volume/(unit area of finned surface)

$= 2\ell\delta_B/S_1$

2 STRAIGHT FIN WITH TRIANGULAR CROSS SECTION

$$\psi = \left[\frac{1}{\ell\, m}\,\frac{I_1(2\ell\, m)}{I_0(2\ell\, m)}\right]$$

I_n = modified Bessel function of the first kind of order n

$$R_{Sf} = (\sqrt{\ell^2 + \delta_B^2})/\frac{S_1}{2}$$

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

$$R_{VA} = \delta_B\ell\ /S_1$$

3 STRAIGHT FIN WITH TRAPEZOIDAL CROSS SECTION

$$\psi = \frac{\mu_0}{2\kappa^2 b_c}\left[\frac{K_1(\mu_e)\,I_1(\mu_0) - I_1(\mu_e)\,K_1(\mu_0)}{I_0(\mu_0)\,K_1(\mu_e) + I_1(\mu_e)\,K_0(\mu_0)}\right]$$

K_n = modified Bessel function, second kind of order n

$$\mu_0 = 2\kappa\left[b_c + \delta_t(1 - \tan\gamma)/\tan\gamma\right]^{1/2}$$

$$\mu_e = 2\kappa\left[\frac{\delta_t(1 - \tan\gamma)}{\tan\gamma}\right]$$

Fin type	Description

$$\kappa = \sqrt{\frac{h}{k\sin\gamma}}$$

$$\gamma = \tan^{-1}\left((\delta_B - \delta_t)/\ell\right)$$

$$b_c = \ell + \delta_t$$

$$R_{Sf} = (2\delta_t + 2\sqrt{\ell^2} + (\delta_B - \delta_t)^2)/S_1$$

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

$$R_{VA} = \ell\ (\delta_t + \delta_B)/S_1$$

4 CIRCULAR (ANNULAR) FIN WITH RECTANGULAR CROSS-SECTION EXTERNAL SURFACE FIN

$r_t > r_B$ Fin on External Surface of Cylinder

$$\psi = \left[\frac{2}{m\ell\left[\frac{r_t}{r_B} + 1\right]}\right]\left[\frac{I_1(mr_t)K_1(mr_B) - I_1(mr_B)K_1(mr_t)}{I_0(mr_B)K_1(mr_t) + I_1(mr_t)K_0(mr_B)}\right]$$

r_t = *tip radius*
r_B = *base radius*

$$\ell = r_t - r_B$$

$$R_{Sf} = [r_t\delta_B + (r_t^2 - r_B^2)/2]/(r_B\frac{S_1}{2})$$

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

Table H1.2.4 (continued)

Fin type	Description

5 SPINE, RIGHT CIRCULAR CYLINDER - TRIANGULAR PATTERN

$$\psi = \frac{1}{m\ell}\tanh(m\ell) \qquad m = \sqrt{2\frac{h}{k\delta_B}}$$

$$R_{Sf} = 2[\ell\ (\delta_B + \delta_t) + \delta_B\delta_t]/(S_1S_2) \qquad P = 4(\delta_B + \delta_t) = \textit{perimeter}$$

$$R_{Sf} = \pi\delta_B(2\ell + \delta_B)/(2S_1S_2)$$

$$R_{SW} = (S_1S_2 - \frac{\pi}{2}\delta_B^2)/(S_1S_2)$$

$$R_{VA} = (\frac{\pi}{2}\delta_B^2\ell\ )/(S_1S_2)$$

6 SPINE, RIGHT CIRCULAR CYLINDER - RECTANGULAR PATTERN

$$\psi = \psi \textit{ for FIN No. 5}$$

$$R_{Sf} = \pi\delta_B(2\ell + \delta_B)/(S_1S_2)$$

$$R_{SW} = (S_1S_2 - \pi\delta_b^2)/(S_1S_2)$$

$$R_{VA} = (\pi\delta_B^2\ell\ )/(S_1S_2)$$

7 SPINE, RECTANGULAR CROSS SECTION - TRIANGULAR PATTERN

$$\psi = \frac{1}{m\ell}\tanh(m\ell\ ) \qquad m = \sqrt{\frac{hP}{kA}}$$

Table H1.2.4 (continued)

Fin type	Description
$R_{SW} = (S_1S_2 - 2\delta_B\delta_t)/(S_1S_2)$	$A = 4(\delta_B\delta_t)$ = *cross-sectional area*
$R_{VA} = (2\delta_B\delta_t\ell\ )/(S_1S_2)$	
$R_{Sf} = 2[\ell\ (\delta_B + \delta_t) + \delta_B\delta_t]/(S_1S_2)$	$P = 4(\delta_B + \delta_t)$ = *perimeter*
8 SPINE, RECTANGULAR CROSS SECTION - RECTANGULAR PATTERN	
$\psi = \psi$ *for FIN No. 7*	
$R_{Sf} = 4[\ell(\delta_B + \delta_t) + \delta_B\delta_t]/(S_1S_2)$	
$R_{SW} = (S_1S_2 - 4\delta_B\delta_t)/(S_1S_2)$	
$R_{VA} = (4\delta_B\delta_t\ell\ )/(S_1S_2)$	

DWG. NO. K/G-80-2687 (4)

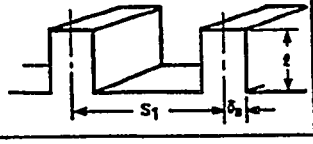
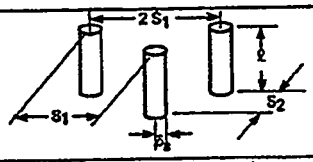
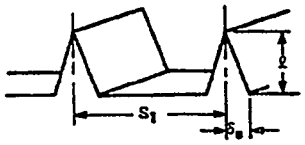
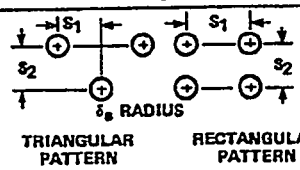
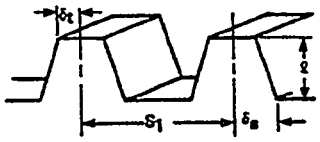
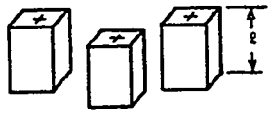
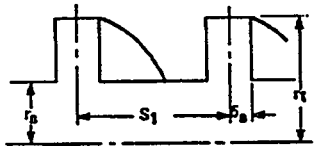
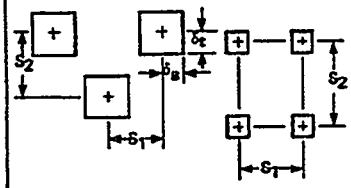
FIN TYPE NO.	DESCRIPTION	FIGURE	FIN TYPE NO.	DESCRIPTION	FIGURE
1	STRAIGHT (LONGITUDINAL) RECTANGULAR CROSS SECTION		5	SPINE RIGHT CIRCULAR CYLINDER TRIANGULAR PATTERN	
2	STRAIGHT (LONGITUDINAL) TRIANGULAR CROSS SECTION		6	SPINE RIGHT CIRCULAR CYLINDER RECTANGULAR PATTERN	
3	STRAIGHT (LONGITUDINAL) TRAPEZOIDAL CROSS SECTION		7	SPINE RECTANGULAR CROSS SECTION TRIANGULAR PATTERN	
4	CIRCULAR (ANNULAR) RECTANGULAR CROSS SECTION EXTERNAL FIN		8	SPINE RECTANGULAR CROSS SECTION RECTANGULAR PATTERN	

Figure H1.2.6 Fin effectiveness models, pictorial

techniques were developed for steady-state flow of heat in fins, they should be reasonably accurate for transient models if the fin size is small compared to the thickness of the surface zone.

The fin effectiveness η_t is the ratio of the heat transfer from the fin to that from the base area of the fin assuming convection to the fluid at the same temperature and convective heat transfer coefficient. The fluid temperature, heat transfer coefficient, and fin material thermal properties are assumed constant along the length of the fin. This concept is extended to finned surface effectiveness η. The finned surface effectiveness is the ratio of the heat transferred by the fin surface and the surface between the fins to that transferred by the surface if the fins were removed:

$$\eta = \frac{Q_{fin} + Q_W}{Q_{base}} = R_{Sf}\,\psi + R_{SW}, \qquad \text{(H1.2.7)}$$

where

Q_{fin} = heat flow from surface of fin,

Q_W = heat flow from portion of base surface not covered by fin,

Q_{base} = heat flow from surface assuming fins removed,

ψ = fin efficiency = $\dfrac{Q_{fin}}{Q_{fin}\,(k=\infty)}$

$Q_{fin}(k=\infty)$ = heat flow from fin surface assuming fin thermal conductivity is infinite,

R_{Sf} = (fin surface area)/(unit area of base surface)

R_{SW} = (base surface area not covered by fins)/(unit area of base surface).

In HTAS1, the fin effectiveness is used to modify the effective conductance for the boundary condition by adjusting the effective heat transfer coefficients as follows:

$$h_c' = h_c\eta \qquad \text{(H1.2.8)}$$

$$h_n' = h_n\eta, \qquad \text{(H1.2.9)}$$

where

η = finned surface effectiveness for that boundary condition and will be the same for both natural or forced convection.

If the surface material properties or the boundary heat transfer coefficient are temperature-dependent, a fin effectiveness temperature-dependent table is generated.

The fin effectiveness technique implemented does not check for inconsistent geometric definitions (e.g., width of fin greater than the fin spacing) or if the node spacing is smaller than the fin spacing. Modeling errors can result from these problems. If the node spacing is much smaller than the fin spacing or if the fin height is significant compared to the surface thickness, use of this technique is not recommended. Fin models 1–4 are 2-D in nature, and conduction along the third dimension is neglected. The code also does not allow for thermal growth of fins.

H1.2.5 MISCELLANEOUS CONSIDERATIONS IN MODELING A PROBLEM

H1.2.5.1 Location of the Neutron Shield, Water Jacket, and Impact Limiter

HTAS1 generates the fine grid lines for the model based on the grid spacing information supplied with the zone data. The axial fine grid lines are based on the axial grid spacing information provided for the cavity, inner-shell shielding, outer shell, and impact limiters. If one of the axial boundaries of the neutron shield and water jacket does not lie on one of these zone boundaries or on one of the fine grid lines generated by HTAS1, then HTAS1 will move the axial boundary of the neutron shield and water jacket to the nearest axial fine grid line. It will also generate a warning message indicating this action. If one of the impact limiters wraps around the package, HTAS1 will locate its axial extent in a similar manner. The radial fine grid lines are based on the radial grid spacing information provided for the cavity, inner shell, shielding, outer shell, neutron shield, water jacket and impact limiter if the impact limiter extends radially beyond the water jacket. If the radius of the impact limiter does not extend beyond the radius of the water jacket, it must lie on one of the boundaries of the neutron shield or water jacket or on one of the fine grid lines within those zones. If this is not the case, HTAS1 will move the radius of the impact limiter to the nearest radial fine grid line and will generate a warning message indicating this action. HTAS1 follows this procedure to minimize the occurrence of an unfavorable distribution of nodes in the model. As an example, large differences in the size of coefficients in the system of equations describing the temperature distribution can lead to numerical problems when an attempt is made to solve the system. This situation can happen when large differences exist between node sizes throughout the model, especially if they are within the same zone. Note that when the boundaries of one of the zones is moved, the resulting model will be slightly different from the one which was input. For instance, the volume and heat flow paths will be slightly changed. This error will decrease as the grid spacing decreases.

H1.2.5.2 Modeling of the Neutron Shield and Water Jacket

The water jacket wraps around the neutron shield and extends to the surface of the outer shell. The top and bottom of the water jacket tend to serve as a heat flow path between the water jacket and outer shell since its thermal conductivity will generally be higher than that of the neutron shield. HTAS1 assumes this heat flow path is small, and thus it is not modeled in order to minimize the occurrence of an unfavorable nodal configuration. The effects of this assumption will be small unless the axial thickness of the water jacket at one of the ends of the neutron shield is large. The effects of radiative heat transfer on the ends of the water jacket are considered since the default values for the emissivities on the surface of the neutron shield are equal to the water jacket surface emissivities.

H1.2.5.3 Modeling of the Impact Limiter

The impact limiter is usually covered by a thin layer of metal, which could extend around the impact limiter to the surface of the outer shell. This layer would serve as a heat flow path since its thermal conductivity would probably be higher than that of the impact limiter. HTAS1 assumes this covering is very thin and as such its heat transfer effects in this analysis are negligible. The effects of radiative heat transfer on the surface of the impact limiter are considered since the default values for the emissivities on the surface of the impact limiter is equal to the emissivities for stainless steel (see Table H1.2.3). Of course these values may be overridden by the emissivities of any material covering the impact limiter.

H1.2.5.4 Other Modeling Considerations

In developing HTAS1, it was assumed the contact resistance between the zones was negligible, and thus it was not considered. The neutron shield will be composed of water under the default conditions. During a prescribed accident, the water jacket may be punctured, and the water in the neutron shield may leak

out. This condition is modeled by deleting the neutron shield. As the default, the water (or material) in the neutron shield will be replaced by air when the neutron shield is deleted. In both cases, HTAS1 only approximates the natural convective heat transfer in the neutron shield by using an effective thermal conductivity for the water or air in the annulus.

For the water-filled neutron shield, HTAS1 will use material 17, denoted as H2OCONV, from its material property library. The effective thermal conductivity of material 17 was designed to simulate the effects of the natural circulation in a 4.5-in.-wide annulus (Ref. 5). This temperature-dependent effective thermal conductivity was derived using a correlation by Liu, Mueller, and Landis for approximating the thermal conductivity due to natural convection through a medium enclosed in an annular space between concentric cylinders (Ref. 10).

As the default for the air-filled neutron shield, HTAS1 will replace the material (default, H2OCONV) in the neutron shield with material 18 from the HTAS1 material property library. Material 18, denoted as AIRCONV, is air with an effective thermal conductivity of 0.1 Btu/hr-ft-°F to simulate the natural convective effects that will occur in the resulting enclosure between the outer shell and the water jacket. The decision to use this value for the default, average effective thermal conductivity of the air in the voided neutron shield, was based on the following analyses on variations of sample problem No. 1. Under normal operating conditions, the maximum temperature on the surface of the outer shell was 281°F and on the surface of the water jacket was 275°F. If the neutron shield was deleted following the prefire steady state, the absolute maximum temperature on the surface of the water jacket during the fire would be the temperature of the fire or 1475°F. Thus, the temperature difference across the air-filled neutron shield will range from approximately 6°F immediately following the rupture of the water jacket to −1225°F during the fire. Since the temperature on the surface of the outer shell will increase during the fire transient and since the temperature on the inner surface of the water jacket will be less than the fire temperature, the temperature difference will not really be that large. It will also vary along the axial length of the water jacket. During the postfire transient, the temperature difference will increase to zero and will gradually increase to a maximum of several hundred degrees Fahrenheit. Thus, the absolute value of the temperature difference across the air-filled annulus will range from 0°F to around 1000°F.

If the average air temperature is assumed to be the average of the temperatures of the opposing surfaces, then it will range from 275°F to around 1000°F. To estimate the effects of natural convection through the annulus, a number of hand calculations were performed using the correlation of Lui, Mueller, and Landis (ref 10) to obtain the effective thermal conductivity of the air-filled zone. The calculations were performed with the average air temperature ranging from 250°F to 1000°F and the temperature difference across the annulus ranging from 10°F to 1000°F. The effective thermal conductivity ranged from 0.06 to 0.15 Btu/hr-ft-°F. The thermal conductivity of air ranges from 0.01944 Btu/hr-ft-°F at 263°F to 0.03483 Btu/hr-ft-°F at 1073°F (Ref. 3). Based on this analysis, the effective thermal conductivity of the air in the annulus would range from a minimum of 0.01944 Btu/hr-ft-°F with pure conduction to around 0.15 Btu/hr-ft-°F with natural convection. Since the effective thermal conductivity of the air will be a function of both the air temperature and the temperature difference across the annulus, since it will be a function of both axial location and time, and since a conservative value during the fire will not necessarily be conservative following the fire and vice versa, a constant value of 0.1 Btu/hr-ft-°F was used for the effective thermal conductivity of material 18, AIRCONV.

An analysis was performed to compare the amount of heat transferred by radiation with that transferred by conduction and natural convection. The emissivities on the opposing surfaces of the annulus were assumed to be the default of 0.5. One set of calculations held the temperature of the outer shell at 280°F while increasing the temperature of the water jacket from 275°F to 1475°F. The ratio of heat transferred by radiation to that transferred by conduction and natural convection with an effective thermal conductivity of 0.1 Btu/hr-ft-°F ranged from 4.3 to 29. The calculations were repeated by allowing the temperature of the outer shell to increase. As the outer-shell temperature approached that of the water jacket, the above ratios increased for each water jacket temperature. Thus, the heat transferred across the annulus was largely controlled by radiation. As a final check on the effective thermal conductivity of the air in the

annulus, a parametric study was run with HTAS1 on sample problem number 1 assuming the water jacket was ruptured following the prefire steady state. The emissivities on the opposing surfaces of the annulus were assumed to be the default of 0.5. Calculations were run with the effective thermal conductivity of the air ranging from 0 (or a void) to 0.2 Btu/hr-ft-°F. The variations in the temperatures along the outer shell were at most a few percent during this parametric study. Thus, 0.1 Btu/hr-ft-°F is a reasonable effective thermal conductivity to simulate the natural convection heat flow across a 4.5-in. annulus for the shipping container similar to the one modeled by sample problem number 1. This value should be reasonable for shipping packages having similar dimensions and material properties. However, the user should analyze the natural convective heat flow across an annulus for shipping packages basically different from sample problem No. 1 prior to using the HTAS1 default properties for air with natural convection or material 18, AIRCONV.

Any support structure or internal fins that may be inside the neutron shield are not modeled. For a specific design, the user may approximate any such effects by developing an effective density and an effective thermal conductivity to simulate any change in the density and heat flow paths due to such a structure inside the neutron shield.

Since the internal heat load is applied as a heat flux across the surface of the inner shell, the actual fuel in the nuclear fuel transport package is not physically modeled, and thus its heat capacity effects are not included in the transient calculations.

H1.2.6 DESCRIPTION OF HTAS1 PLOTTING OPTIONS

Subroutines from REGPLOT6 (see Sect. F14) are included in HTAS1 so that the HEATING input generated by HTAS1 to describe the heat transfer model at each calculational phase can be graphically verified if the user selects the region plotting option. Maps of the regions, the materials, the heat-generation-function numbers, the initial-temperature-function numbers, and the boundary-condition function numbers are generated by plotting the model regions and labeling each region appropriately. By default, plots of the regions, the materials, and the boundary condition function numbers are generated for each calculational phase. HEATING is not executed when region plots are generated. Therefore, a minimum of execution time can be used to verify that the input supplied to HTAS1 has produced the desired HEATING input.

Temperature profile plots may also be generated if the user desires. If the temperature profile plotting option is selected, one temperature distribution plot data set is written by HEATING during the fire transient calculations and another temperature distribution plot data set is written by HEATING during the postfire transient calculations. These data sets are written to logical units 18 and 19, respectively.

By default, three plots are generated. The first plot contains temperature-vs-time curves for the nodes in the center of the inner shell, the shielding, and the outer shell. If a node is not located in exactly the center of a particular zone, the node closest to the center of that zone is used. If the shielding is not modeled, the node that represents the inner shell is located on the radial fine grid line that is the border between the cavity and the inner shell, the node that represents the shielding is located on the radial fine grid line that is the border between the inner shell and the outer shell, and the node that represents the outer shell is located on the radial fine grid line that denotes the outer boundary of the outer shell. The second plot contains a curve that shows maximum temperature over a span of problem time vs the radial distance from the origin for all nodes on the axial center line. The third plot contains a curve that shows the difference in volume-averaged temperatures between the inner shell and the outer shell as a function of time. The temperature at each node in a zone is multiplied by the volume of that node. These products are summed, and the sum is divided by the volume of the entire zone to compute the volume-averaged temperature for a zone.

If both the fire transient and postfire transient calculations are performed by HEATING, the time axis on plots includes problem times from both the fire transient and postfire transient calculational phases. If only the fire transient calculation is performed by HEATING, then the time axis only includes problem times from the fire transient calculational phase. In a similar manner, if only the postfire transient calculation is performed by HEATING, then the time axis only includes problem times from the postfire transient

calculational phase. If neither the fire transient calculation nor the postfire transient calculation are performed by HEATING, then temperature profile plots are not generated.

The user may choose from several options that allow plots to be generated in a manner other than the default plots that include data at all problem times for which temperature distributions exist. The plot of maximum temperature at any problem time vs the radial distance from the origin for all nodes on the axial center line may be omitted, as may the plot of the difference in volume-averaged temperature between the inner shell and the outer shell vs time. The temperature-vs-time curves for the outermost nodes of the inner shell, the shielding, and the outer shell may be drawn on individual plots. These same curves may be generated for temperature change from the initial temperature distribution instead of for the actual temperatures. Finally, a minimum and maximum time may be specified so that the time axis only includes a specified time interval. Combinations of these options may be specified. For example, it is possible to generate curves of temperature change for the inner shell, the shielding, and the outer shell on individual plots between specified minimum and maximum problem times.

PLOTS ARE DISABLED IN CURRENT VERSION. Although the routines and output of summary information remain in the current version, generation of plots has been disabled due to the lack of a suitable graphics package. The output now contains sufficient data for the user to generate these plots.

H1.3 LOGICAL PROGRAM FLOW AND DESCRIPTION OF SUBROUTINES

The input data for HTAS1 are basically composed of five sets. The first set consists of a title card and a parameter card. The parameter card contains the maximum CPU seconds allowed for this execution and the logical unit number for the initial temperature distribution for cases involving the restart of an analytical sequence. The second set of data consists of the zone data used to define the zones present in the model, along with accompanying data to override undesirable default values. This set defines the physical model. The third set of data consists of the thermal analysis data to define the particular analytical sequence to be used in the analysis of the model. This set may contain data to override undesirable default values to include both those that determine the specific thermal analysis to be performed as well as those that determine the numerical technique to be used to perform each thermal analysis. The fourth set consists of data defining the frequency and type of HEATING output for transient calculations. The final set of data simply consists of an end-of-data (EOD) card.

H1.3.1 DISCUSSION OF INTERACTION WITH THE DRIVER, HEATING, AND OCULAR

HTAS1 reads the input data and checks it for errors. If an error is encountered, HTAS1 writes a descriptive message indicating the nature of the error and, if possible, offering suggestions on how it may be corrected. HTAS1 then sets a flag to terminate calculations, but, if it is possible, it continues to examine the input data for additional errors. Thus, as many as possible of the input data errors are located on the first execution of HTAS1. At the end of the execution, HTAS1 generates a summary message which includes the total number of errors it encountered in the input data. If no errors are encountered, HTAS1 processes the input data and generates the HEATING input data for the first thermal analysis in the specified analytical sequence. To identify the thermal analysis to be performed by HEATING, HTAS1 puts the appropriate entry from the following list in column 57–72 of the title card.

- INITIAL SS
- PREFIRE SS
- FIRE TR
- POSTFIRE TR
- FINAL SS

For restart cases HTAS1 copies the initial temperature distribution from the specified logical unit (ITPIN) to logical unit KTPIN and adds information to the HEATING input data telling it to read the initial temperature distribution from unit KTPIN. If it is necessary to save the final temperature distribution from this thermal analysis for the next part of the prescribed analytical sequence, HTAS1 adds the appropriate information to the HEATING input data telling it to save the final temperature distribution on logical unit KTPOUT. Then HTAS1 writes the HEATING input data on a formatted data set and returns to SCALE telling it to call HEATING to perform the desired analysis. After HEATING completes the calculations, it returns to SCALE which then reenters HTAS1. On each subsequent entrance HTAS1 checks the data to determine if the final calculation in the specified analytical sequence has been performed. If so, it performs any wrap-up procedures to include the generation of the data set to be used in restarts of the analytical sequence. HTAS1 will write the final temperature distribution from HEATING on logical unit KTPIN. Then, HTAS1 returns to SCALE telling it to terminate calculations.

If additional calculations remain in the specified analytical sequence, HTAS1 first checks the data set returned by HEATING to determine if the calculations were successfully completed. If they were not, HTAS1 goes through the wrap-up procedures as described above. Otherwise, HTAS1 continues the calculations by modifying the HEATING input data set to properly define the next thermal analysis to be performed by

HEATING. This modification may involve changing some of the boundary conditions (for instance from fire to postfire conditions), changing the HEATING thermal analysis from steady state to transient or vice versa, or deleting some of the zones (for instance, the neutron shield and water jacket or impact limiters). If any of the zones are deleted, HTAS1 must delete the appropriate regions from the HEATING input data. In addition, it must apply new boundary conditions for the regions containing the newly exposed outer surfaces. If the neutron shield has been deleted from the model or has been changed to air, but the water jacket remains, HTAS1 will generate input data for the OCULAR module which will be used to generate additional input to HEATING. This additional input consists of node-to-node connectors representing 2-D radiative heat transfer within the vacated water jacket region. HTAS1 will direct the SCALE driver to call OCULAR immediately before calling HEATING for each of the remaining calculations in the analytical sequence. The user has the option of foregoing this radiation model, in which case HTAS1 would not generate OCULAR input or direct SCALE to call OCULAR, and no radiation heat transfer would be modeled within the annular region between the water jacket and outer shell.

A new set of grid lines must be added to the HEATING input data whenever a zone is deleted. Since HEATING will generate a new set of nodes when a zone is deleted, the final temperature distribution from the previous calculation cannot be used to start the newly defined thermal analysis. Instead HTAS1 must determine the new nodal configuration and map the final temperature distribution from the old model into the initial temperature distribution for the new model. This new initial temperature distribution is written on unit KTPIN.

Finally, HTAS1 updates the Title card as indicated above, adds the data telling HEATING to read the initial temperature distribution from unit KTPIN, updates the flag indicating whether to save the final temperature distribution, updates the parameters indicating the type of thermal analysis to be performed, and adds the appropriate data to define the numerical technique to be used. HTAS1 then writes the input data set for OCULAR (possibly) and HEATING and returns to SCALE telling it to call OCULAR (possibly) and HEATING to perform the calculations. After each HEATING execution HTAS1 directs SCALE to call H7MAPRZ to provide temperature maps of each analysis.

H1.3.2 DESCRIPTION OF LOGICAL UNITS UTILIZED BY HTAS1

The logical units used during an execution of HTAS1 are identified in Table H1.3.1. Data are transmitted between HTAS1, OCULAR, and HEATING using the files created on the logical units identified by KTPIN, KTPOUT, ICONT, IBOUT, and IBIN. If HTAS1 is restarted, the initial temperature distribution must be supplied by the user on the logical unit identified by ITPIN. HTAS1 will save the final temperature distribution on the logical unit identified by KTPIN. If the user references any materials in the Lawrence Livermore National Laboratory material property library (Ref. 2), HEATING will select their values from the library on the logical unit identified by IMATLB.

H1.3.3 RESTARTING HTAS1

HEATING has provisions for restarting a thermal analysis when an earlier calculation was terminated prematurely. HEATING will generate a data set containing the final temperature distribution calculated for steady-state problems and the temperature distribution at the last time level that had satisfied the convergence criteria for transient problems. This temperature distribution may then be used to restart the HEATING calculations at a later date. This feature is used in the option for restarting a HTAS1 analytical sequence. After the final HEATING calculation has been completed, HTAS1 will write the final HEATING temperature distribution on an unformatted data set on the unit KTPIN. Later, the user may restart the analytical sequence by identifying the unit number from which the unformatted temperature distribution will be read. The HTAS1 input data deck must also be modified. Any analytical sequence data blocks that have been successfully completed must be removed. Any zones that were modified during the previous HTAS1 run must

Table H1.3.1 Description of logical units utilized by HTAS1

Unit name	Unit No.	Type of Data	Creating module	User module
KTPIN	1	Binary scratch file with HEATING initial temperatures for next analysis	HTAS1	HEATING
KTPOUT	2	Binary scratch file with HEATING final temperatures from last analysis	HEATING	HTAS1
IN	4	Formatted scratch file with HTAS1 input data	HTAS1	DRIVER
IECHO	5	Standard HTAS1 input data, formatted	User	HTAS1
IO	6	Standard output (default, printer)	HTAS1 HEATING	User
IUF	18	Binary plot scratch file for fire transient data	HTAS1	HTAS1
IUPF	19	Binary plot scratch file for postfire transient data	HTAS1	HTAS1
IMATLB	78	Material property library (default, LLNL, formatted)	HEATING	
ICONT	91	Binary scratch file	HTAS1	HTAS1
IBIN	95	HEATING binary input data	HTAS1	DRIVER
IBOUT	94	OCULAR binary output of connectors	OCULAR	HEATING
ITPIN	Input	Initial temperatures for restart of HTAS1 (binary)	User	HTAS1

be modified in a similar manner in the input data for the restart run. Since HTAS1 does not allow radiativeheat transfer across the neutron shield for the initial model in an analytical sequence, HTAS1 should not be restarted after the neutron shield has been deleted or changed to air. The nodal configuration for the restart model must be identical to the nodal configuration corresponding to the final temperature distribution to be used in the restart run. The logical unit numbers ITPIN and ITPOUT may not be equal to 1, 2, 4, 5, 6, 18, 19 nor greater than 75. In addition, the appropriate data or file definition parameters must be supplied to describe the unformatted data sets or files on units ITPIN and ITPOUT.

H1.3.4 DESCRIPTION OF SUBROUTINES IN HTAS1

MAIN - Allocates buffer space for the necessary input and output units prior to the call to ALOCAT (see Sect. M2.2.1). Enters calculational portion of control module HTAS1 by instructing ALOCAT to call HTAS1A. Upon completion of each set of HTAS1 calculations, MAIN sets up the return to the SCALE driver instructing it to either call HEATING (alias HTNG72) only, OCULAR and HEATING, or to terminate the calculations. Called from HTAS1. Calls HTAS1A and H1PALC. Calls SCALE routine ALOCAT.

BLOCK DATA - Initializes data in labeled common blocks ARYLN1, ARYLNG, FLGTYP, TSTOUT, IOUNIT, MAPFMT, DIVIDR, and WIDTH. Labeled common ARYLN1 contains default dimensions for some of the HTAS1 variably dimensioned arrays. Labeled commons ARYLNG, FLGTYP, TSTOUT, IOUNIT, MAPFMT, and WIDTH are from HEATING. Although some of these variables are used in HTAS1, they are mainly used to generate the OPTION data block for input to HEATING. Values for the variables in these common blocks are initialized in this block data. Values for some of these variables are later computed by HTAS1 based on the model being generated.

CDRD - Reads a double-precision real number from a character variable and converts it to single precision. Called from RGINP.

DOUBLE - Copies the double word stored in the second argument into two consecutive elements of the single word character array identified by the first argument. Called from HIP, OUT123, OUTGRD, OUTITP, OUTPRT, OUTSS, OUTTAB, OUT17, WBC, WMAT and WREG.

ECHO - Reads input data card images from unit IECHO, lists input data card images on unit 10, puts 'END' after each data string, and writes the resulting input data card images on unit IN. Assumes card image with '@' in column 1 is a continuation of the previous card image. Replaces '@' in column 1 with a ' '. Assumes card image with '*' in column 1 is a comment card. Called from H6TAS1.

FGRID - Generates fine grid lines along the appropriate axis based on gross grid RG(IGT0) through RG(IGT1) and the spacings between the respective gross grid lines as stored in the NRG array. Stores generated fine grid lines in the array R and the total number generated in IT. Called from NODMAP.

FILL - Stores the character string 'END ' in the D-array immediately after the data string which extends through D(ID+NREC). Called from HIP, OUT123, OUTBC, OUTEOD, OUTGRD, OUTM, OUTMAT, OUTPRT, OUTREG, OUTSS, OUTTAB, OUTTT, WBC, WMAT, and WREG.

FINDLN - Checks the axial boundaries of the neutron shield, water jacket, and impact limiters. Generates a warning message and moves the respective axial boundary to the nearest axial fine grid line if one of these boundaries does not match a fine grid line generated by HTAS1 for the cavity, inner-shell shielding, or outer shell. Called from GENREG.

GENBC - Generates parameters for the HEATING B2 input data card. In particular, generates the coefficient for radiative heat transfer to include that for surface-to-surface heat transfer across the neutron shield, when appropriate, and the coefficient and exponent for the term simulating the effects of natural convective heat transfer. Generates the terms for each zone and for each calculational phase of the analytical sequence. Called from H6TAS1.

GENDAT- Scans the input data of each zone for obvious errors. In particular, determines if required zones are present, if zones appear in proper combinations, if dimensions of each zone satisfy all constraints, if grid spacing information is defined for each zone, if fin types are properly defined, and if the removal of a zone during calculations is properly defined. When an error is encountered, writes error message, continues to scan remaining input data, if possible, and sets flag to terminate calculations when error scanning is completed. Called from READER.

GENDEL - Determines the gross grid lines bounding the model during each calculational phase of the analytical sequence when the impact limiters or neutron shield and water jacket are deleted following a calculational phase. Called from H6TAS1.

GENREG - Examines each zone and determines the radial and axial gross grid lines and the number of divisions separating consecutive gross grid lines. These data will be used later to generate the HEATING XGRID and ZGRID data blocks. For cases where the radius of the impact limiters is not the outer radius of the model, also matches the radius of the impact limiters with radial fine grid lines generated by HTAS1 for the outer-shell neutron shield, or water jacket. If a match is not found, issues a warning message and moves the radius of the impact limiter to the nearest radial fine grid line. Checks model structure and, if any inconsistencies are located, issues a warning message and attempts to continue. Determines the maximum number of axial and radial gross grid lines, the maximum number of axial and radial fine grid lines, the maximum number of points, and the maximum bandwidth for steady-state models using the direct-solution technique. Called from H6TAS1. Calls FINDLN.

H6TAS1 - Controls flow of the calculations in the HTAS1 control module. Initializes certain parameters for the calculations, calculates starting indices for the variably dimensioned arrays, calculates the starting point for the storage of the HEATING input data in the D-array, calculates the storage requirements for these arrays, notifies the user if the amount of core requested can be reduced or writes an error message and terminates the calculations if not enough core was requested. If errors are detected in the input data or if the calculations cannot be continued, arranges

for HTAS1 control module to tell the SCALE driver to terminate the calculations. On the initial entrance into HTAS1 control module, writes the generated HEATING input data on binary files on unit IBIN. On subsequent entrances, reads HEATING input data for the previous calculation in the analytical sequence, arranges for HIP to modify it for the next calculation, and writes the modified HEATING input data on unit IBIN. Called from HTAS1A. Calls ECHO, GENBC, GENDEL, GENREG, HIP, INITIL, INPUT, MATLIB, NODMAP, OUTDAT, READER, REGPLT, RGPINP, TABDAT and WTITLE. Calls SCALE routines IONUMS, RCRDLN and SCANON (see Sect. M2.2.61).

HIP - Modifies the HEATING input data generated by other routines in the HTAS1 control module. Adds tag to title to indicate type of calculation being performed, passes remaining CPU time to HEATING, arranges for HEATING to save final temperature distribution from a calculation and to read it as the initial temperature distribution in the next calculation of the analytical sequence and adds the proper data block defining the numerical technique to be used by HEATING for the next set of calculations. For models that involve the removal of zones during the calculations, maps the final temperature distribution from the old model into the initial temperature distribution for the new model, modifies the REGION, BOUNDARY CONDITION, XGRID, and ZGRID data blocks. Arranges for HEATING to read the initial temperature distribution for models being restarted. Saves the final temperature distribution in the analytical sequence when requested. Passes data from one entrance into the HTAS1 control module to the next through unit ICONT. Called from H6TAS1. Calls DOUBLE, FILL OUTEOD, OUTGRD, OUTSS, and OUTTT.

HTAS1 - Serves as normal entrance into HTAS1 control module when the SCALE driver encounters #HTAS1 in the input data stream. Stores data passed through the arguments from the SCALE driver into labeled common /CMDATA/ maining the data available to any routine in the HTAS1 control module. Calls MAIN. On return from MAIN, data in labeled common /CMDATA/ are stored back in the dummy arguments, allowing it to be passed back to the SCALE driver. This capability allows data generated on an entrance to the HTAS1 control module to be available on the next entrance to HTAS1. Called from the SCALE driver. Calls MAIN routine in the HTAS1 control module.

HTAS1A - Serves as an interface between the main routine in the HTAS1 control module and its working routines. Closes appropriate units and calls H6TAS1. Called from MAIN. Calls H6TAS1.

INITIL - Initializes variables for the first entrance into the HTAS1 control module. Called from H6TAS1.

INPUT - Reads the TITLE card and card 2 of the HTAS1 input data. Called from H6TAS1. Calls NEXTCD. Calls SCALE routines AREAD and IREAD.

MATLIB - Contains the HTAS1 material property library. Examines the material for each zone. If the material is in HTAS1 material property library, locates that material along with its thermal conductivity, density, and specific heat. If latent heat option is selected for a zone, uses the default latent heat parameters for the material unless input data overrides the defaults. Uses zone 8 for new material in neutron

shield when it is lost during the calculations. Uses default emissivities for each zone and each calculational phase unless the default are overridden. Determines maximum number of tabular functions and maximum number of pairs per tabular function for HEATING. Called from H6TAS1.

NEXTCD- Reads first word of next card image. Writes informative message if end-of-file or end-of-data is encountered. Writes out entire card image if it is a comment and looks at next card image. Otherwise, resets flags so that next read is from first word of this card image. Return 1 implies end-of-data was encountered. Return 2 implies end-of-data for this case was encountered. Called from INPUT, READER, and RPROP. Calls SCALE free-form reading routine AREAD (see Sect. M2.2.3).

NODMAP - Generates the mapping to transform the final temperature distribution for a calculation into the initial temperature distribution for the next calculation of an analytical sequence involving two or more calculations. Determine the nodal configuration for the initial model, determines the next calculational phase, deletes any regions involving zones that may have been deleted at the end of the previous calculational phase, determines the nodal configuration for the new model, and calculates the array NODE1, where NODE1(N2,IP) is the node number in the old model (calculational phase IP-1) that maps into node N2 in the new model (calculational phase IP). Called from H6TAS1. Calls FGRID, POINTS and REGFGL.

OUT123 - Stores the TITLE card and the parameter card for the HEATING input data in the D-array. Called from OUTDAT. Calls DOUBLE and FILL.

OUTBC - Stores the boundary condition keyword for the HEATING input data in the D-array. Prepares the HEATING boundary condition parameters for output for each boundary condition associated with each zone in the model, converts data to appropriate HEATING units. Called from OUTDAT. Calls FILL and WBC.

OUTDAT - Controls the order of calculations for storing the HEATING input data in the D-array. Called from H6TAS1. Calls OUT123, OUTBC, OUTEOD, OUTGRD, OUTITP, OUTMAT, OUTNL, OUTPRT, OUTREG, OUTSS, OUTTAB, and OUTTT.

OUTEOD - Stores the end-of-data (EOD) mark ('% ') for the HEATING input data in the D-array. Called from HIP and OUTDAT. Calls FILL.

OUTGRD - Stores the XGRID and ZGRID data blocks for the HEATING input data in the D-array. Called from HIP and OUTDAT. Calls DOUBLE and FILL.

OUTITP - Stores the initial temperature data block for the HEATING input data in the D-array. Called from OUTDAT. Calls DOUBLE and FILL.

OUTMAT - Stores the materials data block keyword for the HEATING input data in the D-array. Prepares the HEATING input data material parameters for output for each material in the model. Calculates the maximum number of materials for HEATING. Called from OUTDAT. Calls FILL and WMAT.

OUTNL - Generates OPTION data block for the HEATING input data when IDAT is greater than zero. Called from OUTDAT.

OUTOCL - Generates OCULAR input that is added to the HEATING input data. This procedure is only done if the neutron shield is replaced or deleted at some point in the analysis sequence, but the water jacket remains in place.

OUTPRT - Stores the PRINTOUT TIMES data block for the HEATING input data in the D-array. Called from OUTDAT. Calls DOUBLE and FILL.

OUTREG - Stores the REGION data block keyword for the HEATING input data in the D-array. Prepares the HEATING input data region parameters for output for each region associated with each zone in the model. Called from OUTDAT. Calls FILL and WREG.

OUTSS - Stores the steady-state parameters data block for the HEATING input data in the D-array. Called from HIP and OUTDAT. Calls DOUBLE and FILL.

OUTTAB - Stores the TABULAR FUNCTION data block for the HEATING input data in the D-array. Called from OUTDAT. Calls DOUBLE and FILL.

OUTTT - Stores the TRANSIENT PARAMETERS data block for the HEATING input data in the D-array. Called from HIP and OUTDAT. Calls DOUBLE and FILL.

POINTS - Generates arrays NTPI, NTPJ, and NTPK defining the fine grid lines passing through each node, determines the number of nodes for the current model Called from NODMAP.

READER - Reads the HTAS1 input data (except for the TITLE card and card 2) using SCALE's free-form reading routines (see Sect. M3) locates each keyword and either reads the appropriate data from the specified data block or arranges for other routines to read it. Called from H6TAS1. Calls GENDAT, NEXTCD, RMAT, RPROP, and RREAD. Calls SCALE routines AREAD, DREAD, and IREAD.

REGFGL - Determines the fine grid lines that bound each region in a model. Called from NODMAP.

RMAT - Reads the material index for a zone. Called from READER. Calls SCALE routines AREAD and IREAD.

RPROP - Reads the thermal parameter defined by IPROP for the material in the zone defined by IBLOCK. IPROP = 1, 2 or 3 for the thermal conductivity, density, or specific heat, respectively; property may be constant or temperature-dependent. Counts the number of tables defined and checks the number of table entries against the maximum of MXPRS. Called from READER. Calls NEXTCD. Calls SCALE routine DREAD.

RREAD - Reads the appropriate data for each zone in the model from the ZONE data card. Called from READER. Calls SCALE routines AREAD, DREAD, and IREAD (see Sect. M2).

TABDAT - Tabulates or arranges for other routines to tabulate data read or generated by HTAS1. Tabulates data for each zone in the model and for each calculation in the analytical sequence. Generates the printout times for the transient calculations provided they were not supplied by the user. Tabulates the printout times for the transient calculations. Called from H6TAS1. Calls TABDEL and TABMAT.

TABDEL - Generates the message that appears with the tabulation of the HTAS1 data as written by TABDAT to indicate the zones that will be deleted from the model following a particular calculation. Called from TABDAT. Calls TABMAT.

TABMAT - Tabulates the material properties for zone number IZONE which appear with the tabulation of HTAS1 data as written by TABDAT. Called from TABDAT and TABDEL.

WBC - Stores boundary condition data for boundary condition number NBC for the HEATING input data in the D-array. Counts the number of boundary conditions for HEATING. Called from OUTBC. Calls DOUBLE and FILL.

WMAT - Stores material data for material number MZONE(IZONE) for the HEATING input data in the D-array. Counts the number of materials for HEATING and converts data to appropriate units for HEATING. Handles both standard HEATING material cards and material cards referencing the LLNL material property library. Adds conversion factors to material card referencing the LLNL material property library. Called from OUTMAT. Calls DOUBLE and FILL.

WREG - Stores region data for region number NREG for the HEATING input data in the D-array. Counts the number of regions for HEATING. Called from OUTREG. Calls DOUBLE and FILL.

WTITLE - Generates the descriptive heading for the HTAS1 output. Heading contains the code name and version date, the date and time the job was executed, the computer on which the job was executed and the jobname under which the job was executed. Includes the title for the job and the author of the code. Date of the current version of the code appears in the data initialization statement for V(2). Called from H6TAS1.

BCDRAW - Draws the boundary condition symbols when the plot of the model boundary condition function numbers is generated. Called from REGPLT.

H1PALC - Determines the dimension of the master array that contains all variably dimensioned arrays in the HTAS1 temperature plotting subroutines. Called from MAIN. Calls H1PINT.

H1PINT - Calculates starting locations for the variably dimensioned arrays. Writes messages describing which temperature plot will be generated. Called from H1PALC. Calls H1PLOT.

H1PLOT - Generates curves of temperature vs time for the centermost nodes of the inner shell, the shielding, and the outer shell if the curves are drawn on the same plot. Generates the curve of maximum temperature at any problem time vs the radial distance from the origin for all nodes on the axial center line. Called from

H1PINT. Calls MINMAX, NODNUM, ROUND, SEPRAT, SETUP, and VOLAVG.

MINMAX - Determines the minimum and maximum values of the array received in the argument list. Called from H1PLOT, SEPRAT, and VOLAVG.

NODNUM - Determines the node number of the node that is nearest the center of either the inner shell, the shielding, or the outer shell. Called from H1PLOT.

REGPLT - Generates plots of the regions, materials, heat generation function numbers, initial temperature function numbers, and boundary conditions of the model. Called from H6TAS1. Calls BCDRAW.

RGPINP - Stores data in common blocks that are used to generate REGPLOT6-type plots for the current phase of the calculation. Called from H6TAS1.

ROUND - Determines rounded axis numbers based on the minimum and maximum values to be plotted in a certain direction. Called from H1PLOT, SEPRAT, and VOLAVG.

SEPRAT - Generates plots of temperature vs time for the centermost nodes of the inner shell, the shielding, and the outer shell if the curves are drawn on individual plots. Called from H1PLOT. Calls MINMAX, ROUND, and SETUP.

SETUP - Draws the axes and writes the heading for each plot. Called from H1PLOT, SEPRAT, and VOLAVG.

VOLAVG - Generates the plot of a curve showing the difference in volume-averaged temperature between the inner shell and the outer shell vs time. Called from H1PLOT. Calls MINMAX, ROUND, and SETUP.

H1.4 INPUT DATA DESCRIPTION FOR HTAS1

H1.4.1 INTRODUCTION

A detailed discussion of the input data cards is presented to instruct the user in the selection of the various options of the HTAS1 code. The units for each entry are given in the discussion for each data card.

Since the input data for HEATING must be in consistent units, HTAS1 must convert the units for some of the parameters before generating the HEATING input data. The units for the input data for HTAS1, as well as the input data for HEATING generated by HTAS1, are presented in Table H1.4.1.

Table H1.4.1 Units for input data to HTAS1 and HEATING

Parameter	HTAS1 units	HEATING units
Density	$\frac{lb}{ft^3}$	$\frac{lb}{in.^3}$
Emissivity	unitless	unitless
Heat flux	Btu/(hr-ft^2)	Btu/(min-in.^{2})
Heat load	Btu/hr	Btu/min
Latent heat	Btu/lb	Btu/lb
Length	in.	in.
Natural convective heat transfer coefficient	Btu/(hr-ft^2-°F)	Btu/(min-in.^{2}-°F)
Specific heat	Btu/(lb-°F)	Btu/(lb-°F)
Temperature	°F	°F
Thermal conductivity	Btu/(hr-ft-°F)	Btu/(min-in.°F)
Time	min	min
Time step	min	min

The input data for HTAS1 are read using the SCALE free-form reading routines (see Sect. M3) which allow data to be entered in an unformatted manner. With a few exceptions noted below, the data items can begin or end anywhere in columns 1 through 80. If data that are to appear on a card will not fit on one card, they may be entered on the succeeding card denoted as a continuation card. An '@' must appear in column 1 of each continuation card. Otherwise, the code will read the remaining data for that card image as either blank or zero. There is no limit to the number of continuation cards. However, a continuation card may not

immediately follow a title card, an end-of-data card, or a comment card. A single data entry cannot be started on one card and extended onto the next card.

The following discussion concerning the free-form input data was taken from Sect. M3 after some minor revisions. Any alphanumeric data entry such as a keyword must be terminated by two or more blanks. Such an entry cannot be delimited by a comma. Any numeric data entry will be terminated when a blank or a comma is encountered. The use of a D or an E as an exponent does allow a single imbedded blank after the D or E. An exponent is limited to two digits, and the number being read is terminated with the second digit. For this case only, therefore, another number can be started immediately following the second digit of the exponent without an intervening blank or comma. Decimal data may be entered as in FORTRAN input, for example, 1.733-4, 1.733-04, or .0001733 are the same as 1.733×10^{-4}; 1.733+4, 1.733E+4, 1.733E4, and 17330.0 are the same as $1.733 \times 10^{+4}$. Integers may be entered for floating-point data (i.e., 10 will be interpreted as 10.0). Similarly, floating-point data may be entered for integers. Thus, 1.733E+4 would be interpreted as 17330, and 1.733E-4 would be interpreted as zero.

The free-form routines have provisions for multiple entries of the same data value. This step is done by entering the number of repeats, followed by an R, *, or $, followed by the data value to be repeated. For example, 5R2, 5*2, or 5$2 enters five successive 2's in the input data. Blanks are not allowed between the number of repeats and the repeat flag (R,*,$). However, a blank is allowed between the repeat flag and the data item to be repeated. Multiple zeros may be specified by entering nZ where n is the number of zeros to be repeated. No blanks should be present between the n and the Z, but the nZ must be separated from the rest of the data by one or more blanks.

All numeric data are read in double precision and are then converted to the desired form. Exponent indicators can be either a D or an E. The default method of terminating a data field is one or more blanks or a comma. A comma must immediately follow the number if it is used as a terminator (i.e., 5.6, should be used to enter the number 5.6 as data; 5.6 , results in two numbers 5.6 and 0). Thus commas can be used to enter zeros. 5.6,,,,, 8.0 enters 6 numbers as data – 5.6, four zeros, and 8.0 (the comma immediately after the 5.6 terminates that number and does not cause an entry of zero into the data). Similarly, both 5.6 ,,,,, 8.0 and 5.6 , , , , , 8.0 enter seven numbers as data – 5.6, five zeros and 8.0.

A data set for a case consists of a title card, a parameter card, and the data blocks necessary to define the problem being modeled. The user may wish to add comment cards to the input data to assist in documenting the model. Any number of comment cards may appear anywhere in the input data set following the title card, except a comment card may not precede a continuation card. The comment cards are identified by an asterisk (*) in column 1. These comments will be written on the standard output unit as they are encountered.

Seven different data blocks, denoted as zone data blocks, may be used to describe the zones to be modeled by HTAS1 (see Table H1.2.1.). A MATERIAL data block, an EMISSIVITY card, a LATENT HEAT card, and/or a DELETE card may appear in a zone data block to override default values assigned to the zone. The zone data blocks may appear in any order following the parameter card. Every data deck must have a CAVITY, an INNER SHELL, and an OUTER SHELL data block. Also, NEUTRON SHIELD and WATER JACKET data blocks must appear in pairs. Five different data blocks may be used to describe the different calculations that may be performed on a model (see Table H1.4.2.). These are denoted as Analytical Sequence data blocks, and they may appear in any order in any acceptable combination following the zone data blocks. A PRINTOUT TIMES data block may be entered to define the times at which the transient temperature distribution is to be printed by HEATING. A PLOT data card may be entered to generate temperature profile plots. A REGP data block may be entered to generate region plots. Each keyword associated with a data block must consist of at least the first four characters of the respective character string. *Each keyword must be terminated by two or more blanks.*

The final data card in a data set for a case is an end-of-data (EOD) card and must contain a percent (%) in column 1 and a blank in column 2. This card signifies the end of data for a problem. As HTAS1 reads the input data, it sets a flag when an error is encountered and continues to read additional data unless the effort was fatal. When the end-of-data indicator (%) is encountered, HTAS1 terminates reading and

Table H1.4.2 Keywords for analytical sequences for HTAS1 model

INITIAL -	initial steady state
PREFIRE -	steady state immediately before fire
FIRE -	fire transient
POSTFIRE -	transient immediately following fire
FINAL -	final steady state

commences processing the input data. After processing is completed, the code performs the specified calculations unless an error was encountered, in which case it terminates the calculations.

H1.4.2 CARD 1 – TITLE OF PROBLEM

This card, which can contain alphanumeric characters in the first 56 columns, contains a descriptive title for the problem and must be the first card in the data set for each case. The card itself cannot be omitted although it may be left blank. This title serves to identify the output for a case executed on HTAS1 since it appears with a number of tables and messages generated by the code. It is also used as part of the title for each thermal analysis performed by HEATING. The appropriate entry from the following list is added to columns 57–72 of the HTAS1 title to generate the title for each thermal analysis being performed by HEATING.

- INITIAL SS
- PREFIRE SS
- FIRE TR
- POSTFIRE TR
- FINAL SS

H1.4.3 CARD 2 - PROBLEM CONTROL PARAMETERS

H1.4.3.1 Maximum CPU Seconds Allowed (I)

The first entry, MXCPU, specifies the maximum CPU seconds allowed for each HEATING execution. Default value is 500 seconds.

H1.4.3.2 Initial Temperature Input Option (I)

The second entry, ITPIN, on this card specifies whether explicitly specified, lattice-point initial temperatures will be read by HTAS1 from an existing data set or file. If ITPIN is nonzero, HTAS1 will read the initial temperatures in unformatted form from logical unit number ITPIN. If there are no initial

temperatures explicitly specified for HEATING, this entry must be zero. The user must ensure that the appropriate data or file definition parameters have been supplied to describe the data set or file.

This entry must be nonzero for HTAS1 runs that begin with either the fire transient or the postfire transient. If it is zero for one of these cases, HTAS1 will generate an error message. It must also be nonzero for HTAS1 runs that restart a HEATING calculation. This entry is usually zero or blank for HTAS1 calculations that begin by performing the STEADY STATE, PREFIRE, or FINAL steady-state calculations.

H1.4.4 TRANSIENT OUTPUT

H1.4.4.1 Printout Times Data Block

This data block is used to define the times (minutes) at which the transient temperature distribution is to be printed in map form by HEATING. It is used by HTAS1 to generate the PRINTOUT TIMES data block for HEATING. The card consists of the keyword PRINTOUT TIMES. The desired output times then appear in ascending order following the keyword. The output times must be separated from the keyword by at least two blanks. Each entry is a floating-point number. The maximum number of times is MXPRT (currently equal to 50) not counting the automatic printout of the initial temperature distribution. If the PRINTOUT TIMES data block is omitted for a HTAS1 run involving the FIRE or POSTFIRE transient, HTAS1 will generate a PRINTOUT TIMES data block for HEATING with equally spaced times that are multiples of 5 time units. The generated printout times will include the end-of-fire transient and the end-of-postfire transient times if either is defined. If the total number of printout times exceeds MXPRT, either generated or input, HTAS1 will write an error message. This data block is not used for problems involving steady-state-only calculations.

H1.4.5 ZONE DATA BLOCKS

The zones that may be used in HTAS1 to model a radioactive material transport package are depicted in Fig. H1.2.1. Each zone is composed of a homogeneous, right, circular cylinder. Each cylinder may be solid such as the impact limiter or hollow such as the water jacket or it may have a cavity at the center such as the inner shell. The cylinders are all concentric.

Each zone to be included in the model is defined to HTAS1 by entering a zone data card consisting of a zone keyword and physical attributes unique to the zone. The zone keyword must consist of at least the first four characters of the string, as shown in Fig. H1.2.1 and Table H1.2.1, and must be followed by at least two blanks. Data unique to each zone data card are then entered to define the physical dimensions and grid spacing for the zone. Each model must have a CAVITY, an INNER SHELL and an OUTER SHELL. A description of these data appears below for each zone.

H1.4.5.1 Cavity Zone

Keyword - CAVITY

RCAVTY - Radius of the cavity in inches. The entry must be a positive, floating-point number.

NRCAVT - Number of equal increments in the radial direction from the origin to the cavity surface. The entry must be a positive integer.

TCAVTY - Axial distance from the axial midplane of the cavity to its top in inches. The entry must be a positive, floating-point number.

NTCAVT - Number of equal increments in the axial direction from the axial midplane of the cavity to its top. The entry must be a positive integer.

HEAT - Total heat load within the cavity in Btu/hr. The entry must be a positive, floating-point number.

H1.4.5.2 Inner Shell Zone

Keyword - INNER SHELL

RINNER - Radial thickness of the inner shell in inches. The entry must be a positive, floating-point number.

NRINNE - Number of equal increments across the radial thickness of the inner shell. The entry must be a positive integer.

TINNER - Axial thickness of the top of the inner shell in inches. The entry must be a positive, floating-point number.

NTINNE - Number of equal increments across the axial thickness of the top of the inner shell. The entry must be a positive integer.

BINNER - Axial thickness of the bottom of the inner shell in inches. The entry must be a nonnegative, floating-point number. If the entry is zero or blank, then BINNER is set equal to TINNER.

NBINNE - Number of equal increments across the axial thickness of the bottom of the inner shell. The entry must be a nonnegative integer. If the entry is zero or blank, NBINNE is set equal to NTINNE.

H1.4.5.3 Shielding Zone

Keyword - SHIELDING

RSHELD - Radial thickness of the shielding in inches. The entry must be a positive, floating-point number.

NRSHEL - Number of equal increments across the radial thickness of the shielding. The entry must be a positive integer.

TSHELD - Axial thickness of the top of the shielding in inches. The entry must be a nonnegative, floating-point number. If the entry is zero or blank, the distance from the axial center line of the cavity to the top of the shielding will be the same as the distance from the axial center line of the cavity to the top of the inner shell. In other words, the shielding will not extend across the top of the inner shell.

NTSHEL - Number of equal increments across the axial thickness of the top of the shielding. The entry must be a positive integer if TSHELD is greater than zero. The entry is not used if TSHELD is equal to zero.

BSHELD - Axial thickness of the bottom of the shielding in inches. The entry must be a floating-point number. If the entry is zero or blank, then BSHELD is set equal to TSHELD. If the entry is negative, then BSHELD is set equal to zero. If the final value of BSHELD is zero, the distance from the axial center line of the cavity to the bottom of the shielding will be the same as the distance from the axial center line of the cavity to the bottom of the inner shell. In other words, the shielding will not extend across the bottom of the inner shell.

NBSHEL - Number of equal increments across the axial thickness of the bottom of the shielding. The entry must be a nonnegative integer. If the entry is zero or blank, then NBSHEL is set equal to NTSHEL. The entry is not used if the final value of BSHELD is zero.

H1.4.5.4 Outer Shell Zone

Keyword - OUTER SHELL

ROUTER - Radial thickness of the outer shell in inches. The entry must be a positive, floating-point number.

NROUTE - Number of equal increments across the radial thickness of the outer shell. The entry must be a positive integer.

TOUTER - Axial thickness of the top of the outer shell in inches. The entry must be a positive, floating-point number.

NTOUTE - Number of equal increments across the axial thickness of the top of the inner shell. The entry must be a positive integer.

BOUTER - Axial thickness of the bottom of the outer shell in inches. The entry must be a nonnegative, floating-point number. If the entry is zero or blank, BOUTER is set equal to TOUTER.

NBOUTE - Number of equal increments across the axial thickness of the bottom of the outer shell. The entry must be a nonnegative integer. If the entry is zero or blank, NBOUTE is set equal to NTOUTE.

H1.4.5.5 Neutron Shield Zone

Keyword - NEUTRON SHIELD

RNUTRN - Radial thickness of the neutron shield in inches. The entry must be a positive, floating-point number.

NRNUTR - Number of equal increments across the radial thickness of the neutron shield. The entry must be a positive integer.

TNUTRN - Axial distance from the axial midplane of the cavity to the top of the neutron shield in inches. The entry must be a floating number. When the entry is negative, HTAS1 sets the value of TNUTRN to zero and the neutron shield does not extend above the axial midplane of the cavity. When the entry is zero or blank, HTAS1 sets TNUTRN to the distance from the axial midplane of the cavity to the top of the cavity (or TCAVTY).

The neutron shield cannot extend axially beyond the top of the outer shell (i.e., TNUTRN < TCAVTY + TINNER + TSHELD + TOUTER).

BNUTRN - Axial distance from the axial midplane of the cavity to the bottom of the neutron shield in inches. The entry must be a floating-point number. When the entry is negative, HTAS1 sets the value of BNUTRN to zero and the neutron shield does not extend below the axial midplane of the cavity. When this entry is zero or blank and the previous entry, TNUTRN, is zero or blank HTAS1 sets BNUTRN to the distance from the axial midplane of the cavity to the bottom of the cavity (or TCAVTY). When this entry is zero or blank and the previous entry, TNUTRN, is positive, HTAS1 sets the value of BNUTRN to that of TNUTRN. The neutron shield cannot extend axially beyond the bottom of the outer shell.

H1.4.5.6 Water Jacket Zone

Keyword - WATER JACKET

RWATER - Radial thickness of the water jacket in inches. The entry must be a positive, floating-point number.

NRWATE - Number of equal increments across the radial thickness of the water jacket. The entry must be a positive integer.

TWATER - Axial distance from the axial midplane of the cavity to the top of the water jacket in inches. Currently not used. HTAS1 sets the value of TWATER to that of TNUTRN.

BWATER - Axial distance from the axial midplane of the cavity to the bottom of the water jacket in inches. Currently not used. HTAS1 sets the value of BWATER to that of BNUTRN.

H1.4.5.7 Impact Limiter Zone

Keyword - IMPACT LIMITER

RMPACT - Radius of both the top and bottom impact limiters in inches. The entry must be a nonnegative, floating-point number. RMPACT must be greater than or equal to the radius of the outer surface of the transport package as determined by ignoring the neutron shield and water jacket. If the entry is zero or blank, HTAS1 sets RMPACT to the outer radius of the outer shell (i.e., RMPACT = RCAVTY + RINNER + RSHELD + ROUTER).

NRMPAC - Number of equal increments in the radial direction along the portion of the impact limiters that extend radially beyond the outer surface of the model as determined by considering the neutron shield and water jacket, if present, but by ignoring the impact limiters. The entry must be a nonnegative integer. The entry must be zero or blank when the radius of the impact limiters does not exceed the radius of the model without the impact limiters.

TMPACT - Axial thickness of the top impact limiter measured from top of outer shell in inches. The entry must be a nonnegative, floating-point number. If the entry is zero or blank, the top impact limiter is omitted from the model.

NTMPAC - Number of equal increments across the axial thickness of the top impact limiter. The entry must be a nonnegative integer. The entry is ignored, and thus, it may be zero or blank when TMPACT is zero or blank.

BMPACT - Axial thickness of the bottom impact limiter measured from bottom of outer shell in inches. The entry must be a floating-point number. If the entry is zero or blank HTAS1 sets BMPACT equal to TMPACT. If the entry is negative, the bottom impact limiter is omitted from the model and BMPACT is set equal to zero.

NBMPAC - Number of equal increments across the axial thickness of the bottom impact limiter. The entry must be a nonnegative integer. If the entry is zero or blank, NBMPAC is set equal to NTMPAC. The entry is ignored, and thus, it may be zero or blank when the final value of BMPACT is zero.

TWRAP - Axial thickness of the portion of the top impact limiter that wraps around the portion of the outer shell above the axial midplane of the cavity in inches. TWRAP is measured from the top of the outer shell toward the cavity centerline and cannot overlap the neutron shield and water jacket. The entry must be a nonnegative, floating-point number. If the entry is zero or blank, the top impact limiter does not wrap around the sides of the transport package but is a disk that sits on top of it. The entry must be zero or blank when the radius of the impact limiters is the same as the radius of the outer surface of the transport package as determined by ignoring the neutron shield and water jacket.

BWRAP - Axial thickness of the portion of the bottom impact limiter that wraps around the portion of the outer shell below the axial midplane of the cavity in inches. BWRAP is measured from the bottom of the outer shell towards the axial midplane of the cavity and cannot overlap the neutron shield and water jacket. The entry must be a floating-point number. If the entry is zero or blank, HTAS1 sets BWRAP equal to TWRAP. If the entry is negative, HTAS1 sets BWRAP to zero. If the final value of BWRAP is zero, the bottom impact limiter does not wrap around the sides of the transport package but is a disk on which the package sits. The entry must be zero or blank when the radius of the impact limiters is the same as the radius of the outer surface of the transport package as determined by ignoring the neutron shield and water jacket.

H1.4.6. MATERIAL DATA BLOCK

Default values for the thermal conductivity, density, specific heat, emissivity, phase-change or transition temperature, and latent heat are associated with the material in each zone. A MATERIAL data block, EMISSIVITY card, or LATENT HEAT card may be entered immediately following a particular zone card to override any or all of the default values for the zone. The MATERIAL data block, EMISSIVITY card, and LATENT HEAT card may be entered in any combination or any order for each zone.

A default material from the HTAS1 material properties library is associated with each zone. The zones and default materials are identified in Table H1.2.1. A MATERIAL data block may be entered on a card or group of cards following the zone data card to override the default material within a particular zone with the exception of the CAVITY zone. A description of the MATERIAL data block follows:

H1.4.6.1 Material Card

Keyword - MATERIAL

MZONE - Material Index. The entry must be a nonnegative integer. If the entry is positive, it must be one of the material identification numbers from the HTAS1 material property library. See Table H1.2.2. If the integer is not positive, the material name, thermal conductivity, density, and specific heat must be supplied on additional cards as described below.

H1.4.6.2 Material Name Card

This card immediately follows the MATERIAL card when the material index on it is not positive.

ZONENM - Name of the material. This name, which cannot contain any embedded blanks, may consist of up to eight alphanumeric characters. The name must be terminated by two or more blanks. The thermal conductivity, density, and specific heat for the material are then entered on succeeding cards. Another option is to allow HEATING to extract the thermal properties for the material in this zone from the Lawrence Livermore National Laboratory (LLNL) material properties library (Ref. 2). If this option is desired, the first column of the Material Name card must be blank, and the material name must consist of an asterisk (*) in column 2 followed by the material identification number for the desired material from the LLNL material properties library. In this case the material name must consist of five characters and cannot contain any embedded blanks. Again the material name must be terminated by two or more blanks. The thermal conductivity, density, specific heat and phase change parameters are then extracted from the library by HEATING instead of being supplied by the user.

H1.4.6.3 Thermal Conductivity Card

The temperature-dependent thermal conductivity for the material named on the Material Name card is entered on this card. The thermal conductivity must be tabulated as a function of temperature with the temperatures in ascending order, and the data from the resulting table are entered in ordered pairs where the first member of each pair is the temperature and the second member is the thermal conductivity at that temperature. The temperature units must be in degrees Fahrenheit, and the thermal conductivity units must be Btu/(hr-ft-°F). There can be a maximum of MXPRS ordered pairs in the table. MXPRS is currently equal to 20. If the thermal conductivity is constant, its value may appear as the single entry on the thermal conductivity card. If there are only two entries on the card, the first entry must be the temperature and the second entry must be the thermal conductivity. HTAS1 will use the second entry as the constant thermal conductivity in generating the HEATING input data. Each entry is a floating-point number.

H1.4.6.4 Density Card

The temperature-dependent density for the material named on the Material Name card is entered on this card. The density must be tabulated as a function of temperature, with the temperatures in ascending order. Using the conventions presented above for the thermal conductivity, the data from the resulting table are entered in ordered pairs where the first member of each pair is the temperature and the second member is the density. The units for the density must be in (lb/ft^3). Each entry is a floating-point number. The user should note that care must be exhibited in using a temperature-dependent density since HEATING does not allow thermal expansion in its thermal analysis.

H1.4.6.5 Specific Heat Card

The temperature-dependent specific heat for the material named on the Material Name card is entered on this card. The specific heat must be tabulated as a function of temperature with the temperatures in ascending order. Using the conventions presented above for the thermal conductivity, the data from the resulting table are entered in ordered pairs, where the first member of each pair is the temperature and the second member is the specific heat. The units for the specific heat must be in (Btu/lb-°F). Each entry is a floating-point number.

H1.4.7 EMISSIVITY DATA

A set of default emissivities is associated with the surface of each zone for each calculational phase of the problem (INITIAL, PREFIRE, FIRE, POSTFIRE, or FINAL). If the emissivity for a zone is nonzero for a phase and if a surface of that zone is an outer surface of the model, then a radiative boundary condition is applied during that calculational phase. The default emissivities for each zone are shown in Table H1.2.3. One or more of the default values may be overridden by supplying an EMISSIVITY data card after the zone data card defining the particular zone. The EMISSIVITY data card must not be entered for the CAVITY, INNER SHELL, or SHIELDING zones. A description of the EMISSIVITY card follows:

Keyword - EMISSIVITY

EMISIV(1) - Emissivity for the normal operating condition INITIAL steady-state phase.

EMISIV(2) - Emissivity for the PREFIRE steady-state phase.

EMISIV(3) - Emissivity for the FIRE transient phase.

EMISIV(4) - Emissivity for the POST FIRE transient phase.

EMISIV(S) - Emissivity for the FINAL steady-state phase.

If an input emissivity is negative, then HTAS1 will not generate a radiative boundary condition for the outer surfaces of that zone during that particular calculational phase. If an input emissivity is zero, then HTAS1 will use the default value for the emissivity if it generates a radiative boundary condition for the outer surfaces of that zone during that particular phase of the calculations. If an input emissivity is positive, then HTAS1 will use the input value for the emissivity if it generates a radiative boundary condition for the outer surfaces of that zone during that particular phase of the calculations. The emissivities are all floating-point numbers and are unitless.

H1.4.8 CHANGE-OF-PHASE OPTION

A phase-change or transition temperature and latent heat are associated with the material for each zone of the model. If the latent heat is positive, then the material undergoes a change of phase during the transient calculations when its temperature reaches the phase-change or transition temperature. Under default conditions the latent heat is zero for each material in the model, and thus no material is allowed to undergo a change of phase. In this case, the transient calculations are performed using the implicit procedure. If the option is invoked to allow a material to change phase, the transient implicit technique can no longer be used. Instead HTAS1 generates input data telling HEATING to use Levy's modification to the explicit technique to perform the transient calculations. The default Levy time-step factor used by HTAS1 is 10.

The material in a zone is allowed to change phase by supplying a LATENT HEAT data card following the zone data card for the particular zone involved. The LATENT HEAT data card must not be entered for the CAVITY zone. A LATENT HEAT data card has the following format:

Keyword - LATENT HEAT

SLTM - Phase-change or transition temperature for the material associated with the zone. This entry is a floating-point number. The temperature must be in degrees Fahrenheit.

SLHM - Latent heat for the material associated with the zone. This entry is a floating-point number. The units for the latent heat must be in (Btu/lb).

If the input latent heat is negative, HTAS1 will not allow the material to change phase. This is equivalent to not entering a LATENT HEAT card for this zone. A phase-change or transition temperature and latent heat are associated with each material in the HTAS1 material property library. If the input latent heat is zero or blank for a zone whose material thermal properties are extracted from the HTAS1 material property library, then the phase-change or transition temperature and latent heat are also taken from the library. If the input latent heat is positive, HTAS1 will use the input values for the phase-change or transition temperature and latent heat. Some of the materials in the LLNL material properties library have a phase-change or transition temperature and latent heat defined. When the LATENT HEAT card is present for a zone whose material thermal properties are to be extracted from the LLNL material properties library, the phase-change or transition temperature and latent heat are also extracted from the library if the input value for the latent heat is nonnegative on the LATENT HEAT card.

The maximum number of zones that are allowed to undergo a change of phase is five.

H1.4.9 ANALYTICAL SEQUENCE DATA BLOCKS

HTAS1 is designed to prepare HEATING input data to perform five different thermal analyses on a model of a radioactive material transport package. Each thermal analysis is identified by a keyword:

INITIAL - to obtain the steady-state normal operating thermal conditions for the transport package for operating conditions as specified in Part 71 of Title 10, Chapter 1, Code of Federal Regulations-Energy, U.S. Nuclear Regulatory Commission,

PREFIRE - to obtain the steady-state thermal conditions for the transport package prior to the fire transient (the only difference in INITIAL and PREFIRE is that due to the specified accident conditions of 10CFR71.73, the PREFIRE has a zero solar heat load as default),

FIRE - to obtain the transient thermal conditions during a specified accident in which the transport package is subjected to a fire at a stated temperature for a stated period of time,

POSTFIRE - to obtain the transient thermal conditions of the transport package for a specified period of time following exposure to the fire, and

FINAL - to obtain the steady-state operating thermal conditions following the accident and exposure to the fire.

By using acceptable combinations of the above thermal analyses, 15 different analytical sequences may be performed:

1. all five thermal analyses may be performed in a sequence or INITIAL, PREFIRE, FIRE, POSTFIRE, and FINAL,

2. the INITIAL, PREFIRE, FIRE, and POSTFIRE thermal analyses may be performed in a sequence,

3. the INITIAL, PREFIRE, and FIRE thermal analyses may be performed in a sequence,

4. the INITIAL and PREFIRE thermal analyses may be performed in a sequence,

5. the PREFIRE, FIRE, POSTFIRE, and FINAL thermal analyses may be performed in a sequence,

6. the PREFIRE, FIRE, and POSTFIRE thermal analyses may be performed in a sequence,

7. the PREFIRE and FIRE thermal analyses may be performed in a sequence,

8. the FIRE, POSTFIRE, and FINAL thermal analyses may be performed in a sequence,

9. the FIRE and POSTFIRE thermal analyses may be performed in a sequence,

10. the POSTFIRE and FINAL thermal analyses may be performed in a sequence,

11. the INITIAL thermal analysis may be performed separately,

12. the PREFIRE thermal analysis may be performed separately,

13. the FIRE thermal analysis may be performed separately,

14. the POSTFIRE thermal analysis may be performed separately, and

15. the FINAL thermal analysis may be performed separately.

The initial temperature distribution for any analytical sequence that begins with a FIRE thermal analysis must be taken from the final temperature distribution of a PREFIRE thermal analysis that was executed previously. Likewise, the initial temperature distribution for any analytical sequence that begins with a POSTFIRE thermal analysis must be taken from the final temperature distribution of a FIRE thermal analysis that was executed previously.

HTAS1 will define the appropriate calculations to HEATING based on the combination of keywords it encounters in the input data. If an unacceptable sequence of keywords is encountered, HTAS1 will write an error message and terminate calculations. Basically, all five Analytical Sequence Data Blocks are similar. Each is identified by the appropriate keyword followed by at least two blanks. Data unique to each analytical sequence may be entered after the two or more blanks following the keyword. If the input value of any data item on the INITIAL, PREFIRE, FIRE, POSTFIRE, or FINAL data cards is negative, then the value of the appropriate variable is set to zero and that option is not used for the model. If the input value of any data item is zero or blank, then the value of the appropriate variable is set to the default value. Otherwise, the input value of any data item is used for the value of the appropriate variable for the model. If a data card contains only one of the Analytical Sequence Data Block keywords, INITIAL, PREFIRE, FIRE, POSTFIRE, or FINAL, the value of each variable associated with the keyword is set to the default value. If none of the Analytical Sequence Data Blocks is present in the input data, then HTAS1 will generate a model for HEATING to perform the complete analytical sequence, INITIAL, PREFIRE, FIRE, POSTFIRE, and FINAL, using all of the default values. Any data card containing one of the Analytical Sequence Data Block keywords may be continued by beginning the continuation card with an "@" in column 1.

In order to override the default numerical technique for a particular thermal analysis, an additional data card or cards may be entered following the Analytical Sequence Data Block keyword card. For the INITIAL, PREFIRE, and FINAL thermal analyses, the additional card contains the parameter values defining the numerical technique to be used to solve for the steady-state temperature distribution. For the FIRE and POSTFIRE thermal analysis, a group of data cards must be entered. The first such data card must contain the keyword IMPLICIT or EXPLICIT to select either an implicit or explicit numerical technique. The IMPLICIT data card must be followed by two additional data cards that contain the parameter values defining the numerical technique to be used to solve for the transient temperature distribution. HEATING will not allow a transient implicit technique for models allowing materials with change of phase (i.e., when a LATENT HEAT card is present in the HTAS1 input data). The EXPLICIT data card must be followed by a data card containing the initial time-step size and Levy's time step factor. The variables, which may be defined in each of the Analytical Sequence Data Blocks, are described below.

H1.4.9.1 INITIAL Steady-State Thermal Analysis

a. INITIAL Data Card

Each entry on the INITIAL data card is discussed below:

DBDTP - ambient temperature of the transport package, default 100°F,

DCONCR - coefficient for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 0.18 Btu/(hr-ft^2-°F^n), where n is equal to DCONER plus 1.0,

DCONER - exponent for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 1/3,

DCONCA - coefficient for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 0.19 Btu/(hr-ft^2-°F), where n is equal to DCONEA plus 1.0,

DCONEA - exponent for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 1/3, and

DFLUX - solar heat load to be applied to all external surfaces of the transport package, default 122.92 Btu/(hr-ft^2).

b. Default Numerical Technique

As the default, HTAS1 will generate input data for HEATING to perform the INITIAL thermal analysis using the direct-solution technique. For linear problems this technique requires only one pass through the numerical algorithm to obtain the steady-state temperature distribution. Nonlinear problems must be solved iteratively using the direct-solution technique, and the HTAS1 default values allow a maximum of 20 iterations and a heat residual convergence criterion of 1.0×10^{-5}.

c. Overriding the Default Numerical Technique

If the user wishes to override the default values or if he wishes to specify that HEATING use the SOR technique to obtain the steady-state temperature distribution, the following SS card may be added to the HTAS1 input data immediately following the data card containing the keyword INITIAL. HTAS1 will use the values on the SS data card for the steady-state technique parameters instead of the default values.

The parameters that are defined on the SS data card are summarized below:

Steady-State Technique Flag (I)

One of the three steady-state numerical techniques can be chosen by setting the first entry to 1 for the SOR, 2 for the direct, or 3 for the conjugate gradient techniques.

Maximum Number of Steady-State Iterations Allowed (I)

This entry defines the maximum number of iterations allowed before the steady-state calculations are terminated. Typically 200 to 500 iterations are sufficient to converge to the solution using the SOR technique. For linear problems, the direct-solution technique requires only one iteration to obtain the solution. Experience has indicated that 20 iterations are usually sufficient to obtain a converged solution for nonlinear steady-state problems using the direct-solution technique. If this entry is zero, the code will use the DIRECT technique with a default of 20 iterations. If the maximum number of steady-state iterations is reached, and the convergence criterion is not satisfied, the HEATING program will write "END STEADY-STATE CALCULATIONS, CONVERGENCE NOT SATISFIED" and will terminate the calculations and attempt to read the next problem.

Steady-State Convergence Criterion (R)

For the SOR technique, this entry contains the value of ϵ in Eq. (F10.2.14), which defines the steady-state convergence criterion. For the direct-solution technique, this entry contains the convergence criterion, as discussed in Sect. F10.2.2.2. The steady-state calculation will continue until the convergence criterion is met. Since the criterion that ensures convergence varies from case to case, the user must rely on his own judgment and experience in determining the correct value for his particular problem. If this entry is zero, the code uses a default of 10^{-5}.

Steady-State Overrelaxation Factor (R)

The value of [see Eq. (F10.2.13)] is the third entry on this card and its value must be in the range $1 \leq \beta < 2$. If a zero is entered for steady-state problems using the SOR solution technique, the code assumes that the initial value of β is 1.9. This entry is not used for the direct-solution technique.

Updating Temperature-Dependent Properties (I)

The fourth entry on this card specifies the number of iterations which are allowed before the temperature-dependent thermal properties are reevaluated for steady-state problems using the SOR solution technique. Once the convergence criterion has been satisfied the code continues to iterate. However, the temperature-dependent thermal properties are now reevaluated after every iteration until the convergence criterion is satisfied a second time. Some nonlinear problems will converge in fewer iterations if the thermal properties are not evaluated at each iteration, and certainly, the computing time per iteration will be less. It

is recommended that this parameter be on the order of 10 or 20. If it is zero, then the default value is unity for nonlinear problems. This entry is not used for the direct solution or conjugate gradient technique.

H1.4.9.2 PREFIRE Steady-State Thermal Analysis

a. PREFIRE Data Card

Each entry on the PREFIRE data card is discussed below.

DBDTP - ambient temperature of the transport package, default 100°F,

DCONCR - coefficient for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 0.18 Btu/(hr-ft^2-°F^n), where n is equal to DCONER plus 1.0,

DCONER - exponent for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 1/3,

DCONCA - coefficient for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 0.19 Btu/(hr-ft^2-°F^n), where n is equal to DCONEA plus 1.0,

DCONEA - exponent for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 1/3, and

DFLUX - solar heat load to be applied to all external surfaces of the transport package, default 0 Btu/(hr-ft^2).

b. Default Numerical Technique

As the default, HTAS1 will generate input data for HEATING to perform the PREFIRE steady-state thermal analysis using the direct-solution technique. As with the INITIAL thermal analysis, the HTAS1 default values allow a maximum of 20 iterations and a heat residual convergence criterion of 1.0×10^{-5}.

c. Overriding the Default Numerical Technique

If the user wishes to override the default values or if he wishes to specify that HEATING use the SOR technique to obtain the PREFIRE steady-state temperature distribution, then a SS data card may be added to the HTAS1 input data immediately following the data card containing the keyword PREFIRE. HTAS1 will use the values on the SS data card for the steady-state technique parameters instead of the default values. See the section on the INITIAL thermal analysis for a description of the SS data card (Sect. H1.4.9.1b).

H1.4.9.3 FIRE Transient Thermal Analysis

a. FIRE Data Card

Each entry on the FIRE data card is discussed below.

DTIMEF - duration of the fire transient, default 30 min,

DEMISF - emissivity coefficient of the fire, default 0.9,

DBDTP - temperature of the fire, default 1475°F,

DCONCR - coefficient for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (third data entry), default 0 Btu/(hr-ft^2-°F^n), when n is equal to DCONER plus 1.0,

DCONER - exponent for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (third data entry), default 0,

DCONCA - coefficient for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (third data entry), default 0 Btu/(hr-ft^2-°F^n), where n is equal to DCONEA plus 1.0,

DCONEA - exponent for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (third data entry), default 0, and

DFLUX - solar heat load to be applied to all external surfaces of the transport package, default 0 Btu/(hr-ft^2).

b. Default Numerical Technique

Normally, HTAS1 will generate input data for HEATING to perform the FIRE thermal analysis using the implicit transient technique. Under the default conditions, HTAS1 will use an initial time-step size of zero which causes HEATING to choose an initial time-step size equal to the stability criterion as calculated for the explicit procedure. Other HTAS1 default values give a maximum time step size of 5 min and allow HEATING to adjust the time step size to keep the maximum percent of relative temperature change allowed at a node from one time level to the next one to 2%. HTAS1 allows HEATING to use its own default values for the remaining implicit transient technique parameters.

c. Overriding the Default Numerical Technique

If the user wishes to override the default option and choose the numerical technique to solve for the FIRE transient temperature distribution, he may do so by supplying a group of data cards immediately following the data card containing the keyword FIRE. The first card in the group must contain one of the keywords IMPLICIT or EXPLICIT to choose either an implicit or explicit

numerical technique. HTAS1 IP and TP cards must immediately follow the data card containing the keyword IMPLICIT. Only one TP data card may be supplied. HTAS1 will use the values on the IP and TP cards for the implicit transient technique parameters instead of the default values.

If the data card immediately following the FIRE analytical sequence keyword contains the keyword EXPLICIT, an additional data card must be supplied to define the explicit transient technique. This data card is summarized below:

1. The first entry, a real value, is the initial time step. An initial time step of zero causes HEATING to choose an initial time step size equal to the stability criterion as calculated for the explicit procedure.

2. The second entry, an integer, is the factor by which the stable time increment is multiple to form the time increment for Levy's explicit method. If the entry is 0 or 1, then Levy's method will not be used.

If the data card immediately following the FIRE analytical sequence keyword contains the keyword IMPLICIT, two additional data cards must be supplied to define the explicit transient technique. These data cards are summarized below:

Card IP

This entire card may be left blank or any of its entries may be zero, and the default values will be used. They are based on experiences with a few 2-D RZ models. They are certainly not the best values that can be used for a given problem, but they are probably good starting points. Eight entries are on this card.

1. The first entry, a real value, contains the convergence criterion, which must be met in order for the iterative technique to terminate successfully at each time step. This convergence criterion corresponds to ϵ_1 in Eq. (F10.2.52). The default is 10^{-5}.

2. The second entry, an integer, indicates the number of iterations between tests for convergence in the linear loop. Experience has shown that for problems requiring large numbers of iterations (over 50) for the linear loop to converge, a significant saving in computer time can be achieved by not performing the calculations necessary for convergence tests at every iteration. However, the number entered applies for all of the transient calculations. The default is 1.

3. The third entry, a real value, contains the convergence criterion for problems involving temperature-dependent parameters. This convergence criterion corresponds to ϵ_2 in Eq. (F10.2.55). The default is 10^{-5}.

4. This entry, the fourth, defines the implicit technique that will be used to solve the transient problem. It refers to θ in Eq. (F10.2.49) and must be chosen so that $0.5 \leq, \theta \leq 1.0$. The default is 0.5. This entry is a real value.

5. The fifth entry, a real value, defines the initial value of the point successive overrelaxation iteration acceleration parameter [ω in Eq. (F10.2.49)]. It also defines the method that will be used to update the acceleration parameter. If this entry is positive, then the acceleration parameter will remain constant throughout the calculations and will be equal to the value of this entry. If it is zero, then the acceleration parameter will be optimized empirically as a function of time. This appears to be the best option for nonlinear problems. If it is negative, then the acceleration parameter will be calculated using Carre's technique (Sect. F10.2.3.3.4). The absolute value of this must be less than 2.0.

6. This entry, an integer, defines the number of time steps between attempts to optimize the acceleration parameter empirically [referred to as N_ω in Sect. F10.2.3.3.4]. It is used only when Entry 5 is zero. The default value is 1.

7. For the case when the acceleration parameter will be updated empirically (Entry 5 is zero), then this entry, the seventh, defines the change-in-number-of-iterations criterion (referred to as I_ω in Sect. F10.2.3.3.4) which must be met before the acceleration parameter will be updated. The default is 5. For the case when the SOR acceleration parameter will be updated using Carre's technique, then this entry defines the number of iterations between updates. The default is 12. This entry is an integer.

8. The last entry, an integer, is the change-in-number-of-iterations criterion (referred to as J_ω in Sect. F10.2.3.3.4) which is used to determine when a good estimate to the optimum acceleration parameter has been found. This entry is used only when the acceleration parameter will be updated empirically (Entry 5 on this card is zero). The default is 2.

Card TP

When an implicit scheme is used to solve a transient problem, the time step may be variable. This allows the time step to increase as the solution smoothes out and to decrease when some parameter varies rapidly with time. The information controlling the value of the time step is contained on one of the TP cards. The size of the time step is automatically adjusted in order to get printouts of the temperature distribution at the specified time. If the size of the coefficients in the system of equations varies by orders of magnitude (10^5 or greater), it has been observed that point-successive overrelaxation iteration may converge very slowly (it may appear to not converge at all). This occurs when the grid spacing or thermal properties vary by orders of magnitude over the problem. It can be observed by examining the stability criterion table in the output. If this appears to be happening, either further subdivide some of the larger nodes or combine some of the smaller ones. In some cases, it may help to use a larger time step size. All seven entries are floating-point numbers. For some of these parameters, the indicated default value will be used when the corresponding entry is zero.

1. The first entry is the initial time step. If this entry is zero, HEATING will choose an initial time step size equal to the stability criterion as calculated for the explicit procedure.

2. After the temperature distribution has been calculated, the current time step is multiplied by a factor. The value of this factor is entered in the second field of the TP card. The default value is 1.0. For many problems whose parameters vary mildly with time and/or temperature, values between 1.0 and 1.3 have been acceptable.

3. The maximum value of the time step is the third entry. Once the time step reaches this value, it is no longer increased. The default is 10^{50}.

4. The fourth entry contains the maximum time that the time-step information on this card applies. If the time reaches this value, then a new TP card is read. The default is 10. This parameter must not be used with HTAS1.

5. The fifth entry contains the maximum temperature change allowed at a node over a time step. The time step is adjusted according to the procedure outlined in Sect. F10.2.3.3.5. If this entry is zero, this feature is not invoked in calculating the time-step size.

6. The sixth entry contains the maximum percentage of relative temperature change allowed at a node from one time level to the next one. The time-step size is adjusted according to the procedure outlined in Sect. F10.2.3.3.5. If this entry is zero, then this feature is not invoked in calculating the time-step size.

7. The seventh and final entry on this card contains the minimum value of the time step. Once the time-step size reaches this value, it is no longer decreased. The default is one-tenth of the initial time-step size.

H1.4.9.4 POSTFIRE Transient Thermal Analysis

a. POSTFIRE Data Card

Each entry on the POSTFIRE data card is discussed below.

DTIMPF - duration of the transient analysis following the fire, default 180 min,

DBDTP - ambient temperature of the transport package, default 100°F,

DCONCR - coefficient for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (second data entry), default 0.18 Btu/(hr-ft^2-°F^n) where n is equal to DCONER plus 1.0,

DCONER - exponent for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (second data entry), default 1/3,

DCONCA - coefficient for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (second data entry), default 0.19 Btu/(hr-ft^2-°F^n), where n is equal to DCONEA plus 1.0,

DCONEA - exponent for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (second data entry), default 1/3, and

DFLUX - solar heat load to be applied to all external surfaces of the transport package, default 0 Btu/(hr-ft^2).

b. Default Numerical Technique

Normally, HTAS1 will generate input data for HEATING to perform the POSTFIRE thermal analysis using the implicit transient technique. As with the FIRE thermal analysis, HTAS1 default conditions will use an initial time-step size of zero which causes HEATING to choose an initial time-step size equal to the stability criterion as calculated for the explicit procedure. Other HTAS1 default values give a maximum time-step size of 5 min and allow HEATING to adjust the time-step size to keep the maximum percentage of relative temperature change allowed at a node from one time level to the next one to 2%. HTAS1 allows HEATING to use its own default values for the remaining implicit transient technique parameters.

c. Overriding the Default Numerical Technique

If the user wishes to override the default option and choose the numerical technique to solve for the POSTFIRE transient temperature distribution, he may do so by supplying a group of data cards immediately following the data card containing the keyword POSTFIRE. The first card in the group must contain one of the keywords IMPLICIT or EXPLICIT to choose either an implicit or explicit numerical technique. HTAS1 IP and TP cards must immediately follow the data card containing the keyword IMPLICIT. Only one TP data card may be supplied. HTAS1 will use the values on the IP and TP cards for the implicit transient technique parameters instead of the default values.

See the FIRE thermal analysis section (Sect. H1.4.9.3) for a summary of the HTAS1 IP and TP data cards.

If the data card immediately following the POSTFIRE analytical sequence keyword contains the keyword EXPLICIT, an additional data card as described in Sect. H1.4.9.3 must be supplied to define the EXPLICIT transient technique.

H1.4.9.5 FINAL Steady-State Thermal Analysis

a. FINAL Data Card

Each entry on the FINAL data card is discussed below.

DBDTP - ambient temperature of the transport package, default 100°F,

DCONCR - coefficient for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 0.18 Btu/(hr-ft^2-°F^n), where n is equal to DCONER,

DCONER - exponent for the term simulating the effects of natural convective heat transfer from the smooth radial surfaces of the transport package (assumed to be long, horizontal cylinders) to still air at a temperature of DBDTP (first data entry), default 1/3,

DCONCA - coefficient for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 0.19 Btu/(hr-ft^2-°F^n), where n is equal to DCONEA plus 1.0,

DCONEA - exponent for the term simulating the effects of natural convective heat transfer from the smooth axial surfaces of the transport package (assumed to be vertical plates) to still air at a temperature of DBDTP (first data entry), default 1/3, and

DFLUX - solar heat load to be applied to all external surfaces of the transport package, default 0 Btu/(hr-ft^2).

b. Default Numerical Technique

As the default, HTAS1 will generate input data for HEATING to perform the FINAL steady-state thermal analysis using the direct-solution technique. As with the INITIAL thermal analysis, the

HTAS1 default values allow a maximum of 20 iterations and a heat residual convergence criterion of 1.0×10^{-5}.

c. Overriding the Default Numerical Technique

If the user wishes to override the default values or if he wishes to specify that HEATING use the SOR technique to obtain the FINAL steady-state temperature distribution, a SS data card may be added to the HTAS1 input data immediately following the data card containing the keyword FINAL. HTAS1 will use the values on the SS data card for the steady-state technique parameters instead of the default values. See the section on the INITIAL thermal analysis for a description of the SS data card.

H1.4.10 MODIFYING THE MODEL DURING AN ANALYTICAL SEQUENCE

The zones denoted by the keywords NEUTRON SHIELD, WATER JACKET, and IMPACT LIMITERS may be deleted from the model at the completion of one of the thermal analyses denoted by the keywords INITIAL, PREFIRE, FIRE, and POSTFIRE. When one of the zones is deleted, HTAS1 must modify HEATING input data to reflect the designated changes in the model. HTAS1 must also map the final temperature distribution from the old model into the initial temperature distribution for the new model. HTAS1 then tells HEATING to perform the next thermal analysis as designated by the input data.

These options have been added to HTAS1 to model some of the variations in a prescribed accident involving a shipping container. For instance, the removal of the neutron shield can be used to model a rupture in the water jacket followed by the loss of a liquid neutron shield. The removal of the water jacket and neutron shield can be used to model a shipping container in an accident resulting in shearing off of the complete water jacket. The removal of the impact limiters can be used to model a shipping container in an accident resulting in shearing off of one or both impact limiters.

The model modifications outlined above are elected by supplying a DELETE card with the input data for the NEUTRON SHIELD, WATER JACKET, and/or IMPACT LIMITERS. The DELETE card may be entered in any order with other data blocks or cards defining the particular zone. The format of the DELETE card for each zone follows:

H1.4.10.1 Neutron Shield

Keyword - DELETE

ADELET - Neutron shield removal time keyword. This entry must contain one of the keywords INITIAL, PREFIRE, FIRE, or POSTFIRE and must be separated from the keyword DELETE by at least two blanks. The neutron shield will be removed from the model following the thermal analysis identified by this keyword.

MZONE - Material Index. The entry must be an integer and must be separated from the previous entry by at least two blanks. If the entry is zero or blank, HTAS1 will replace the neutron shield by material 18 (see Table H1.2.2) in the HTAS1 material property library. This material is currently air with an effective thermal conductivity to simulate the natural convective effects across the annulus. A positive entry denotes the identification number for the material from the HTAS1 material property library that will replace the neutron shield. If the entry is negative, the neutron shield will be replaced by a void and heat will not be transferred by conduction across the resulting gap.

EMISIV(I) - Emissivity of the portion of the outer surface of the outer shell formerly covered by the neutron shield. This entry, a floating-point number, is unitless and has a default value of 0.5.

EMISIV(2) - Emissivity of the inner surface of the water jacket formerly covering the neutron shield. This entry, a floating-point number, is unitless and has a default value of 0.5.

If one of the above emissivities is negative, radiative heat transfer will not be allowed across the deleted neutron shield. If one of the above entries is zero or blank, the default value is used for the respective emissivity.

H1.4.10.2 Water Jacket

Keyword - DELETE

ADELET - Water jacket removal time keyword. This entry must contain one of the keywords INITIAL, PREFIRE, FIRE, or POSTFIRE and must be separated from the keyword DELETE by at least two blanks. Both the neutron shield and the water jacket will be removed from the model following the thermal analysis identified by the keyword.

H1.4.10.3 Impact Limiter

Keyword - DELETE

ADELET - Impact limiter removal time keyword. This entry must contain one of the keywords INITIAL, PREFIRE, FIRE, or POSTFIRE and must be separated from the keyword DELETE by at least two blanks. The portion of the impact limiters identified by the next entry will be removed from the model following the thermal analysis identified by this keyword.

ADELIM - Impact limiter removal zone keyword. This entry must contain one of the keywords TOP, BOTTOM, or BOTH or it may be omitted. It must be separated from the previous entry by at least two blanks. This keyword identifies the portion of the impact limiter which will be removed from the model following the thermal analysis identified by the previous keyword, the impact limiter removal time keyword. These keywords are self-explanatory with TOP indicating the top impact limiter, BOTTOM indicating the bottom impact limiter, and BOTH indicating both the top and bottom impact limiters. If the impact limiter removal-zone keyword is omitted, the keyword BOTH is assumed.

H1.4.11 FINNED SURFACE OPTION

The HTAS1 steady-state fin-effectiveness technique may be applied along the outer surfaces of the model of the shipping container.

If fins are defined on the outer radial surface of the outer shell and if the water jacket and neutron shield and/or one or both impact limiters are removed during the analytical sequence, the resulting uncovered surfaces of the outer shell are assumed to be smooth. However, the fins on the original uncovered portion of the outer shell surface are assumed to remain intact. This option is invoked along an outer surface or surfaces by entering a FINS data block in the data block for the zone or zones containing the particular surface or surfaces. The FINS data block may be entered in any order with other data blocks or cards defining the particular zone. A FINS data block may not be entered in the CAVITY, INNER SHELL, or SHIELDING data blocks. The format of the FINS data block for each zone follows:

Keyword - FINS

IFINR - Radial fin flag. This entry, a nonnegative integer, contains the HEATING fin type (as defined in Fig. H1.2.6) which is to be applied along the outer radial surface of the zone. If this entry is zero or blank, then the fin effectiveness option is not invoked for the outer radial surfaces of the zone.

IFINZ - Axial fin flag. This entry, a nonnegative integer, contains the HEATING fin type as defined in Fig. H1.2.6 that is to be applied along the outer axial surface of the zone. If this entry is zero or blank, then the fin-effectiveness option is not invoked for the outer axial surfaces of the zone.

F1 cards must follow the FINS data card to define the fin parameters for the radial and axial outer surfaces, respectively. The F1 card for the radial outer surface must precede the F1 card for the axial outer surface. If IFINR is zero or blank, the corresponding F1 card is omitted. Likewise, if IFINZ is zero or blank, the corresponding F1 card is omitted. The fin descriptor card, F1, containing five floating-point numbers is described below:

FINLEN - height of the fin from the base surface in inches.

DELBAS - half-width of fin at base in inches (for rectangular spine, DELBAS is the halfwidth in the first direction).

DELTIP - half-width of fin at tip in inches (for rectangular spine, DELTIP is the halfwidth perpendicular to DELBAS).

S1 - fin spacing in inches (centerline to centerline).

S2 - spine spacing in inches (centerline to centerline) perpendicular to S1. Enter zero if not spine.

For spines, the actual direction of DELBAS, DELTIP or S1, S2 is not important, but DELBAS must be perpendicular to DELTIP and S1 must be perpendicular to S2.

H1.4.12 PLOTTING DATA BLOCKS

NOTE: In the current version only the summary data are printed out for each of the plot type described.

Either region plots or temperature profile plots may be generated for the model that is defined by the HEATING input generated by HTAS1. If region plots are desired, the region plots data block must be the final data block listed in the HTAS1 input. If temperature profile plots are desired, the temperature profile plots data card may appear anywhere in the input after the title card and the problem control parameters card and before the end of data card. If both the temperature profile plots data card and the region plot data block are included in the input, only the region plots are generated because HEATING is not executed when region plots are generated. Therefore, no temperature distribution plot data sets exist from which temperature profile plots can be generated. The temperature profile plots data card must precede the region plots data block in this case.

H1.4.12.1 Temperature Profile Plots Data Card

Keyword - PLOT

MAXZVR - 0, generates a plot containing a curve that shows maximum temperature at any problem time vs the radial distance from the origin for all nodes on the axial center line (default).

1, above plot is not generated.

IVA - 0, generates a plot containing a curve that shows the difference in volume-averaged temperatures between the inner shell and the outer shell vs time (default).

1, above plot is not generated.

ISEP - 0, the temperature-vs-time curves for the centermost nodes of the inner shell, the shielding, and the outer shell are generated on the same plot (default).

1, each of the above curves is generated on an individual plot.

IDELT - 0, temperature-vs-time curves are generated for the actual temperatures (default).

1, temperature-vs-time curves are generated for temperature change from the initial temperature distribution.

TIMMIN - The problem time below which temperature distributions are not considered in the temperature-vs-time plots and the volume-averaged temperature plot. If TIMMIN is zero, the initial temperature distribution written by HEATING is the first one used when generating these plots. The entry must be a nonnegative floating-point number. The default is zero.

TIMMAX - The problem time above which temperature distributions are not considered in the temperature-vs-time plots and the volume-averaged temperature plot. If TIMMAX is zero, the final temperature distribution written by HEATING is the last one used when generating these plots. The entry must be a nonnegative floating-point number. The default is zero.

If the only entry on this card is the keyword PLOT, then the three default temperature profile plots described in Sect. H1.2.6 are generated.

H1.4.12.2 Region Plots Data Block

The first card in the plots data block contains only the keyword REGP. If no other cards are included in this data block, then by default plots of the regions, the materials, and the boundary condition function numbers are generated for each thermal analysis specified in the analytical sequence data blocks (Sect. H1.4.9).

Up to five plot description cards, one for each type of plot, may follow the keyword card if plots other than the default region plots are desired. The first entry on a plot description is an integer. All other entries are floating-point numbers. The entries are described below.

1TYPE - The number corresponding to the type of plot generated.

= 1 Plots are generated with region numbers inside the region boundaries for each calculational phase.

= 2 Plots are generated with material names inside the region boundaries for each calculational phase.

= 3 Plots are generated with heat generation function numbers inside the region boundaries for each calculational phase.

= 4 Plots are generated with initial temperature function numbers inside the region boundaries for each calculational phase.

= 5 Plots are generated with boundary condition function numbers inside the region boundaries for each calculational phase.

XSCALE - The scaling factor in units per inch for the horizontal axis of region plots for every calculational phase. If XSCALE is zero, the scaling factor is computed by the program for each calculational phase. The default is zero.

YSCALE - The scaling factor in units per inch for the vertical axis of region plots for every calculational phase. If YSCALE is zero, the scaling factor is computed by the program for each calculational phase. The default is zero.

XREG1 - The minimum r value of the area for which region plots are generated for every calculational phase. If XREG1 is zero, the minimum r value of the model at each calculational phase is used. The default is zero.

XREG2 - The maximum r value of the area for which region plots are generated for every calculational phase. If XREG2 is zero, the maximum r value of the model at each calculational phase is used. The default is zero.

YREG1 - The minimum z value of the area for which region plots are generated for every calculational phase. If YREG1 is zero, the minimum z value of the model at each calculational phase is used. The default is zero.

YREG2 - The maximum z value of the area for which region plots are generated for every calculational phase. If YREG2 is zero, the maximum z value of the model at each calculational phase is used. The default is zero.

H1.4.13 DATA BLOCK TERMINATION CARD

Each problem (or case) must be terminated with a data block termination card. This card consists of a percent sign (%) in column 1 followed by a blank in column 2.

H1.4.14 SUMMARY AND FORMAT OF INPUT

Table H1.4.3 is a summary of the information needed to prepare the input data. Columns 73 through 80 of each card are reserved for identification. The table in this column gives proposed identification names for the cards and, in parentheses, the reference sections in the report where more information can be found. The first line in each format box includes the variable name used in the program and, in parentheses, the type of that variable. The rest of the box includes a short explanation of the input in that box. In some cards, where free space is available, additional notes have been included to describe the way the input information will be used in the program.

Table H1.4.3 Summary of HTAS input

TITLE
Job Title – up to 56 alphanumeric characters

MXCPU Maximum number of CPU seconds allowed.	ITPIN Unit number from which initial temperature distribution is to be read.										Required
PRINTOUT TIMES		-- At least two blanks.	First printout time.	Second printout time.	--	Last printout time					Optional
CAVITY		-- At least two blanks.	RCAVTY Radius of the cavity in inches.	NRCAVT Radial increments in the cavity.	TCAVTY Distance from the midplane to the top of the cavity in inches.	NTCAVT Axial increments between the midplane and the top of the cavity.	HEAT Total heat load in the cavity in BTU/hr.				Required
INNER SHELL		-- At least two blanks.	RINNER Radial thickness of the inner shell in inches.	NRINNE Radial increments across the thickness of the inner shell.	TINNER Axial thickness of the top of the inner shell in inches.	NTINNE Axial increments across the inner shell top thickness.	BINNER Axial thickness of the bottom of the inner shell in inches.	NBINNE Axial increments across the inner shell bottom thickness.			Required
MATERIAL		-- At least two blanks.	MZONE Material index.								Optional
ZONENM Material name											Required if MZONE = 0

Table H1.4.3 (continued)

First temperature for thermal conductivity in °F or constant thermal conductivity in BTU/hr-ft-°F.	First thermal conductivity in BTU/hr-ft-°F if temperature dependent.	Second temperature for temperature-dependent thermal conductivity in °F.	Second thermal conductivity in BTU/hr-ft-°F if temperature dependent.	--	Last temperature for temperature-dependent thermal conductivity in °F.	Last thermal conductivity in BTU/hr-ft-°F if temperature dependent.					Include only if MZONE = 0 and the LLNL library is not to be used by HEATING for this material.
First temperature for density in °F or constant density in lb/ft³.	First density in lb/ft³ if temperature dependent.	Second temperature for temperature-dependent density in °F.	Second density in lb/ft³ if temperature dependent.	--	Last temperature for temperature-dependent density in °F.	Last density in lb/ft³ if temperature dependent.					
First temperature for specific heat in °F or constant, specific heat in BTU/lb-°F.	First specific heat in BTU/lb-°F if temperature dependent.	Second temperature for temperature-dependent specific heat in °F.	Second specific heat in BTU/lb-°F if temperature dependent.	--	Last temperature for temperature-dependent specific heat in °F.	Last specific heat in BTU/lb-°F if temperature dependent.					
LATENT HEAT		-- At least two blanks.	SLTM Phase change temperature in °F.	SLHM Latent heat in BTU/lb.							Optional
SHIELDING		-- At least two blanks.	RSHELD Radial thickness of the shielding in inches.	NRSHEL Radial increments across the shielding thickness.	TSHELD Axial thickness of the top of the shielding in inches.	NTSHEL Axial increments across the shielding top thickness.	BSHELD Axial thickness of the bottom of the shielding in inches.	NBSHELD Axial increments across the shielding bottom thickness.			Optional
Can insert MATERIAL description (up to 5 cards) as described above.											Optional
Can insert a LATENT HEAT card as described above.											Optional

Table H1.4.3 (continued)

OUTER SHELL		-- At least two blanks.	ROUTER Radial thickness of the outer shell in inches.	NROUTE Radial increments across the outer shell thickness.	TOUTER Axial thickness of the top of the outer shell in inches.	NTOUTE Axial increments across the top thickness of the outer shell.	BOUTER Axial thickness of the bottom of the outer shell in inches.	NBOUTE Axial increments across the bottom thickness of the outer shell.			Required
Can insert MATERIAL description (up to 5 cards) as described above.											Optional
Can insert LATENT HEAT card as described above.											Optional
EMISSIVITY		-- At least two blanks.	EMISIV(1) INITIAL Steady-state emissivity.	EMISIV(2) PREFIRE Steady-state emissivity.	EMISIV(3) FIRE Transient emissivity.	EMISIV(4) POSTFIRE Transient emissivity.	EMISIV(5) FINAL Steady-state emissivity.				Optional
FINS		-- At least two blanks.	IFINR HEATING Fin type for outer radial surface.	IFINZ HEATING Fin type for outer axial surface.							Optional
FINLEN Height of fin from the outer radial surface in inches.	DELBAS Half-width of fin at base in inches for the outer radial surface.	DELTIP Half-width of fin at tip in inches for the outer radial surface.	S1 Fin spacing in inches for the outer radial surface.	S2 Spine spacing in inches for the outer radial surface.							Include only if IFINR $\neq$ 0
FINLEN Height of fin from the outer axial surface in inches.	DELBAS Half-width of fin at base in inches for the outer axial surface.	DELTIP Half-width of fin at tip in inches for the outer axial surface.	S1 Fin spacing in inches for the outer axial surface.	S2 Spine spacing in inches for the outer axial surface.							Include only if IFINZ $\neq$ 0

Table H1.4.3 (continued)

NEUTRON SHEILD	-- At least two blanks.	RNUTRN Radial thickness of neutron shield in inches.	NRNUTR Radial increments across the neutron shield thickness.	TNUTRN Axial distance from the midplane to the top of the neutron shield in inches.	BNUTRN Axial distance from the midplane to the bottom of the neutron shield in inches.					Optional
Can insert MATERIAL description (up to 5 cards) as described above.										Optional
Can insert LATENT HEAT card as described above.										Optional
Can insert EMISSIVITY card as described above.										Optional
Can insert FIN description (up to 3 cards) as described above.										
DELETE	-- At least two blanks.	ADELET Neutron shield removal time keyword.	MZONE Material index.	EMISIV(1) Emissivity of the portion of the outer shell formerly covered.	EMISIV(2) Emissivity of the portion of the water jacket formerly covered.					Optional
WATER JACKET	-- At least two blanks.	RWATER Radial thickness of the water jacket in inches.	NRWATE Radial increments across the water jacket thickness.	TWATER Axial distance from the midplane to the top of the water jacket in inches.	BWATER Axial distance from the midplane to the bottom of the water jacket in inches.					Optional
Can insert MATERIAL description (up to 5 cards) as described above.										Optional
Can insert LATENT HEAT card as described above.										Optional
Can insert EMISSIVITY card as described above.										Optional
Can insert FIN description (up to 3 cards) as described above.										Optional

Table H1.4.3 (continued)

DELETE	-- At least two blanks.	ADELET Water jacket removal time keyword.								Optional
IMPACT LIMITER	-- At least two blanks.	RMPACT Radius of both top and bottom impact limiters in inches.	NRMPAC Additional radial increments needed to discretize the impact limiters.	TMPACT Axial thickness of the top impact limiter in inches.	NTMPAC Axial increments across the top impact limiter.	BMPACT Axial thickness of the bottom impact limiter in inches.	NBMPAC Axial increments across the bottom impact limiter.	TWRAP Axial thickness of top impact limiter that wraps around the outer shell in inches.	BWRAP Axial thickness of bottom impact limiter that wraps around the outer shell in inches.	Optional
Can insert MATERIAL description (up to 5 cards) as described above.										Optional
Can insert LATENT HEAT card as described above.										Optional
Can insert EMISSIVITY card as described above.										Optional
Can insert FIN description (up to 3 cards) as described above.										Optional
DELETE	-- At least two blanks.	ADELET Impact limiter removal time keyword.	ADELIM Top, bottom or both.							Optional
INITIAL	-- At least two blanks.	DBDTP Ambient temperature in °F.	DCONCR Natural convection coefficient for radial surfaces.	DCONER Natural convection exponent for radial surfaces.	DCONCA Natural convection coefficient for axial surfaces.	DCONEA Natural convection exponent for axial surface.	DFLUX Solar heat load in BTU/hr-ft^2.			Optional

Table H1.4.3 (continued)

MAXIT Maximum number of iterations for steady-state solution. If MAXIT ≥ 0, then use SOR, else direct.	EPS Steady-state convergence criterion.	BETA Steady-state over-relaxation factor.	TDP Number of iterations between property re-evaluation.								Optional
PREFIRE		At least two blanks.	DBDTP Ambient temperature in °F.	DCONCR Natural convection coefficient radial surfaces.	DCONER Natural convection exponent for radial surfaces.	DCONCA Natural convection coefficient for axial surfaces.	DCONEA Natural convection exponent for axial surfaces.	DFLUX Solar heat load in BTU/hr-ft².			Optional
Can insert solution technique SS card as shown after the INITIAL block.											Optional
FIRE		At least two blanks	DTIMEF Duration of the fire transient in minutes.	DEMISF Emissivity of the fire.	DBDTP Temperature of the fire in °F.	DCONCR Natural convection coefficient for radial surfaces.	DCONER Natural convection exponent for radial surfaces.	DCONCA Natural convection coefficient for axial surfaces.	DCONEA Natural convection exponent for axial surfaces.	DFLUX Solar heat load in BTU/hr-ft².	Optional
IMPLICIT											
RESDUL Convergence criterion per time step.	NITREZ Iterations between convergence tests.	ABSDIF Convergence criterion per time step with temperature dependence.	THETA Implicitness factor.	BETAT Acceleration parameter.	NUPBTA Iterations between attempts to optimize BETAT.	ITLRCO Iterations between updates using Carre's technique.	ITLRCI Change in number-of-iteration criterion.				Optional

Table H1.4.3 (continued)

DELTAT Initial time step in minutes.	TSFACT Time-step multiplication factor.	TSMAX Maximum allowable time step in minutes.	TSCHGB Maximum time for application of this card in minutes.	TPCGMX Maximum temperature change allowed at a node per time step in °F.	PDPCGM Maximum percent of relative change in temperature allowed per time step.	TSMIN Minimum time step allowed in minutes.					Optional
EXPLICIT											Optional
DELTAT Initial time step in minutes.	KTMFCT Levy factor.										
POSTFIRE		– At least two blanks.	DTIMPF Duration of the postfire transient in minutes.	DBDTP Ambient temperature in °F.	DCONCR Natural convection coefficient for radial surfaces.	DCONER Natural convection exponent for radial surfaces.	DCONCA Natural convection coefficient for axial surfaces.	DCONEA Natural convection exponent for axial surfaces.	DFLUX Solar heat load in BTU/hr-ft²,		Optional
Can insert solution technique description with IMPLICIT or EXPLICIT as shown above.											Optional
FINAL		– At least two blanks.	DBDTP Ambient temperature in °F.	DCONCR Natural convection coefficient for radial surfaces.	DCONER Natural convection exponent for radial surfaces.	DCONCA Natural convection coefficient for axial surfaces.	DCONEA Natural convection exponent for axial surfaces.	DFLUX Solar heat load in BTU/hr-ft².			Optional
Can insert solution technique SS card as shown after the INITIAL block											Optional

Table H1.4.3 (continued)

PLOT		-- At least two blanks.	MAXZVR = 0, generate maximum temperature vs radial distance plots; = 1, suppress.	IVA =0, generate volume-averaged temperature plots; =1, suppress.	ISEP =0, temperature vs time curves are on same plot; =1 different plots.	IDELT =0, temperature vs time curves are for actual temperature; =1, for temperature changes.	TIMMIN Minimum time for plots in minutes.	TIMMAX Maximum time for plots in minutes.			Optional
REGP											Optional
ITYPE Type of plot.	XSCALE Horizontal axis scaling factor.	YSCALE Vertical axis scaling factor.	XREG1 Minimum r-value in inches.	XREG2 Maximum r-value in inches.	YREG1 Minimum z-value in inches.	YREG2 Maximum z-value in inches.					
% Data block termination card.											Required

H1.5 SAMPLE PROBLEMS FOR HTAS1

This section contains two sample problems to demonstrate the use of some of the options available in HTAS1. The first sample problem makes extensive use of HTAS1 defaults to indicate the case of performing a detailed thermal analysis of a shipping container using HTAS1. The second sample problem invokes a number of options available in HTAS1 to include the use of alternative methods of defining material thermal parameters.

The first sample problem is defined below. The diameter of the cavity is 13.5 in. (radius, 6.75 in.), and its total height is 178 in. (half height, 89 in.). The total heat load within the cavity is 11.5 kW (39247 Btu/hr). The radial thickness of the inner shell is 0.31 in., and its axial thickness at both top and bottom is 0.25 in. The shielding has a radial thickness of 6.63 in., and its axial extent is equal to that of the inner shell. The outer shell has a radial thickness of 1.25 in. The axial thickness of the top and bottom of the outer shell is 7.5 and 7.75 in., respectively. The diameter and total thickness of each impact limiter is 78 in. (radius 39 in.) and 38.5 in., respectively. The shipping container extends into each impact limiter a distance of 11 in. Thus, the axial thickness of each impact limiter is 27.5 in., and each impact limiter has a wraparound of 11 in. The radial thickness of the neutron shield and water jacket is 4.5 and 0.16 in., respectively. The neutron shield and water jacket extend axially to each impact limiter so their axial distance above and below the horizontal midplane is 85.5 and 86 in., respectively. The inner shell, outer shell and water jacket are composed of 304 stainless steel. The shielding is lead, and the impact limiters are balsa wood. The neutron shield is water, and it is desired to model the natural convective heat transfer effects across the neutron shield with an effective thermal conductivity. Thus, one can use the HTAS1 default material associated with each zone. The emissivity associated with the outer surfaces of the water jacket and impact limiters is 0.5.

The shipping container is in a horizontal position, and for purposes of defining the steady-state conditions for the accident scenario of 10CFR71, the solar heat load is assumed to be zero. The loaded shipping container is allowed to reach steady-state operating conditions with an ambient temperature of 100°F. The shipping container is cooled by natural convection and radiation to the surrounding environment. It is then subjected to a fire at a temperature of 1475°F for 30 min. The emissivity of the fire is 0.9, and the absorptivity of the surfaces of the shipping container during the fire is 0.8. After the fire, the shipping container is allowed to cool by natural convection and radiation to the surrounding environment at an ambient temperature of 100°F. The emissivity on the surfaces of the shipping container remains at 0.8 following the fire.

It is desired to obtain the prefire steady-state operating temperature distribution, the transient temperature distribution during the fire, the transient temperature distribution for three hours following the fire, and the final steady-state temperature distribution after the fire. The default numerical technique will be used to perform each set of calculations. The input data for HTAS1 to perform this analytical sequence and to generate the default temperature profile plots for the first sample problem are shown in Table H1.5.1. The radial and axial grid divisions indicated for each zone are necessary to yield accurate solutions. Their values were determined by performing a series of analytical sequences using grid divisions that were both more coarse and more fine than the ones indicated in Table H1.5.1.

The standard output from the initial entry to HTAS1 is presented in Table H1.5.2. The temperature distributions at the prefire steady state, at the end of the 30-min fire transient, at the end of the three-hour cooldown period, and at the final steady state are presented in Tables H1.5.3, H1.5.4, H1.5.5, and H1.5.6, respectively. The HTAS1 output that describes the temperature profile plots generated for the first sample problem is presented in Table H1.5.2.

Table H1.5.1 Input data for first sample problem for HTAS1

HTAS1 SAMPLE PROBLEM 1							
CAVITY	6.75	5	89	5	39247		
INNER SHELL	0.31	1	0.25	1			
SHIELDING	6.63	5					
OUTER SHELL	1.25	2	7.25	4	7.75	4	
NEUTRON SHIELD	4.5	4	85.5	86			
WATER JACKET	0.16	1					
IMPACT LIMITER	39	5	27.5	5	0	0	11
PREFIRE							
FIRE							
POSTFIRE							
FINAL							
%							

Table H1.5.2 Standard output from initial entry into HTAS1

```
*********************************************
* control module htas1    has been accessed. *
*********************************************
print input card images w/card columns indicated every 10th card--
card
no./col. 1.......10........20........30........40........50........60........70........80
    1    htas1 sample problem 1
    2        0     0
    3    cavity           6.75 5 89 5 39247
    4    inner shell      0.31 1 0.25 1
    5    shielding        6.63 5
    6    outer shell      1.25 2 7.25 4 7.75 4
    7    neutron shield   4.5 4 85.5 86
    8    water jacket     0.16 1
    9    impact limiter   39 5 27.5 5 0 0 11
   10    prefire
no./col. 1.......10........20........30........40........50........60........70........80
   11    fire
   12    postfire
   13    final
   14    plot
   15    %


code    : htas1          date: 06/11/93          computer: ibmaixws
version: 05/12/93        time: 15:43:41          jobname : geg
htas1: heat transfer analysis sequence number 1 for the scale system.
htas1 is a control module for generating input data for heating for
two-dimensional rz models analyzing a class of shipping containers.
written by:c.k.cobb, w.d.turner, m.w.wendel, g.e.giles
contact:
     g.e. giles
     computing applications division
     oak ridge national laboratory
     building k-1007, mail stop number 7039
     martin marietta energy systems, inc.
     post office box 2003
     oak ridge, tennessee 37831-7039
     phone - 615-574-8667
tabulation of input data
job description -- htas1 sample problem 1
cavity parameters
     radius                                          6.7500000D+00
     radial divisions                                           5
     top height                                      8.9000000D+01
     axial divisions for top                                    5
     bottom height                                   8.9000000D+01
     axial divisions for bottom                                 5
     heat load                                       3.9247000D+04
inner shell parameters
     radial thickness                                3.1000000D-01
     radial divisions                                           1
     axial thickness at top                          2.5000000D-01
     axial divisions                                            1
     axial thickness at bottom                       2.5000000D-01
     axial divisions                                            1
     material number                                           13
     material name                                        sst304
          number     temperature      conductivity
            1      3.2000000D+01    8.1000000D+00
            2      2.1200000D+02    8.7000000D+00
            3      3.9200000D+02    8.7000000D+00
            4      5.7200000D+02    9.4000000D+00
            5      7.5200000D+02    1.0000000D+01
            6      1.1120000D+03    1.1000000D+01
            7      1.4720000D+03    1.3000000D+01
          number     temperature        density
                                     4.9100000D+02
```

Table H1.5.2 (continued)

```
          number      temperature      specific heat
            1       3.2000000D+01    1.2000000D-01
            2       7.5200000D+02    1.3500000D-01
shielding parameters
     radial thickness                                  6.6300000D+00
     radial divisions                                              5
     axial thickness at top                            0.0000000D+00
     axial divisions                                               0
     axial thickness at bottom                         0.0000000D+00
     axial divisions                                               0
     material number                                              11
     material name                                              lead
          number      temperature      conductivity
            1       3.2000000D+01    2.0300000D+01
            2       2.1200000D+02    1.9300000D+01
            3       3.9200000D+02    1.8200000D+01
            4       5.7200000D+02    1.7200000D+01
            5       6.3000000D+02    1.2100000D+01
            6       7.1700000D+02    9.7000000D+00
            7       8.0000000D+02    9.0000000D+00
            8       9.8000000D+02    8.7000000D+00
            9       1.2760000D+03    8.6600000D+00
          number      temperature         density
                                       7.1000000D+02
          number      temperature      specific heat
            1       3.2000000D+01    3.0500000D-02
            2       2.1200000D+02    3.1500000D-02
            3       6.2150000D+02    3.3800000D-02
            4       6.2170000D+02    3.4000000D-02
            5       1.8320000D+03    3.2800000D-02
outer shell parameters
     radial thickness                                  1.2500000D+00
     radial divisions                                              2
     axial thickness at top                            7.2500000D+00
     axial divisions                                               4
     axial thickness at bottom                         7.7500000D+00
     axial divisions                                               4
     emissivity
          initial steady state                         5.0000000D-01
          prefire steady state                         5.0000000D-01
          fire transient                               8.0000000D-01
          postfire transient                           8.0000000D-01
          final steady state                           8.0000000D-01
     material number                                              13
     material name                                           sst304
          number      temperature      conductivity
            1       3.2000000D+01    8.1000000D+00
            2       2.1200000D+02    8.7000000D+00
            3       3.9200000D+02    8.7000000D+00
            4       5.7200000D+02    9.4000000D+00
            5       7.5200000D+02    1.0000000D+01
            6       1.1120000D+03    1.1000000D+01
            7       1.4720000D+03    1.3000000D+01
          number      temperature         density
                                       4.9100000D+02
          number      temperature      specific heat
            1       3.2000000D+01    1.2000000D-01
            2       7.5200000D+02    1.3500000D-01
neutron shield parameters
     radial thickness                                  4.5000000D+00
     radial divisions                                              4
     top height                                        8.5500000D+01
     bottom height                                     8.6000000D+01
     emissivity
          initial steady state                         5.0000000D-01
          prefire steady state                         5.0000000D-01
          fire transient                               8.0000000D-01
          postfire transient                           8.0000000D-01
          final steady state                           8.0000000D-01
```

Table H1.5.2 (continued)

```
     material number                                                  17
     material name                                                h2oconv
          number     temperature     conductivity
            1      1.5000000D+02    1.4750000D+01
            2      2.0000000D+02    1.7330000D+01
            3      2.5000000D+02    1.9150000D+01
            4      3.0000000D+02    2.0830000D+01
            5      4.0000000D+02    2.3350000D+01
          number     temperature       density
                                     6.0000000D+01
          number     temperature     specific heat
            1      3.2000000D+01    1.0072000D+00
            2      6.8000000D+01    9.9861000D-01
            3      1.0400000D+02    9.9780000D-01
            4      1.4000000D+02    9.9921000D-01
            5      1.7600000D+02    1.0021000D+00
            6      2.1200000D+02    1.0068000D+00
            7      2.4800000D+02    1.0149000D+00
            8      2.8400000D+02    1.0228000D+00
            9      3.2000000D+02    1.0369000D+00
           10      3.5600000D+02    1.0548000D+00
           11      3.9200000D+02    1.0758000D+00
           12      4.2800000D+02    1.1009000D+00
           13      4.6400000D+02    1.1357000D+00
           14      5.0000000D+02    1.1818000D+00
           15      5.3710000D+02    1.2437000D+00
           16      5.7200000D+02    1.3678000D+00
water jacket parameters
     radial thickness                                    1.6000000D-01
     radial divisions                                               1
     top height                                          8.5500000D+01
     bottom height                                       8.6000000D+01
     emissivity
          initial steady state                           5.0000000D-01
          prefire steady state                           5.0000000D-01
          fire transient                                 8.0000000D-01
          postfire transient                             8.0000000D-01
          final steady state                             8.0000000D-01
     material number                                                13
     material name                                             sst304
          number     temperature     conductivity
            1      3.2000000D+01    8.1000000D+00
            2      2.1200000D+02    8.7000000D+00
            3      3.9200000D+02    8.7000000D+00
            4      5.7200000D+02    9.4000000D+00
            5      7.5200000D+02    1.0000000D+01
            6      1.1120000D+03    1.1000000D+01
            7      1.4720000D+03    1.3000000D+01
          number     temperature       density
                                     4.9100000D+02
          number     temperature     specific heat
            1      3.2000000D+01    1.2000000D-01
            2      7.5200000D+02    1.3500000D-01
impact limiter
     radius                                              3.9000000D+01
     radial divisions from  1.9600000D+01                           5
     axial thickness of top impact limiter               2.7500000D+01
     axial divisions                                                5
     axial thickness of top impact limiter
          along outer surface of container               1.1000000D+01
     axial thickness of bottom impact limiter            2.7500000D+01
     axial divisions                                                5
     axial thickness of bottom impact limiter
          along outer surface of container               1.1000000D+01
     emissivity
          initial steady state                           5.0000000D-01
          prefire steady state                           5.0000000D-01
          fire transient                                 8.0000000D-01
          postfire transient                             8.0000000D-01
```

Table H1.5.2 (continued)

```
          final steady state                          8.0000000D-01
     material number                                          19
     material name                                        balsa
          number      temperature      conductivity
                                       4.8400000D-02
          number      temperature         density
                                       2.0000000D+01
          number      temperature      specific heat
                                       5.5000000D-01


code   : htas1           date: 06/11/93          computer: ibmaixws
version: 05/12/93        time: 15:43:41          jobname : geg
job description -- htas1 sample problem 1
*******************************************************************************
heating input data will be generated for the prefire steady state thermal analysis.
*******************************************************************************
the steady state temperature distribution for the shipping container model
will be obtained subject to the following boundary conditions:
     ambient temperature                          1.0000000D+02
     convection at radial boundary
          convective coefficient                  1.8000000D-01
          convective exponent                     3.3333333D-01
     convection at axial boundary
          convective coefficient                  1.9000000D-01
          convective exponent                     3.3333333D-01
     radiation to surrounding medium at ambient
          temperature with emissivity coefficients
          as specified along each surface
     solar heat flux                              0.0000000D+00
the steady state temperature distribution will be
solved using the direct solution technique.
     maximum number of iterations will be                   20
     convergence criterion will be                1.0000000D-05


code   : htas1           date: 06/11/93          computer: ibmaixws
version: 05/12/93        time: 15:43:41          jobname : geg
job description -- htas1 sample problem 1
*******************************************************************************
heating input data will be generated for the fire transient thermal analysis.
*******************************************************************************
the transient temperature distribution for the shipping container model will be
obtained during exposure to a fire subject to the following boundary conditions:
     duration of fire                             3.0000000D+01
     fire temperature                             1.4750000D+03
     convection at radial boundary
          convective coefficient                  0.0000000D+00
          convective exponent                     0.0000000D+00
     convection at axial boundary
          convective coefficient                  0.0000000D+00
          convective exponent                     0.0000000D+00
     radiation from fire
          fire emissivity coefficient                    .9000
          surface absorption coefficients are
          as specified for the materials
          along each surface.
     solar heat flux                              0.0000000D+00
the implicit procedure will be used to calculate the transient temperature distribution.
maximum normalized heat residual convergence criterion = 0.00000D+00
(corresponds to epsilon sub 1, default=1.0d-5)
number-of-iterations between tests for convergence, linear loop (default = 1) =  0
average l1 norm of relative temperature difference convergence criterion
for temperature dependent properties = 0.00000D+00
(corresponds to epsilon sub 3, default=1.0d-5)
theta (0.5 for crank-nicolson,1.0 for classical implicit) = 0.00000D+00
(default = 0.5)
the sor acceleration parameter (beta) will be optimized empirically.
beta = 0.00000D+00
```

Table H1.5.2 (continued)

```
a beta update will be attempted every    0 time steps (default=1).
number-of-iterations tolerance for beta update calculations, outer loop (default=5) = 0
number-of-iterations tolerance for beta update calculations, inner loop (default=2) = 0
the following time step parameters will be used to compute the fire transient.
     time step  0.0000000D+00
     the maximum time step allowed is  5.0000000D+00
     new time step parameters will be read in at time =  3.0000000D+01
     if the maximum temperature change at a node exceeds  2.0000000D+00 per cent over a
     time step, then the time step size will be decreased accordingly.
code   : htas1          date: 06/11/93          computer: ibmaixws
version: 05/12/93       time: 15:43:41          jobname : geg
job description -- htas1 sample problem 1
********************************************************************************
heating input data will be generated for the postfire transient thermal analysis.
********************************************************************************
the transient temperature distribution for the shipping container model will be
obtained following exposure to a fire subject to the following boundary conditions:
     duration of post-fire transient                1.8000000D+02
     ambient temperature                            1.0000000D+02
     convection at radial boundary
          convective coefficient                    1.8000000D-01
          convective exponent                       3.3333333D-01
     convection at axial boundary
          convective coefficient                    1.9000000D-01
          convective exponent                       3.3333333D-01
     radiation to surrounding medium at ambient
          temperature with emissivity coefficients
          as specified along each surface
     solar heat flux                                0.0000000D+00
the implicit procedure will be used to calculate the transient temperature distribution.
maximum normalized heat residual convergence criterion = 0.00000D+00
(corresponds to epsilon sub 1, default=1.0d-5)
number-of-iterations between tests for convergence, linear loop (default = 1) =  0
average l1 norm of relative temperature difference convergence criterion
for temperature dependent properties = 0.00000D+00
(corresponds to epsilon sub 3, default=1.0d-5)
theta (0.5 for crank-nicolson,1.0 for classical implicit) = 0.00000D+00
(default = 0.5)
the sor acceleration parameter (beta) will be optimized empirically.
beta = 0.00000D+00
a beta update will be attempted every    0 time steps (default=1).
number-of-iterations tolerance for beta update calculations, outer loop (default=5) = 0
number-of-iterations tolerance for beta update calculations, inner loop (default=2) = 0
the following time step parameters will be used to compute the post-fire transient.
     time step  0.0000000D+00
     the maximum time step allowed is  5.0000000D+00
     new time step parameters will be read in at time =  2.1000000D+02
     if the maximum temperature change at a node exceeds  2.0000000D+00 per cent over a
     time step, then the time step size will be decreased accordingly.
code   : htas1          date: 06/11/93          computer: ibmaixws
version: 05/12/93       time: 15:43:41          jobname : geg
job description -- htas1 sample problem 1
********************************************************************************
heating input data will be generated for the final steady state thermal analysis.
********************************************************************************
the steady state temperature distribution for the shipping container model
will be obtained subject to the following boundary conditions:
     ambient temperature                            1.0000000D+02
     convection at radial boundary
          convective coefficient                    1.8000000D-01
          convective exponent                       3.3333333D-01
     convection at axial boundary
          convective coefficient                    1.9000000D-01
          convective exponent                       3.3333333D-01
     radiation to surrounding medium at ambient          temperature with emissivity coefficients
          as specified along each surface
     solar heat flux                                0.0000000D+00
the steady state temperature distribution will be
solved using the direct solution technique.
```

Table H1.5.2 (continued)

```
     maximum number of iterations will be                    20
     convergence criterion will be                  1.0000000D-05
code    : htas1           date: 06/11/93          computer: ibmaixws
version: 05/12/93         time: 15:43:41          jobname : geg
job description -- htas1 sample problem 1
transient printout times
     output         output
     number          time
          1      5.00000D+00
          2      1.00000D+01
          3      1.50000D+01
          4      2.00000D+01
          5      2.50000D+01
          6      3.00000D+01
          7      3.50000D+01
          8      4.00000D+01
          9      4.50000D+01
         10      5.00000D+01
         11      5.50000D+01
         12      6.00000D+01
         13      6.50000D+01
         14      7.00000D+01
         15      7.50000D+01
         16      8.00000D+01
         17      8.50000D+01
         18      9.00000D+01
         19      9.50000D+01
         20      1.00000D+02
         21      1.05000D+02
         22      1.10000D+02
         23      1.15000D+02
         24      1.20000D+02
         25      1.25000D+02
         26      1.30000D+02
         27      1.35000D+02
         28      1.40000D+02
         29      1.45000D+02
         30      1.50000D+02
         31      1.55000D+02
         32      1.60000D+02
         33      1.65000D+02
         34      1.70000D+02
         35      1.75000D+02
         36      1.80000D+02
         37      1.85000D+02
         38      1.90000D+02
         39      1.95000D+02
         40      2.00000D+02
         41      2.05000D+02
         42      2.10000D+02
*** warning *** the axial thickness of the portion of the lower  impact
*** warning *** limiter that wrapped around the  shipping container was
*** warning *** changed to eliminate an unfavorable axial grid spacing.
*** warning *** the boundary was moved from  3.8500000D+01 to
*** warning ***  3.5500000D+01.
*** warning *** the axial thickness of the lower  portion of the neutron
*** warning *** shield and water jacket was changed to eliminate an
*** warning *** unfavorable axial grid spacing.  the boundary was
*** warning *** moved from  3.5500000D+01 to  3.5500000D+01.
*** warning *** the axial thickness of the portion of the upper  impact
*** warning *** limiter that wrapped around the  shipping container was
*** warning *** changed to eliminate an unfavorable axial grid spacing.
*** warning *** the boundary was moved from  2.1000000D+02 to
*** warning ***  2.1350000D+02.
in h6tas1, the maximum dimension of the double precision array is 100000 which uses 782k
 bytes.
(this is set in htmain as the variable limitd.)
this use of the variably dimensioned double precision array require 14880 elements or 117k
 bytes of memory.
```

Table H1.5.2 (continued)

```
the variable dimensioned character array has 782k bytes left for storage of heating input
data in binary form.
htas1 used a total of 1617 elements in the character-array which required a total
of 13k bytes of core.  the core requirements for the htas1 portion of the
analysis could be reduced by 768k bytes.
*************************************************************************************
* exit from control module htas1    and direct scale to execute heating7 (htng72  ). *
*************************************************************************************

*********************************************
* control module htas1    has been accessed. *
*********************************************
htas1 will generate heating input data for the fire tr      thermal analysis.
      title:  htas1 sample problem 1                                  -- prefire ss
      number of nodes read:        654       number of nodes written:        654
  time found in plot data set:    0.0000000D+00
htas1 used a total of 1633 elements in the character-array which required a total
of 13k bytes of core.  the core requirements for the htas1 portion of the
analysis could be reduced by 768k bytes.

*************************************************************************************
* exit from control module htas1    and direct scale to execute heating7 (htng72  ). *
*************************************************************************************
*********************************************
* control module htas1    has been accessed. *
*********************************************
htas1 will generate heating input data for the postfire tr  thermal analysis.
      title:  htas1 sample problem 1                                  -- fire tr
      number of nodes read:        654       number of nodes written:        654
  time found in plot data set:    0.0000000D+00
  time found in plot data set:    5.0000000D+00
  time found in plot data set:    1.0000000D+01
  time found in plot data set:    1.5000000D+01
  time found in plot data set:    2.0000000D+01
  time found in plot data set:    2.5000000D+01
  time found in plot data set:    3.0000000D+01
htas1 used a total of 1633 elements in the character-array which required a total
of 13k bytes of core.  the core requirements for the htas1 portion of the
analysis could be reduced by 768k bytes.

*************************************************************************************
* exit from control module htas1    and direct scale to execute heating7 (htng72  ). *
*************************************************************************************

*********************************************
* control module htas1    has been accessed. *
*********************************************
htas1 will generate heating input data for the final ss     thermal analysis.
      title:  htas1 sample problem 1                                  -- postfire tr
      number of nodes read:        654       number of nodes written:        654
  time found in plot data set:    0.0000000D+00
  time found in plot data set:    5.0000000D+00
  time found in plot data set:    1.0000000D+01
  time found in plot data set:    1.5000000D+01
  time found in plot data set:    2.0000000D+01
  time found in plot data set:    2.5000000D+01
  time found in plot data set:    3.0000000D+01
  time found in plot data set:    3.5000000D+01
  time found in plot data set:    4.0000000D+01
  time found in plot data set:    4.5000000D+01
  time found in plot data set:    5.0000000D+01
  time found in plot data set:    5.5000000D+01
  time found in plot data set:    6.0000000D+01
  time found in plot data set:    6.5000000D+01
  time found in plot data set:    7.0000000D+01
  time found in plot data set:    7.5000000D+01
  time found in plot data set:    8.0000000D+01
  time found in plot data set:    8.5000000D+01
  time found in plot data set:    9.0000000D+01
```

Table H1.5.2 (continued)

```
 time found in plot data set:    9.5000000D+01
 time found in plot data set:    1.0000000D+02
 time found in plot data set:    1.0500000D+02
 time found in plot data set:    1.1000000D+02
 time found in plot data set:    1.1500000D+02
 time found in plot data set:    1.2000000D+02
 time found in plot data set:    1.2500000D+02
 time found in plot data set:    1.3000000D+02
 time found in plot data set:    1.3500000D+02
 time found in plot data set:    1.4000000D+02
 time found in plot data set:    1.4500000D+02
 time found in plot data set:    1.5000000D+02
 time found in plot data set:    1.5500000D+02
 time found in plot data set:    1.6000000D+02
 time found in plot data set:    1.6500000D+02
 time found in plot data set:    1.7000000D+02
 time found in plot data set:    1.7500000D+02
 time found in plot data set:    1.8000000D+02
 time found in plot data set:    1.8500000D+02
 time found in plot data set:    1.9000000D+02
 time found in plot data set:    1.9500000D+02
 time found in plot data set:    2.0000000D+02
 time found in plot data set:    2.0500000D+02
 time found in plot data set:    2.1000000D+02
htas1 used a total of 1601 elements in the character-array which required a total
of 13k bytes of core.  the core requirements for the htas1 portion of the
analysis could be reduced by 768k bytes.

*********************************************************************************************
* exit from control module htas1    and direct scale to execute heating7 (htng72  ). *
*********************************************************************************************
**********************************************
* control module htas1    has been accessed. *
**********************************************

*****************************************************
* the temperature plotting option has been invoked *
* this version does not generate plots             *
* but reports out the plot data                    *
*****************************************************

plots will include temperature distributions from the fire transient and postfire
transient heating calculations

temperature vs. time curves for the inner shell, shielding, and outer shell will be
generated on one plot

temperature distributions at every printout time will be used

a plot will be generated showing a curve of maximum temperature at any time
at each center axial node vs. the r distance from the origin

a plot will be generated showing a curve of the difference in the volume averaged
temperatures of the inner shell and the outer shell

      title:  htas1 sample problem 1                                    -- final ss
      number of nodes read for ploting:         654
    43 time steps read from plot dataset

   start time 0.00000E+00 end time  210.00
     maximum temperatures as a function of time:
   time (min)     inner shell     shield     outer shell
     0.00000E+00    264.56        255.67       246.28
      5.0000        264.59        255.86       251.44
      10.000        266.43        260.27       277.22
      15.000        275.26        273.74       313.13
      20.000        292.70        295.38       351.42
```

Table H1.5.2 (continued)

25.000	316.91	322.56	389.19
30.000	345.46	352.99	425.91
35.000	376.51	385.05	457.12
40.000	407.53	414.70	470.97
45.000	433.93	437.59	475.59
50.000	453.74	453.77	476.74
55.000	467.61	464.68	476.40
60.000	476.88	471.73	475.32
65.000	482.79	476.03	473.80
70.000	486.27	478.36	472.02
75.000	488.04	479.31	470.07
80.000	488.59	479.28	468.01
85.000	488.28	478.57	465.88
90.000	487.37	477.39	463.71
95.000	486.05	475.87	461.52
100.00	484.44	474.13	459.33
105.00	482.64	472.24	457.13
110.00	480.70	470.24	454.95
115.00	478.67	468.19	452.78
120.00	476.60	466.09	450.63
125.00	474.49	463.98	448.49
130.00	472.37	461.86	446.38
135.00	470.25	459.74	444.28
140.00	468.13	457.63	442.21
145.00	466.02	455.53	440.16
150.00	463.93	453.45	438.13
155.00	461.85	451.39	436.12
160.00	459.79	449.34	434.14
165.00	457.75	447.32	432.18
170.00	455.73	445.32	430.23
175.00	453.73	443.34	428.31
180.00	451.76	441.37	426.42
185.00	449.80	439.43	424.54
190.00	447.87	437.52	422.68
195.00	445.95	435.62	420.84
200.00	444.06	433.74	419.02
205.00	442.19	431.88	417.23
210.00	240.57	231.73	222.40

maximum temperature vs. radius on axial center plane
from 0.00000E+00 to 210.00 minutes

radius	temperature
6.7500	488.59
7.0600	486.58
8.3860	482.65
9.7120	479.31
11.038	476.74
12.364	474.86
13.690	474.15
14.315	476.74
14.940	488.53
16.065	504.87
17.190	525.55
18.315	573.08
19.440	630.75
19.600	652.47

title: htas1 sample problem 1 -- final ss
number of nodes read for ploting: 654
43 time steps read from plot dataset
start time 0.00000E+00 end time 210.00
difference between inner and outer shield
volume-averaged temperatures

time (min)	temperature
0.00000E+00	13.245
5.0000	9.1623
10.000	-7.3223
15.000	-23.939
20.000	-34.294
25.000	-38.268

Table H1.5.2 (continued)

```
      30.000     -37.827
      35.000     -31.263
      40.000     -13.266
      45.000      6.3346
      50.000      22.145
      55.000      33.530
      60.000      41.262
      65.000      46.270
      70.000      49.323
      75.000      50.998
      80.000      51.715
      85.000      51.773
      90.000      51.384
      95.000      50.699
      100.00      49.822
      105.00      48.826
      110.00      47.763
      115.00      46.668
      120.00      45.565
      125.00      44.470
      130.00      43.394
      135.00      42.343
      140.00      41.321
      145.00      40.330
      150.00      39.372
      155.00      38.447
      160.00      37.554
      165.00      36.694
      170.00      35.864
      175.00      35.063
      180.00      34.292
      185.00      33.548
      190.00      32.830
      195.00      32.137
      200.00      31.468
      205.00      30.821
      210.00      13.058
*******************************************************************************
* exit from control module htas1    and direct scale to terminate this run. *
* control module htas1    was successfully accessed    8 times.             *
*******************************************************************************
```

Table H1.5.3 Temperature distribution at the prefire steady state

htas1 sample problem 1 -- prefire ss Fri Jun 11 15:43:44 1993

Steady-State Temperature Distribution at Time 0.0000E+00

31	248.50	102.44	102.43	102.42	102.39	102.36	102.32	102.31	102.25	102.19	102.12	102.04	101.96	101.92	101.87
30	243.00	122.59	122.54	122.39	122.15	121.81	121.37	121.26	120.73	120.10	119.40	118.63	117.79	117.38	116.95
29	237.50	146.01	145.91	145.62	145.12	144.43	143.55	143.32	142.22	140.93	139.48	137.85	136.07	135.19	134.27
28	232.00	176.00	175.85	175.39	174.63	173.56	172.18	171.81	170.07	168.00	165.60	162.86	159.78	158.21	156.57
27	226.50	216.05	215.86	215.28	214.32	212.99	211.27	210.82	208.65	206.04	202.91	199.15	194.56	192.02	189.20
26	221.00	268.92	268.65	267.86	266.64	265.08	263.35	262.96	261.27	259.71	258.36	257.28	256.46	256.15	255.86
25	219.19	270.00	269.70	268.83	267.46	265.71	263.78	263.34	261.48	259.80	258.36	257.22	256.45	256.23	256.11
24	217.38	273.23	272.84	271.71	269.88	267.51	264.86	264.28	261.90	259.82	258.07	256.70	255.76	255.50	255.39
23	215.56	279.22	278.71	277.16	274.56	270.94	266.61	265.72	262.41	259.70	257.44	255.58	254.17	253.72	253.52
22	213.75	288.91	288.29	286.39	282.95	277.42	268.59	266.82	262.69	259.38	256.52	253.97	251.60	250.00	248.90
21	213.50	290.59	289.98	288.06	284.61	279.03	268.85	266.63	262.69	259.36	256.46	253.88	251.51	249.20	246.85
20	195.70						265.98	263.89	260.21	257.07	254.33	251.89	249.69	247.58	245.56
19	177.90						265.18	263.08	259.42	256.29	253.56	251.14	248.97	246.88	244.87
18	160.10						264.79	262.70	259.03	255.91	253.18	250.76	248.59	246.51	244.51
17	142.30						264.61	262.52	258.85	255.73	253.00	250.59	248.42	246.33	244.34
16	124.50						264.56	262.46	258.80	255.67	252.95	250.53	248.37	246.28	244.29
15	106.70						264.61	262.52	258.85	255.72	253.00	250.58	248.42	246.33	244.34
14	88.90						264.79	262.69	259.03	255.90	253.17	250.76	248.59	246.50	244.51
13	71.10						265.16	263.07	259.40	256.27	253.55	251.13	248.95	246.86	244.86
12	53.30						265.95	263.86	260.19	257.05	254.30	251.86	249.67	247.56	245.53
11	35.50	290.15	289.54	287.65	284.24	278.74	268.77	266.56	262.62	259.30	256.41	253.83	251.46	249.16	246.82
10	35.25	288.47	287.86	285.97	282.58	277.12	268.48	266.74	262.62	259.32	256.46	253.92	251.55	249.97	248.90
9	33.31	278.23	277.74	276.26	273.78	270.34	266.26	265.41	262.24	259.63	257.44	255.65	254.30	253.88	253.69
8	31.38	272.05	271.70	270.65	268.98	266.81	264.39	263.85	261.65	259.72	258.09	256.81	255.94	255.70	255.59
7	29.44	268.78	268.52	267.74	266.52	264.97	263.25	262.86	261.19	259.67	258.36	257.33	256.62	256.42	256.31
6	27.50	267.69	267.46	266.77	265.69	264.33	262.81	262.46	260.96	259.57	258.36	257.37	256.62	256.33	256.05
5	22.00	215.71	215.52	214.97	214.06	212.77	211.11	210.68	208.57	206.02	202.95	199.23	194.68	192.16	189.37
4	16.50	175.93	175.78	175.33	174.59	173.54	172.17	171.82	170.09	168.05	165.68	162.96	159.90	158.34	156.71
3	11.00	146.02	145.93	145.63	145.14	144.46	143.58	143.35	142.26	140.99	139.54	137.93	136.16	135.28	134.37
2	5.50	122.61	122.56	122.42	122.17	121.84	121.40	121.29	120.76	120.14	119.45	118.68	117.84	117.43	117.00
1	.00	102.44	102.43	102.42	102.40	102.36	102.32	102.31	102.26	102.19	102.12	102.05	101.96	101.92	101.88
		.00	1.35	2.70	4.05	5.40	6.75	7.06	8.39	9.71	11.04	12.36	13.69	14.32	14.94
		1	2	3	4	5	6	7	8	9	10	11	12	13	14

Table H1.5.3 (continued)

htas1 sample problem 1 -- prefire ss Fri Jun 11 15:43:44 1993

Steady-State Temperature Distribution at Time 0.0000E+00

31	248.50	101.79	101.71	101.62	101.53	101.52	101.20	100.88	100.59	100.31	100.05
30	243.00	116.15	115.33	114.48	113.61	113.49	110.43	107.50	104.85	102.49	100.40
29	237.50	132.57	130.79	128.97	127.12	126.85	120.37	114.38	109.14	104.64	100.72
28	232.00	153.47	150.21	146.85	143.46	142.98	131.38	121.35	113.17	106.54	101.00
27	226.50	183.35	177.03	170.57	164.18	163.29	142.83	127.20	115.90	107.64	101.15
26	221.00	234.55	217.06	202.10	188.84	187.06	150.59	128.16	114.99	106.82	101.02
25	219.19	238.46	222.60	208.07	194.38	192.48	149.12	125.51	113.07	105.84	100.88
24	217.38	240.80	227.26	214.09	200.58	198.58	144.54	120.97	110.28	104.51	100.69
23	215.56	242.96	233.23	223.15	211.20	209.17	134.70	114.17	106.64	102.88	100.45
22	213.75	244.79	241.80	238.79	234.35	232.91	114.81	104.95	102.32	101.03	100.17
21	213.50	244.87	243.02	241.29	239.66	239.17	110.40	103.57	101.71	100.77	100.13
20	195.70	243.98	242.50	241.11	239.81	239.42					
19	177.90	243.31	241.85	240.48	239.18	238.79					
18	160.10	242.95	241.49	240.12	238.83	238.44					
17	142.30	242.78	241.32	239.95	238.66	238.28					
16	124.50	242.73	241.27	239.90	238.61	238.23					
15	106.70	242.78	241.32	239.95	238.66	238.27					
14	88.90	242.95	241.49	240.11	238.82	238.44					
13	71.10	243.30	241.84	240.46	239.17	238.78					
12	53.30	243.95	242.48	241.09	239.79	239.40					
11	35.50	244.84	242.99	241.25	239.62	239.14	110.50	103.61	101.73	100.79	100.13
10	35.25	244.78	241.80	238.80	234.31	232.86	114.97	105.00	102.36	101.05	100.17
9	33.31	242.93	232.96	222.65	210.56	208.54	135.91	114.91	107.03	103.06	100.47
8	31.38	240.84	227.13	213.83	200.31	198.33	145.91	122.06	110.92	104.82	100.73
7	29.44	238.63	222.69	208.13	194.49	192.60	150.36	126.65	113.82	106.21	100.94
6	27.50	234.70	217.18	202.23	189.04	187.28	151.55	129.18	115.72	107.20	101.08
5	22.00	183.54	177.25	170.82	164.48	163.59	143.31	127.70	116.29	107.86	101.18
4	16.50	153.62	150.38	147.05	143.67	143.19	131.64	121.61	113.37	106.66	101.01
3	11.00	132.67	130.91	129.09	127.25	126.98	120.51	114.52	109.25	104.70	100.73
2	5.50	116.21	115.38	114.54	113.68	113.55	110.49	107.56	104.90	102.52	100.41
1	.00	101.80	101.71	101.63	101.54	101.52	101.20	100.89	100.59	100.31	100.05
		16.07	17.19	18.32	19.44	19.60	23.48	27.36	31.24	35.12	39.00
		15	16	17	18	19	20	21	22	23	24

Table H1.5.4 Temperature distribution at the end of the 30-minute fire

htas1 sample problem 1 -- fire tr Fri Jun 11 15:43:53 1993

Transient Temperature Distribution at Time 3.0000E+01

31	248.50	1465.67	1465.67	1465.67	1465.67	1465.67	1465.67	1465.67	1465.66	1465.66	1465.66	1465.66	1465.65	1465.65	1465.65
30	243.00	133.29	133.24	133.09	132.84	132.50	132.07	131.96	131.42	130.80	130.10	129.33	128.49	128.07	127.65
29	237.50	146.06	145.96	145.66	145.17	144.48	143.59	143.36	142.26	140.98	139.52	137.90	136.12	135.23	134.32
28	232.00	176.00	175.85	175.39	174.63	173.56	172.18	171.81	170.07	168.00	165.60	162.86	159.78	158.21	156.57
27	226.50	216.05	215.86	215.28	214.32	212.99	211.27	210.82	208.65	206.04	202.92	199.15	194.57	192.03	189.21
26	221.00	269.06	268.83	268.14	267.09	265.82	264.49	264.19	263.00	262.05	261.38	260.92	260.45	260.07	259.51
25	219.19	270.32	270.09	269.43	268.46	267.35	266.28	266.06	265.22	264.73	264.65	264.86	265.04	264.96	264.76
24	217.38	273.97	273.75	273.18	272.47	271.95	271.83	271.84	272.04	272.94	274.71	277.14	279.44	279.92	279.80
23	215.56	280.64	280.50	280.22	280.36	281.85	285.30	285.99	288.51	292.40	298.45	306.54	315.50	318.78	319.84
22	213.75	290.89	290.85	291.06	292.77	299.09	316.81	319.59	324.23	332.76	346.43	365.74	391.27	412.30	429.93
21	213.50	292.58	292.55	292.76	294.49	300.98	324.83	324.15	327.56	336.39	350.65	370.82	397.76	431.50	474.01
20	195.70						346.49	345.25	347.21	354.12	365.61	381.57	402.03	427.76	460.21
19	177.90						346.06	344.81	346.76	353.58	364.93	380.70	400.93	426.46	458.72
18	160.10						345.69	344.44	346.39	353.21	364.56	380.33	400.57	426.11	458.38
17	142.30						345.52	344.27	346.22	353.04	364.39	380.17	400.41	425.96	458.23
16	124.50						345.46	344.22	346.16	352.99	364.34	380.12	400.36	425.91	458.19
15	106.70						345.51	344.27	346.21	353.03	364.39	380.17	400.41	425.96	458.23
14	88.90						345.68	344.44	346.38	353.20	364.55	380.33	400.57	426.11	458.38
13	71.10						346.04	344.80	346.74	353.56	364.91	380.69	400.92	426.45	458.71
12	53.30						346.46	345.21	347.18	354.08	365.58	381.54	402.00	427.73	460.19
11	35.50	292.17	292.15	292.41	294.22	300.78	324.50	323.83	327.27	336.12	350.40	370.58	397.53	431.25	473.77
10	35.25	290.48	290.46	290.70	292.49	298.88	316.43	319.22	323.92	332.49	346.18	365.51	391.09	411.89	429.07
9	33.31	279.61	279.47	279.19	279.30	280.63	283.74	284.37	286.72	290.39	296.07	303.64	311.93	314.88	315.78
8	31.38	272.72	272.51	271.96	271.26	270.69	270.46	270.44	270.51	271.21	272.68	274.72	276.63	277.00	276.87
7	29.44	269.04	268.83	268.23	267.33	266.29	265.25	265.03	264.19	263.63	263.42	263.47	263.51	263.42	263.23
6	27.50	267.80	267.59	266.97	266.03	264.88	263.65	263.37	262.25	261.30	260.60	260.07	259.57	259.22	258.75
5	22.00	215.71	215.52	214.97	214.06	212.77	211.12	210.68	208.57	206.02	202.95	199.23	194.69	192.17	189.37
4	16.50	175.93	175.78	175.33	174.59	173.54	172.17	171.82	170.09	168.05	165.68	162.96	159.90	158.34	156.71
3	11.00	146.07	145.97	145.68	145.19	144.50	143.63	143.40	142.31	141.04	139.59	137.98	136.21	135.33	134.42
2	5.50	133.31	133.26	133.11	132.87	132.53	132.10	131.99	131.45	130.84	130.14	129.37	128.54	128.12	127.70
1	.00	1465.67	1465.67	1465.67	1465.67	1465.67	1465.67	1465.67	1465.66	1465.66	1465.66	1465.66	1465.65	1465.65	1465.65
		.00	1.35	2.70	4.05	5.40	6.75	7.06	8.39	9.71	11.04	12.36	13.69	14.32	14.94
		1	2	3	4	5	6	7	8	9	10	11	12	13	14

Table H1.5.4 (continued)

htas1 sample problem 1 -- fire tr Fri Jun 11 15:43:53 1993

Transient Temperature Distribution at Time 3.0000E+01

31	248.50	1465.65	1465.64	1465.64	1465.64	1465.63	1465.62	1465.61	1465.60	1465.78	1474.96
30	243.00	126.85	126.02	125.18	124.31	124.19	121.13	118.21	115.79	137.78	1469.53
29	237.50	132.61	130.84	129.01	127.16	126.90	120.41	114.43	109.42	129.45	1469.49
28	232.00	153.47	150.21	146.85	143.46	142.98	131.38	121.35	113.40	131.30	1469.50
27	226.50	183.35	177.03	170.57	164.18	163.29	142.83	127.20	116.14	132.40	1469.50
26	221.00	234.70	217.06	202.10	188.84	187.06	150.59	128.16	115.22	131.58	1469.50
25	219.19	238.90	222.62	208.07	194.39	192.49	149.15	125.55	113.34	130.64	1469.50
24	217.38	242.36	227.46	214.28	200.87	198.90	146.10	122.57	112.11	130.85	1469.50
23	215.56	251.21	238.47	230.08	221.26	219.97	181.14	161.27	154.03	174.01	1469.67
22	213.75	362.90	382.60	417.28	467.19	479.88	979.70	978.97	977.62	985.87	1472.99
21	213.50	512.74	560.69	618.99	688.01	713.23	1444.40	1444.43	1444.35	1444.86	1474.88
20	195.70	489.44	527.80	575.39	633.08	654.76					
19	177.90	487.80	526.04	573.56	631.23	652.94					
18	160.10	487.47	525.73	573.25	630.93	652.64					
17	142.30	487.32	525.59	573.12	630.79	652.51					
16	124.50	487.28	525.55	573.08	630.75	652.47					
15	106.70	487.32	525.58	573.11	630.79	652.51					
14	88.90	487.46	525.72	573.25	630.92	652.63					
13	71.10	487.79	526.03	573.55	631.22	652.93					
12	53.30	489.41	527.78	575.37	633.06	654.74					
11	35.50	512.54	560.50	618.80	687.82	713.04	1443.03	1443.05	1442.96	1443.50	1474.87
10	35.25	359.20	377.87	411.56	460.19	472.50	957.79	956.84	955.45	964.08	1472.91
9	33.31	250.29	237.42	228.53	219.10	217.70	175.44	155.01	147.41	167.29	1469.65
8	31.38	242.17	227.28	213.97	200.53	198.57	147.08	123.25	112.34	130.75	1469.50
7	29.44	238.97	222.71	208.13	194.49	192.61	150.39	126.68	114.08	131.00	1469.50
6	27.50	234.81	217.18	202.23	189.04	187.28	151.55	129.18	115.96	131.96	1469.50
5	22.00	183.54	177.25	170.82	164.48	163.59	143.31	127.70	116.53	132.61	1469.51
4	16.50	153.62	150.38	147.05	143.67	143.19	131.64	121.61	113.61	131.42	1469.50
3	11.00	132.72	130.95	129.14	127.29	127.03	120.56	114.56	109.52	129.51	1469.49
2	5.50	126.91	126.08	125.24	124.37	124.25	121.19	118.27	115.83	137.81	1469.53
1	.00	1465.65	1465.64	1465.64	1465.64	1465.64	1465.62	1465.61	1465.60	1465.78	1474.96
		16.07	17.19	18.32	19.44	19.60	23.48	27.36	31.24	35.12	39.00
		15	16	17	18	19	20	21	22	23	24

Table H1.5.5 Temperature distribution at the end of the three-hour, cool-down transient

htas1 sample problem 1 -- postfire tr Fri Jun 11 15:44:17 1993

Transient Temperature Distribution at Time 2.1000E+02

31	248.50	137.91	137.91	137.90	137.90	137.88	137.86	137.86	137.84	137.82	137.79	137.76	137.72	137.71	137.69
30	243.00	144.26	144.21	144.06	143.82	143.48	143.05	142.94	142.40	141.79	141.09	140.32	139.48	139.07	138.65
29	237.50	147.22	147.12	146.83	146.33	145.64	144.76	144.53	143.43	142.14	140.69	139.06	137.28	136.40	135.48
28	232.00	176.11	175.96	175.51	174.76	173.69	172.32	171.95	170.21	168.15	165.76	163.02	159.92	158.35	156.70
27	226.50	220.10	219.94	219.45	218.63	217.47	215.93	215.52	213.51	211.04	208.01	204.26	199.48	196.62	193.26
26	221.00	390.94	390.87	390.67	390.30	389.75	389.03	388.84	387.93	386.89	385.73	384.45	382.96	382.07	380.96
25	219.19	393.21	393.12	392.84	392.36	391.65	390.74	390.50	389.41	388.22	386.96	385.71	384.54	384.07	383.71
24	217.38	398.15	398.01	397.58	396.83	395.72	394.29	393.94	392.34	390.70	389.09	387.58	386.31	385.88	385.59
23	215.56	405.78	405.58	404.93	403.75	401.90	399.35	398.75	396.20	393.74	391.40	389.20	387.29	386.61	386.26
22	213.75	416.24	415.99	415.16	413.54	410.64	405.50	404.16	400.15	396.56	393.17	389.85	386.40	383.92	382.18
21	213.50	417.92	417.67	416.84	415.21	412.29	406.57	404.43	400.38	396.71	393.25	389.87	386.44	382.97	379.19
20	195.70						429.90	427.79	423.59	419.75	416.14	412.68	409.31	405.93	402.26
19	177.90						438.57	436.47	432.23	428.31	424.60	421.01	417.49	413.97	410.17
18	160.10						440.20	438.10	433.86	429.92	426.17	422.53	418.95	415.37	411.53
17	142.30						440.35	438.25	434.00	430.06	426.30	422.66	419.06	415.47	411.62
16	124.50						440.34	438.23	433.99	430.05	426.29	422.64	419.05	415.45	411.60
15	106.70						440.35	438.24	434.00	430.06	426.30	422.65	419.06	415.47	411.62
14	88.90						440.19	438.09	433.84	429.91	426.16	422.52	418.94	415.36	411.52
13	71.10						438.51	436.40	432.16	428.25	424.54	420.96	417.44	413.92	410.12
12	53.30						429.51	427.40	423.20	419.37	415.77	412.33	408.98	405.61	401.97
11	35.50	413.45	413.24	412.58	411.25	408.84	404.16	402.05	398.08	394.51	391.17	387.91	384.63	381.31	377.70
10	35.25	411.76	411.56	410.90	409.57	407.17	402.88	401.67	397.78	394.30	391.02	387.82	384.50	382.12	380.49
9	33.31	400.39	400.23	399.73	398.79	397.29	395.19	394.67	392.39	390.15	387.98	385.96	384.20	383.59	383.26
8	31.38	391.90	391.80	391.49	390.92	390.06	388.92	388.63	387.29	385.87	384.44	383.10	381.96	381.56	381.27
7	29.44	386.33	386.26	386.07	385.73	385.22	384.52	384.34	383.46	382.46	381.39	380.28	379.21	378.78	378.43
6	27.50	383.76	383.72	383.59	383.34	382.96	382.43	382.28	381.57	380.71	379.71	378.56	377.15	376.29	375.23
5	22.00	219.46	219.31	218.83	218.04	216.90	215.40	215.00	213.04	210.61	207.62	203.91	199.19	196.39	193.08
4	16.50	176.04	175.89	175.45	174.70	173.66	172.30	171.94	170.23	168.19	165.82	163.10	160.03	158.47	156.83
3	11.00	147.23	147.13	146.84	146.35	145.67	144.79	144.56	143.47	142.20	140.76	139.14	137.37	136.49	135.58
2	5.50	144.28	144.23	144.09	143.84	143.51	143.08	142.97	142.44	141.82	141.13	140.36	139.53	139.12	138.70
1	.00	137.91	137.91	137.91	137.90	137.88	137.87	137.86	137.84	137.82	137.79	137.76	137.73	137.71	137.69
		.00	1.35	2.70	4.05	5.40	6.75	7.06	8.39	9.71	11.04	12.36	13.69	14.32	14.94
		1	2	3	4	5	6	7	8	9	10	11	12	13	14

Table H1.5.5 (continued)

htas1 sample problem 1 -- postfire tr Fri Jun 11 15:44:17 1993

Transient Temperature Distribution at Time 2.1000E+02

31	248.50	137.66	137.63	137.60	137.56	137.56	137.44	137.33	137.28	136.15	106.75
30	243.00	137.85	137.03	136.19	135.33	135.20	132.17	129.53	130.79	156.59	118.45
29	237.50	133.78	132.00	130.18	128.33	128.06	121.59	115.89	114.93	142.33	117.85
28	232.00	153.55	150.26	146.89	143.50	143.02	131.43	121.69	117.79	143.23	117.92
27	226.50	185.48	177.86	170.83	164.24	163.33	142.86	127.52	120.51	144.29	117.99
26	221.00	289.83	236.69	207.97	190.29	188.07	151.38	129.27	120.38	144.16	117.97
25	219.19	299.80	247.48	218.17	199.75	197.42	156.39	133.53	125.33	149.04	118.25
24	217.38	314.03	266.63	239.23	221.72	219.44	174.06	152.52	145.85	166.99	119.12
23	215.56	342.75	310.64	290.91	276.80	274.61	202.83	185.93	181.64	194.08	118.98
22	213.75	376.66	370.21	364.28	356.21	353.54	144.60	135.83	134.68	136.80	107.36
21	213.50	376.18	372.84	369.19	365.21	363.69	127.01	121.90	121.25	122.43	104.81
20	195.70	399.56	396.56	393.27	389.71	388.31					
19	177.90	407.36	404.25	400.85	397.18	395.72					
18	160.10	408.69	405.55	402.12	398.42	396.96					
17	142.30	408.78	405.64	402.20	398.50	397.04					
16	124.50	408.76	405.62	402.19	398.48	397.02					
15	106.70	408.78	405.63	402.20	398.50	397.03					
14	88.90	408.68	405.54	402.11	398.41	396.95					
13	71.10	407.31	404.20	400.80	397.13	395.68					
12	53.30	399.27	396.28	393.00	389.44	388.04					
11	35.50	374.79	371.53	367.94	364.00	362.49	127.85	122.74	122.08	123.13	104.90
10	35.25	375.71	369.59	363.78	355.64	352.98	146.04	137.23	136.06	137.96	107.49
9	33.31	338.83	306.18	286.10	271.86	269.70	202.04	184.67	180.12	193.26	119.17
8	31.38	309.72	262.83	235.66	218.16	215.88	171.17	149.12	142.05	163.67	118.97
7	29.44	295.84	245.17	216.75	198.69	196.39	155.84	132.77	124.18	147.80	118.18
6	27.50	286.06	235.00	207.42	190.24	188.08	152.09	130.03	120.86	144.32	117.98
5	22.00	185.47	177.99	171.05	164.52	163.62	143.33	128.01	120.89	144.50	118.00
4	16.50	153.70	150.44	147.09	143.71	143.23	131.69	121.95	118.00	143.34	117.92
3	11.00	133.88	132.12	130.30	128.46	128.19	121.74	116.03	115.03	142.39	117.85
2	5.50	137.91	137.09	136.25	135.39	135.27	132.24	129.59	130.84	156.61	118.45
1	.00	137.66	137.63	137.60	137.56	137.56	137.44	137.33	137.28	136.15	106.75
		16.07	17.19	18.32	19.44	19.60	23.48	27.36	31.24	35.12	39.00
		15	16	17	18	19	20	21	22	23	24

Table H1.5.6 Temperature distribution at the final steady state

htas1 sample problem 1 -- final ss Fri Jun 11 15:45:06 1993

Steady-State Temperature Distribution at Time 2.1000E+02

31	248.50	101.52	101.52	101.51	101.49	101.47	101.44	101.44	101.40	101.36	101.32	101.26	101.21	101.18	101.15
30	243.00	118.82	118.78	118.66	118.45	118.16	117.79	117.70	117.24	116.72	116.13	115.47	114.77	114.42	114.06
29	237.50	138.89	138.81	138.55	138.13	137.53	136.77	136.58	135.63	134.53	133.28	131.89	130.37	129.62	128.84
28	232.00	164.62	164.49	164.09	163.43	162.49	161.29	160.97	159.46	157.67	155.60	153.24	150.59	149.24	147.84
27	226.50	199.15	198.98	198.45	197.58	196.38	194.84	194.44	192.51	190.21	187.48	184.20	180.23	178.04	175.62
26	221.00	245.33	245.07	244.28	243.06	241.51	239.79	239.40	237.72	236.18	234.85	233.79	233.01	232.73	232.48
25	219.19	246.40	246.10	245.23	243.86	242.12	240.19	239.76	237.91	236.24	234.82	233.71	232.96	232.75	232.64
24	217.38	249.61	249.23	248.09	246.27	243.90	241.25	240.67	238.30	236.23	234.50	233.14	232.22	231.97	231.86
23	215.56	255.59	255.08	253.53	250.92	247.29	242.96	242.07	238.77	236.08	233.83	231.99	230.58	230.14	229.94
22	213.75	265.27	264.66	262.74	259.30	253.75	244.88	243.11	239.00	235.71	232.87	230.33	227.98	226.38	225.28
21	213.50	266.96	266.34	264.42	260.96	255.36	245.13	242.91	239.00	235.69	232.81	230.24	227.88	225.57	223.22
20	195.70						242.07	239.98	236.33	233.21	230.49	228.07	225.88	223.77	221.74
19	177.90						241.20	239.11	235.47	232.36	229.65	227.25	225.09	223.00	221.00
18	160.10						240.80	238.71	235.07	231.97	229.26	226.86	224.71	222.62	220.63
17	142.30						240.62	238.53	234.89	231.79	229.08	226.69	224.53	222.45	220.45
16	124.50						240.57	238.47	234.84	231.73	229.03	226.63	224.48	222.40	220.40
15	106.70						240.62	238.52	234.89	231.78	229.08	226.68	224.53	222.45	220.45
14	88.90						240.80	238.70	235.06	231.96	229.26	226.86	224.71	222.62	220.62
13	71.10						241.19	239.10	235.46	232.35	229.64	227.24	225.08	222.99	220.99
12	53.30						242.05	239.96	236.31	233.19	230.47	228.05	225.87	223.75	221.72
11	35.50	266.53	265.92	264.02	260.60	255.08	245.06	242.85	238.94	235.63	232.76	230.20	227.84	225.54	223.20
10	35.25	264.84	264.23	262.34	258.94	253.46	244.78	243.04	238.94	235.65	232.82	230.29	227.94	226.36	225.28
9	33.31	254.62	254.13	252.64	250.16	246.71	242.63	241.78	238.62	236.01	233.84	232.07	230.73	230.31	230.13
8	31.38	248.45	248.10	247.06	245.38	243.21	240.80	240.26	238.07	236.15	234.53	233.27	232.41	232.19	232.08
7	29.44	245.20	244.94	244.16	242.95	241.40	239.69	239.30	237.64	236.13	234.85	233.84	233.15	232.96	232.86
6	27.50	244.13	243.90	243.21	242.14	240.78	239.26	238.92	237.43	236.05	234.86	233.91	233.19	232.93	232.68
5	22.00	198.82	198.65	198.15	197.33	196.18	194.70	194.31	192.44	190.20	187.52	184.29	180.36	178.19	175.78
4	16.50	164.55	164.42	164.03	163.38	162.47	161.29	160.98	159.49	157.72	155.67	153.33	150.70	149.37	147.97
3	11.00	138.90	138.82	138.57	138.15	137.56	136.81	136.61	135.68	134.59	133.35	131.97	130.46	129.71	128.93
2	5.50	118.84	118.80	118.68	118.47	118.18	117.82	117.72	117.27	116.75	116.17	115.52	114.81	114.46	114.10
1	.00	101.52	101.52	101.51	101.50	101.47	101.45	101.44	101.40	101.36	101.32	101.27	101.21	101.19	101.16
		.00	1.35	2.70	4.05	5.40	6.75	7.06	8.39	9.71	11.04	12.36	13.69	14.32	14.94
		1	2	3	4	5	6	7	8	9	10	11	12	13	14

Table H1.5.6 (continued)

htas1 sample problem 1 -- final ss Fri Jun 11 15:45:06 1993

Steady-State Temperature Distribution at Time 2.1000E+02

31	248.50	101.10	101.05	100.99	100.94	100.93	100.72	100.53	100.34	100.18	100.02
30	243.00	113.38	112.69	111.98	111.25	111.15	108.58	106.14	103.93	101.97	100.23
29	237.50	127.38	125.87	124.32	122.74	122.52	117.01	111.94	107.52	103.73	100.42
28	232.00	145.17	142.38	139.51	136.62	136.21	126.32	117.81	110.88	105.29	100.59
27	226.50	170.58	165.15	159.62	154.15	153.38	135.94	122.68	113.14	106.17	100.68
26	221.00	214.12	199.07	186.20	174.83	173.31	142.25	123.32	112.28	105.46	100.60
25	219.19	217.32	203.58	191.04	179.28	177.65	140.80	120.99	110.63	104.64	100.52
24	217.38	219.04	207.20	195.78	184.15	182.44	136.66	117.06	108.26	103.54	100.40
23	215.56	220.42	211.75	202.90	192.57	190.83	127.99	111.22	105.17	102.18	100.25
22	213.75	221.21	218.27	215.38	211.32	210.06	110.70	103.38	101.54	100.66	100.08
21	213.50	221.14	219.20	217.39	215.68	215.19	106.89	102.22	101.03	100.45	100.05
20	195.70	220.09	218.53	217.08	215.70	215.32					
19	177.90	219.36	217.83	216.39	215.02	214.64					
18	160.10	218.99	217.46	216.02	214.66	214.28					
17	142.30	218.82	217.29	215.85	214.50	214.12					
16	124.50	218.77	217.24	215.81	214.45	214.07					
15	106.70	218.82	217.29	215.85	214.50	214.11					
14	88.90	218.99	217.46	216.02	214.66	214.28					
13	71.10	219.35	217.82	216.38	215.01	214.63					
12	53.30	220.07	218.52	217.06	215.69	215.30					
11	35.50	221.12	219.18	217.36	215.65	215.17	106.97	102.24	101.04	100.45	100.05
10	35.25	221.21	218.28	215.39	211.28	210.02	110.82	103.42	101.57	100.67	100.08
9	33.31	220.44	211.58	202.53	192.08	190.34	129.04	111.85	105.50	102.33	100.26
8	31.38	219.13	207.16	195.63	183.99	182.29	137.87	117.99	108.80	103.79	100.42
7	29.44	217.52	203.73	191.16	179.44	177.83	141.91	121.98	111.27	104.95	100.55
6	27.50	214.31	199.23	186.38	175.07	173.56	143.11	124.21	112.91	105.78	100.64
5	22.00	170.77	165.37	159.86	154.43	153.67	136.37	123.12	113.47	106.35	100.70
4	16.50	145.32	142.55	139.69	136.81	136.40	126.56	118.04	111.06	105.38	100.60
3	11.00	127.48	125.98	124.43	122.86	122.64	117.14	112.06	107.61	103.78	100.43
2	5.50	113.44	112.74	112.03	111.31	111.20	108.64	106.19	103.97	101.99	100.23
1	.00	101.11	101.05	101.00	100.94	100.93	100.73	100.53	100.35	100.18	100.02

16.07	17.19	18.32	19.44	19.60	23.48	27.36	31.24	35.12	39.00
15	16	17	18	19	20	21	22	23	24

The second sample problem is designed to demonstrate the use of some of the more useful options in HTAS1. It is the same as the first sample problem with the following changes. The inner shell is composed of carbon steel (1.5%), with thermal properties as presented in Table H1.5.7. The outer shell is composed of stainless steel 347. Its material properties are for material number 3135 from the LLNL material property library (Ref. 2). The water jacket is composed of carbon steel (1%), with thermal properties from material No. 14 in the HTAS1 material property library. The water in the neutron shield will be lost after the prefire steady state. The water will be replaced by a void so that heat will be transferred across the resulting gap by radiation only. The emissivity for each radial surface (outer surface of the outer shell and inner surface of the water jacket) of the resulting gap is 0.6 (the default emissivity on each surface is 0.5). The bottom impact limiter will be deleted following the fire transient. The emissivity on the outer surface of the outer shell not including the portion covered by the water jacket is 0.9 during the postfire transient and final steady state. This section represents the portion of the outer surface previously covered by the bottom impact limiter. The default emissivity for the outer shell during this part of the calculations is 0.8. The ambient temperature during the prefire steady state, the postfire transient and the final steady state is 130°F instead of the default of 100°F. It is desired to compute the transient for the first 4 hours of the cooldown period following the fire. The transient temperature distribution is needed every 5 min during the 30-min fire, every 10 min for the first hour of the cooldown period following the fire, and every 20 min for the remaining cooldown period. After running several cases by varying the restrictions on the time-step size, it was determined that an accurate solution could be obtained by adjusting the time-step size while keeping the maximum relative change in temperature over a time step to 5%. The time-step size should not exceed 5 min. The transient temperature distributions were made using the Crank-Nicolson implicit procedure subject to the above restrictions on the time-step size.

The input data necessary for HTAS1 to perform the analytical sequence are shown in Table H1.5.8.

Table H1.5.7 Thermal properties for one and 1.5% carbon steel

Temperature (°F)	Thermal conductivity[a] Btu/(hr-ft-°F)	Density[a] (lb/ft^3)	Temperature (°F)	Specific heat$_b$ Btu/(lb-°F)
32	21	484	32	0.105
212	21		167	0.120
392	21		392	0.135
572	20		752	0.15
752	19		1112	0.17
1112	18		1292	0.20
1472	16			

[a]Reference 1.
[b]Reference 2.

Table H1.5.8 Input data for second sample problem for HTAS1

```
HTAS1 SAMPLE PROBLEM 2

CAVITY 6.75 5 89 5 39247
INNER SHELL 0.31 1 0.25 1
*
* EXAMPLE OF OVERRIDING THE DEFAULT MATERIAL FOR THE INNER SHELL BY
* EXPLICITLY SPECIFYING THE MATERIAL AND ITS THERMAL PROPERTIES.
MATERIAL
CARBONST
 32 21
@ 212  21
@ 392  21
@ 572  20
@ 752  19
@1112  18
@1472  16
484
 32 0.105
@ 167 0.12
@ 392 0.135
@ 752 0.15
@1112 0.17
@1292 0.20
SHIELDING 6.63 5
OUTER SHELL 1.25 2 7.25 4 7.75 4
*
* EXAMPLE OF OVERRIDING DEFAULT EMISSIVITIES OF THE OUTER SHELL FOR
* THE POSTFIRE TRANSIENT AND FINAL STEADY STATE CALCULATIONS.
EMISSIVITIES 0 0 0 0.9 0.9
*
* EXAMPLE OF OVERRIDING THE DEFAULT MATERIAL FOR THE OUTER SHELL BY
* REPLACING IT WITH A MATERIAL FROM THE LLNL MATERIAL PROPERTY LIBRARY
* (MATERIAL NUMBER 3135 - STAINLESS STEEL 347).
MATERIAL
*3135
NEUTRON SHIELD 4.5 4 85.5 86
*
* EXAMPLE OF REPLACING THE NEUTRON SHIELD WITH A VOID AFTER THE PREFIRE
* STEADY STATE CALCULATIONS.  ALSO, OVERRIDE THE DEFAULT EMISSIVITIES
* FOR THE RADIATIVE HEAT TRANSFER ACROSS THE RESULTING GAP.
DELETE PREFIRE -1 0.6 0.6
WATER JACKET 0. 16 1

*
* EXAMPLE OF OVERRIDING THE DEFAULT MATERIAL IN THE WATER JACKET BY
* REPLACING IT WITH MATERIAL NUMBER 14 FROM THE HTAS1 MATERIAL PROPERTY
* LIBRARY.
MATERIAL 14
IMPACT LIMITER 39 5 27.5 5 0 0 11

*
* EXAMPLE OF REMOVING THE BOTTOM IMPACT LIMITER AFTER THE FIRE
* TRANSIENT CALCULATIONS.
DELETE FIRE BOTTOM
*
```

Table H1.5.8 (continued)

```
* EXAMPLE OF REQUESTING PRINTED OUTPUT OF THE TRANSIENT TEMPERATURE
* DISTRIBUTIONS AT SELECTED TIMES.PRINTOUT TIMES 5 10 15 20 25 30 40 50 60 70 80 90 110 130 150 170 190
@ 210 230 250 270
*
* EXAMPLE OF OVERRIDING THE DEFAULT AMBIENT TEMPERATURE FOR THE PREFIRE
* STEADY STATE CALCULATIONS.
PREFIRE 130
FIRE
*
* EXAMPLE OF OVERRIDING THE DEFAULT NUMERICAL TECHNIQUE FOR THE FIRE
* TRANSIENT CALCULATIONS.  USE CRANK-NICOLSON WITH A MAXIMUM TIME STEP
* SIZE OF 5 MINUTES AND ADJUST THE TIME STEP SIZE TO KEEP THE MAXIMUM
* RELATIVE CHANGE IN TEMPERATURE NEAR 5 PER CENT OVER A TIME STEP.
IMPLICIT

0 0 5 0 0 5
* EXAMPLE OF OVERRIDING THE DEFAULT DURATION TIME AND AMBIENT
* TEMPERATURE FOR THE POSTFIRE TRANSIENT CALCULATIONS.
POSTFIRE 240 130
*
* EXAMPLE OF OVERRIDING THE DEFAULT NUMERICAL TECHNIQUE FOR THE POSTFIRE
* TRANSIENT CALCULATIONS.  USE CRANK-NICOLSON WITH A MAXIMUM TIME STEP
* SIZE OF 5 MINUTES AND ADJUST THE TIME STEP SIZE TO KEEP THE MAXIMUM
* RELATIVE CHANGE IN TEMPERATURE NEAR 5 PER CENT OVER A TIME STEP.

IMPLICIT
0 0 5 0 0 5
*
* EXAMPLE OF OVERRIDING THE DEFAULT AMBIENT TEMPERATURE FOR THE FINAL
* STEADY STATE CALCULATIONS.
FINAL 130
%
```

H1.6 REFERENCES

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