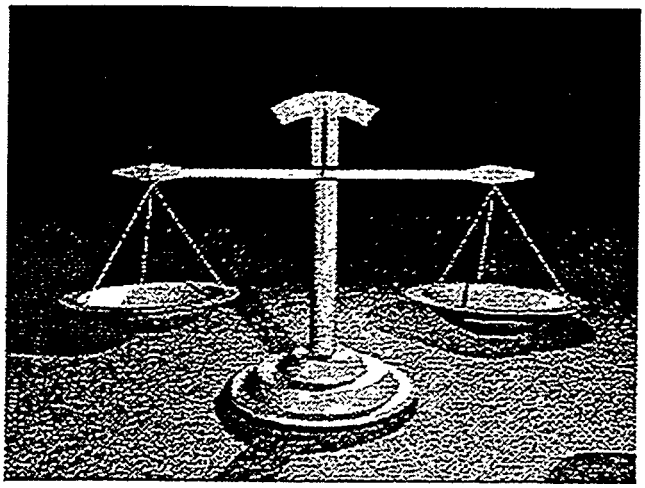
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Vol. 1, Part 2

# SCALE

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



## Control Modules, Part 2

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

## Control Modules S1–H1

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*Obsolete with SCALE-4.0 release.

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# PREFACE

## Background

This Manual represents Revision 5 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 Computational Physics and Engineering 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, C6, S1– S4, and H1), Volume 2 for the functional module documentation (Sections F1–F17), 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 included 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 the primary 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. CSAS6 is a new criticality control module to provide automated problem-dependent cross-section processing and criticality calculations via the new KENO-VI functional module. 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.

The capability to perform a point-kernel shielding analysis within the SCALE system has been developed in the QADS control module which has been added in this 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 in this version of SCALE or as a separate data package from the software distribution centers.

## Major Enhancements in SCALE-4.3

### New ENDF/B-V libraries

SCALE-4.3 includes 238GROUPNDF5, a 238-group, AMPX master-format neutron cross-section library that contains data for all the nuclides available in ENDF/B-V. The library has Bondarenko shielding factors included for nuclides with unresolved resonances, nuclides with Adler-Adler resonance data (U-233 and Pu-241), and the nonresonance nuclides Li-7, F-19, Al-27, and Si-14. Bondarenko factors are used for the latter nuclides because they exhibit resonance structure in the point data. The initial development of this library included only s-wave resonance data in the resonance parameters that are passed to the Nordheim treatment in NITAWL. Although demonstrated sufficient for thermal systems, it was found that p-wave and perhaps d-wave resonances can have a significant effect on the results for shielding applications and for unmoderated, intermediate energy problems. Thus, p-wave and d-wave data were added to the library. Users, however, will not be able to readily access the p- and d-wave resonance data until SCALE-4.3 has been made available to RSIC in 1995.

Several spectra suitable for collapsing this fine-group library to a broad-group structure are included as part of the library. A 44-group derivative of the 238-group library, 44GROUPNDF5, collapsed using a spectrum for a pressurized-water-reactor fuel pin lattice, is also included in the package. This broad-group library has a similar group structure as that provided in the SCALE 27-group ENDF/B-IV library, except that additional groups were added to ensure more accurate treatment of the 0.3-eV resonance of $^{239}$Pu. Based on an analysis of a set of 93 thermal and fast critical experiments, the ENDF/B-V 44-group library has demonstrated markedly improved performance over similar analyses performed with the ENDF/B-IV 27-group library ("Validation of SCALE-4 Criticality Sequences Using ENDF/B-V Data," *Proceedings of the Topical Meeting on Physics and Methods in Criticality Safety*, September 19–23, 1993). In addition, by comparing SAS2H/ORIGEN-S results with measured isotopic data, the library has demonstrated improved results in the prediction of spent fuel isotopics (*Validation of the SCALE System for PWR Spent Fuel Isotopic Composition Analyses*, ORNL/TM-12667, March 1995).

### KENO-VI

KENO-VI is a new version of the KENO Monte Carlo Criticality Safety Code developed at Oak Ridge National Laboratory. It constructs and processes geometry data as sets of quadratic equations. A lengthy set of simple, easy-to-use geometric functions, similar to those provided in KENO-V.a, and the ability to build more complex geometric shapes (represented by sets of quadratic equations) are the heart of the geometry package in KENO-VI. The code's flexibility is increased by allowing the following features: intersecting geometry regions; hexagonal as well as cuboidal arrays; regions, holes, arrays, and units rotated to any angle and truncated to any position; and the use of an array boundary that intersects the array.

KENO-VI maintains all the flexibility and options of KENO-V.a plus a variety of new options. In KENO-VI, units can be constructed using both the simple geometric shapes provided and the tailored geometric shapes constructed using quadratic equations. It includes the new 2-D color plotting capability that has been added to KENO-V.a (see "Improvements to KENO-V.a Include 2-D

Color Plot Capability"). A new SCALE Criticality Safety Analysis Sequence, CSAS6, has been added for running KENO-VI.

Users should be aware that the added geometry features in KENO-VI can result in significantly longer run times than KENO-V.a. A KENO-VI problem that can also be modeled with KENO-V.a will typically run twice as long as the same problem using KENO-V.a. Thus, the new version VI is not a replacement for the existing version V.a, but an additional version for complex geometries that could not be modeled previously.

**New criticality search on material concentrations**

A new search feature has been added to the criticality search sequences in SCALE. Searches may now be done on the concentration of standard compositions in one or more mixtures in the problem. During a concentration search, if the search convergence criteria have not been met, the atom densities of the specified standard compositions are updated, problem-dependent resonance processing is performed using BONAMI, NITAWL, and applicable sections of the material information processor, and a new $k_{eff}$ is calculated using KENO-V.a. Concentration searches cannot be performed on materials contained in cell-weighted mixtures.

In all search sequences (both geometry and concentration), problem-dependent resonance processing of the cross sections is now performed for each iteration prior to the execution of KENO. Heterogeneous effects, Dancoff factors, and self-shielding are now accounted for between iterations. Prior to the addition of concentration searches, a search sequence would update only the specified geometry, but not the cross sections, prior to calculating a new $k_{eff}$ using KENO-V.a. Previously, to ensure that the converged result was acceptable, the problem needed to be rerun with the converged geometry data. The recent changes to the search sequences eliminate the need to rerun a converged problem to account for changes in cross sections.

**Enhanced graphical capabilities**

The graphical display of KENO-V.a and KENO-VI geometry models has been dramatically improved by the new capability to produce high-resolution 2-D color plot files that can be viewed on-screen using appropriate viewer software or printed on a color printer. This new option is activated by using the parameter scr=yes in the KENO plot data. A plot file using up to 256 colors is generated. The plot data parameter "clr=" can be used to override the default color assignments. These plots can be generated only on UNIX workstations and MS-DOS-based personal computers (PC).

In addition to the 2-D color plots, fractional values are now valid for the lpi= parameter in the plot data, which will make it easier to print circles on laser printers.

**KENO-V.a enhancements**

Enhancements to KENO-V.a fall into one of three categories: removed limitations, editing changes, or added capabilities.

Two independent limitations to KENO-V.a were removed. The first limitation involved HOLE boundaries touching other HOLE or adjacent geometry region boundaries. Significant errors

in $k_{eff}$ (as much as 1%) occurred when HOLE boundaries touched with no indication of a problem. HOLE boundaries may now touch other HOLE or adjacent geometry region boundaries.

The second limitation involved the number of scattering angles allowed. Although the parameter sct= (number of scattering angles) was limited to 13, no check was made to avoid overstoring data. Any number of scattering angles are now allowed.

The mixing table edit has been changed to sort mixture data by mixture number. The mixture number and density make up the first line of the data for each mixture. The following lines, which represent the nuclides in the mixture, are sorted by nuclide number. Each line contains a nuclide number, atom density, weight fraction, ZA number, atomic weight, and nuclide title. This provides the user a concise table of the components that make up the mixtures used in the problem.

Three new capabilities were also added to KENO-V.a which provide the user with useful information for analyzing and checking the problem.

The energy corresponding to the average lethargy causing fission is now calculated and the printing of this information (i.e., NUB=YES) is now a default parameter. This is useful for determining trends in $k_{eff}$ as a function of neutron energy to look for problem-type biases.

System total fissions and absorptions by region are now calculated. A parameter to suppress printing fissions and absorptions by region for each group has been added. Set GAS=NO to print only the system totals by group. These values have several uses, such as helping to verify proper problem sampling and determining region importance.

Finally, the total mass of each mixture in the problem is now calculated and printed. These values can be used to help verify the geometry and material masses of the problem.

**New cross-section processing features**

The cross-section processing portion of the SCALE system has been upgraded to add major improvements to the NITAWL-II code. NITAWL-II has been modified to perform the resonance calculation in double precision. The mesh generation for a resonance has been modified to better span higher energy resonances and to reduce excessive numbers of mesh points.

In addition, this new version of NITAWL-II is able to interpolate the available thermal-scattering matrices to obtain data for the temperature requested by user input (via direct input to NITAWL-II or via the SCALE Standard Composition data). Previously, NITAWL-II had no such capability and selected the thermal-scattering data that was closest to the requested temperature. Thermal-scattering data for moderator materials, such as hydrogen and graphite, are available at many more temperatures in the new ENDF/B-V SCALE libraries than in the older ENDF/B-IV SCALE libraries. However, even with the new ENDF/B-V libraries, the interpolation should better determine the effect that a change in moderator temperature will have on the system multiplication factor.

The CSAS and SAS1–SAS4 modules also have been modified via MIPLIB to provide two new parameters in the optional MORE DATA input:

MLV= maximum L value for which resonance calculation will be done (L = 0 is s-wave, L = 1 includes p-wave, L = 2 includes d-wave). The default value is L = 2.

MSH= maximum number of mesh points per resonance. The default value is 2001.

Note that if NITAWL-II is run stand-alone, the default values for MLV and MSH are 0 and 501, respectively.

## New KENO-V.a sample problems

The KENO-V.a sample problems have been updated to improve the range of functionality testing and provide more flexibility in using other cross-section libraries. The SCALE-4.2 sample problems used the 27-group ENDF/B-IV cross-section library. The cross sections were processed by NITAWL-II prior to the execution of KENO-V.a. The new sample problems use BONAMI, which is not necessary for the 27-group library, as well as NITAWL-II for resonance processing of cross sections so that the sample problems can easily be run with other cross-section libraries that require the use of BONAMI. The NITAWL-II input data were updated to specify 2001 mesh points per resonance and the highest resonance L-value of 2. The previous input data used the default values of 501 mesh points and an L-value of 0.

Eight new problems were added to the existing 25 sample problems. Sample problems 26 through 28 are variations of sample problem 1, modeled as hemicylinders with chords and origins, and are extensions of sample problems 23 through 25, which are modeled using chords without origins. Sample problem 29 is a bare critical sphere, and sample problems 30 through 32 are the same critical system modeled using hemispheres with origins. Sample problem 33 is a critical triangular pitched array of partially flooded cylindrical annuli of low-enriched-uranium metal.

## Standard Composition Library updated for ENDF/B-VI compatibility

The Standard Composition Library has been expanded for compatibility with ENDF/B-VI cross-section libraries. In addition, the Material Information Processor Library (MIPLIB) has also been updated so that all the control modules can use ENDF/B-VI cross-section libraries via the new expanded Standard Composition Library. The changes were necessary because the cross sections for the natural-element identifiers such as **FE** for iron are no longer available in the ENDF/B-VI data. Most problems set up to use other cross-section libraries should now run without any changes using ENDF/B-VI libraries.

The changes to the Standard Composition Library were very extensive and fall into several categories. Additions were made so that nearly all the elements are given by both their full name and by their chemical symbol. The full-name elements are all given as naturally occurring abundance nuclides, while a few of the chemical symbol nuclides are given as the principal isotope. For instance, **HYDROGEN** would include trace amounts of deuterium, while **H** would be 100% $^{1}H$.

The isotopic distribution table was changed to include most of the elements. Arbitrary materials may now contain more than one multiple-isotope nuclide. In addition, the specially weighted elements in stainless steel and in Inconel were added, specifying the natural abundance of each.

Atomic masses for isotopes were taken from ENDF/B-VI, if available. Atomic masses for naturally occurring elements were taken from ENDF/B-V, if available. Remaining atomic masses were taken from *GE Chart of the Nuclides* or the *CRC Handbook of Chemistry and Physics.*

## QAD-CGGP and QADS

The 3-D point-kernel shielding code, QAD-CGGP, and its associated SCALE control module have been added. QADS performs multidimensional point-kernel estimation of gamma transport through practically any type of shielding materials using a simplified input scheme that follows the

general input philosophy of the SCALE shielding sequences. QADS was designed to capture the flexibility and power of the QAD technique for problems amenable to point-kernel solution while allowing for an easy-to-use input interface. The QADS module is called via the SCALE driver and preprocesses the actual input for the QAD-CGGP code. The driver then calls and executes QAD-CGGP automatically. The SCALE standard composition library is used to allow simplified input of materials. The problem geometry is coded using the well-known MORSE combinatorial geometry package. Finally, the dose portion of the input follows the XSDOSE input data format in SAS1. The combined use of the SCALE standard compositions and free-form input with the multidimensional geometry capabilities and generally short running time of point-kernel techniques produces a very powerful procedure for shielding analysis of a wide variety of problems.

**SCALE-4.3 minor modifications**

In addition to the major enhancements noted above, SCALE-4.3 contains many minor modifications, including corrections to errors in SCALE-4.2 and changes to improve portability to other computing platforms.

**SCALE driver**: The driver was modified to improve portability to other types of workstations. Modifications to accept upper or lower case input files were also added.

**KENO-V.a:** (1) Corrected error that sometimes occurred when the boundary of a HOLE touched another HOLE or adjacent geometry region. The error can produce erroneous results, either conservative or nonconservative, without triggering warning or error messages. The effect on $k_{eff}$ can be very significant in some cases (~ 1%). (2) Fixed to allow more than 13 scattering angles. Although the parameter "sct=" was limited to 13, no check was made to avoid overstoring data. (3) Corrected error causing core dump on some workstations when a global unit wasn't explicitly defined. (4) Corrected error that permitted a case with a negative radius to run. (5) Added calculation of the energy corresponding to the average lethargy causing fission and made the printing of this information (i.e., NUB=YES) a default parameter. (6) Corrected errors in the starting points edit obtained when PSP=YES. (7) Corrected an error that occurred when a history encountered an edge where differential albedos were used. Other minor fixes were made for (8) printing densities of mixtures that have other mixtures added in and (9) printing plot coordinates for problems ending in a bare array. (10) Output was enhanced to print information on start and plot input parameters that were previously omitted.

**NITAWL**: (1) Corrected the grayness correction to self-shielding in annular regions. (2) Corrected an error passing a variable of the wrong type that resulted in incorrect self-shielding of thermal groups below 0.5 eV.

**All Control Modules (MIPLIB)**: (1) Added checks to avoid the use of negative number densities when solutions with physically unrealistic parameters are entered. (2) Corrected an error that caused CSAS to loop if the collapse option was specified and an input nuclide ID was not found in the cross-section library. (3) Modified MIPLIB to check for resonance data on the cross-section library used to determine whether to perform resonance corrections for a nuclide. Previously, a flag in the Standard Composition Library was used to make this determination. (4) Corrected calculated thickness ("lbar") of cylindrical and spherical annuli for input to BONAMI. (5) Modified reading of Dancoff factor keywords in MORE DATA to detect and prevent erroneous keyword input. (6) Changed the label "lbar" printed by CSAS in PARM=CHECK output to "abar." (7) Replaced the 123GROUP and 218GROUP cross-section-library keywords with 44GROUP and

238GROUP. The former libraries, which were the least used of the standard SCALE libraries, were removed as defaults so the new ENDF/B-V libraries, which give more accurate results, could be accessed directly via keyword input.

**CSAS/MODIFY**: Added an option in the CSAS4 and CSAS4X sequences to perform a criticality search on nuclide concentration. Modified the search sequences to update unit cell data or number densities (depending on the type of search) and execute BONAMI and NITAWL prior to every KENO-V.a calculation.

**SAS2:** (1) Modified for compatibility with recent MIPLIB changes. (2) Corrected the soluble boron concentration to change linearly when NLIB/CYC>1. (3) Modified to allow use of the SYMMSLABCELL geometry in MIPLIB and more than one fuel zone. (4) Automated model setup when burnable poison rods occupy some but not all guide tubes in a fuel assembly. (5) Added THERM, RES, FAST, and the two energy boundaries for converting cross sections to the total flux normalization. (6) Modified the AMPX cross-section library defaults to match MIPLIB, including the use of unit 70 for unrecognized libraries. (7) Corrected an error that occurred if light element nuclides are in both the ORIGEN-S light element and fission product libraries and are input as individual nuclides in the MIPLIB input.

**ORIGEN-S** : (1) Replaced call to INQOPN with call to OPNFIL for standard input (unit 5) to improve portability to other computers. (2) Initialize arrays only within the array boundaries for better portability. (3) Added EXTERNAL statements for BLOCK DATA files to improve portability. (4) Improved coding for the integral option using the actinide library. (5) Program was corrected to execute a continuation subcase when using the integral option. (6) Corrected call to subroutine STOP.

**ORIGEN-S Libraries**: (1) Corrected Cf-249 data in lowest energy group in Master Photon Library. It was high by factor of 100. (2) Corrected the half-life of Se-79. It was low by factor of 10. (3) Corrected Br-86m decay data that was erroneously changed in ENDF/B-VI update.

**COUPLE**: (1) Added check for correct ordering of fission product nuclides by atomic weight in input library. (2) Added EXTERNAL statement for BLOCK DATA files to improve portability to other computers. (3) Modified output format for THERM, RES, and FAST from floating point (F) to exponential (E). (4) Corrected an error that occurred when only fission product yield data were being updated. Note that this error did not occur when using COUPLE in the SAS2 sequence.

**Standard Composition Library**: (1) Revised the resonance energy scattering and/or total cross sections for 197 materials based on the 44-group ENDF/B-V cross-section library. Consistent values were specified for both the natural element and individual isotopes B, Zr, Eu, Hf, and W. (2) Added new composition ZIRC2 for Zircaloy-2 when using ENDF/B-V cross-section libraries. (3) Replaced $\sigma_s$ and $\sigma_t$ values in Nuclide Information Table with average values calculated from ENDF/B-V or ENDF/B-VI libraries. (4) Density for ZIRCALLOY and ZIRC2 was corrected from 6.506 to 6.56 g/cc.

**All Cross-Section Libraries:** The atomic masses of nuclides were modified to all be in terms of neutron mass for consistency.

**XSDRNPM**: (1) Modified to scale the weighting flux so that minimum value is 1E-20. This modification was made to reduce the likelihood that an underflow would occur when creating a weighted cross-section library for problems where there are large variations in the flux (many orders of magnitude). (2) Corrected an error that caused broad-group-flux edits to print bad values. (3) Corrected an error that would occur when creating a gamma-only broad-group library.

**XSDRNPM/SAS4**: Adjoint calculation in XSDRNPM for SAS4 was corrected. Only affects fixed-source calculations with upscatter on machines whose single- and double-precision formats are different (includes IBM workstations). Any such calculations should be rerun to determine impact of correction.

**SAS4**: (1) Increased the number of mesh intervals for both neutrons and gammas in the XSDRN adjoint calculation to improve the likelihood of convergence. Made additional minor changes to improve portability. (2) Updated for consistency with new nuclide ID numbering scheme in MIPLIB.

**MORSE**: Corrected a problem caused by the use of an incorrect normalization factor on standard deviations at the end of each batch. This occurred when NMOST was equal to NSTRT.

**BONAMI**: (1) Restored Bondarenko factor printout that was inadvertently deleted in July 1990 modification. Results were not impacted. (2) Corrected so that calculations with more than one nuclide specified with a zero number density will run.

**SAS1**: (1) Modified to force the pointer for the double-precision flux array to start on a double word boundary. This change improves performance significantly on some workstations other than IBM. (2) Corrected setting of termination flag so that SCALE driver can run other modules when cases are stacked in an input file.

**AIM**: Corrected error that created a bad magic word in a binary library if a magic word position occurred as the last position of a transfer array in the BCD data.

**HEATING**: A coding flaw was found and corrected in HEATING that prevented the proper application of the unit system conversion factors for the material properties database. This option allows the user to select a material from the database and convert the property values to the user's unit system. Due to the flaw, the material property values were not converted and values were used in the calculations that were not correct for the unit system. This flaw would affect only HEATING or HTAS1 problems that specify unit conversion factors for the material properties database.

**HTAS1**: A coding flaw was found and corrected in HTAS1 that prevented the building and the use of enclosure radiation connectors for models that replace the material in the neutron shield with a void (no material). A normal (and the default) analysis would replace the material in the neutron shield with air. Any other material or a void can be placed in the neutron shield volume. As long as any type of material (not a void) is in the neutron shield then the thermal radiation connectors are built in OCULAR and the analysis procedures correctly. However, if a void volume is modeled in HTAS1 then the flaw prevented the building and use of the connectors. Thus, no heat would be transferred across the neutron shield, which could significantly and potentially nonconservatively alter the thermal history of the shipping cask.

**All modules (UNIXLIB)**: Modified subroutine DATIM to read the date and time from the file "datetime.std" if it exists. This option will be useful for comparing sample problem output files.

**KENO-V.a, SAS2 (SUBLIB)**: Modified subroutine YREAD to correctly read an array of numbers separated by commas.

## Portability

Version 4.3 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 and DEC

workstations. In addition, the system has been applied by ORNL on SUN and HP workstations. Information needed to install SCALE on each of these systems is included with the software package distributed by the code centers. A separate SCALE software package, designated SCALE-PC, is available for the execution of the SCALE system, except heat transfer modules, on a MS-DOS 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 MS-DOS 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 SCALE-PC version includes an updated version of the ORIGEN-S processor coupled with the ARP code, which interpolates on standard LWR ORIGEN-S binary libraries, in the ORIGEN-ARP system (Section F7.A).

**Availability**

The SCALE code system and the other software designated under Related Developments have been packaged by the Radiation Shielding Information Center (RSIC). The SCALE system and the related software may be obtained by contacting

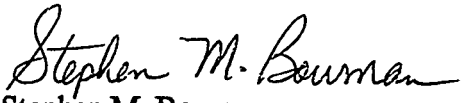
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FAX: (615) 574-6182
E-mail: pdc@ornl.gov

**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. K. Martin, who is responsible for implementing and controlling software 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 C. V. Parks, who has served as the SCALE Project Leader for the past 15 years, and 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.



Stephen M. Bowman
SCALE Project Leader
January 1997

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5. N. M. Greene, J. W. Arwood, R. Q. Wright, C. V. Parks, *The LAW Library-A Multigroup Cross-Section Library for Use in Radioactive Waste Analysis Calculations*, ORNL/TM-12370, Martin Marietta Energy Systems, Inc., Oak Ridge Natl. Lab., August 1994.

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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<br>3-D Monte Carlo calculation of neutron multiplication<br>Problem-dependent cross-section processing<br>Multiplication search or spacing | BONAMI<br>NITAWL-II<br>XSDRNPM<br>KENO V.a<br>ICE | C4 |
| CSAS6 | 3-D Monte Carlo calculation of neutron multiplication | BONAMI<br>NITAWL-II<br>XSDRNPM<br>KENO-VI | C6 |
| SAS1 | 1-D deterministic calculation of radiation transport through shield and dose evaluation at a point<br>Calculation of dose at detector based on leakage from critical volume | BONAMI<br>NITAWL-II<br>XSDRNPM<br>XSDOSE | S1 |
| SAS2 | Point depletion/decay of nuclear fuel<br>1-D radial shielding analysis in cylindrical geometry | BONAMI<br>NITAWL-II<br>XSDRNPM<br>COUPLE<br>ORIGEN-S<br>XSDOSE | S2 |
| SAS3 | Dose evaluation using MORSE Monte Carlo code | BONAMI<br>NITAWL-II<br>XSDRNPM<br>MORSE-SGC | S3 |
| SAS4 | Calculation of dose outside of transportation package using MORSE code and automated biasing techniques | BONAMI<br>NITAWL-II<br>XSDRNPM<br>MORSE-SGC | S4 |
| QADS | 3-D point-kernel gamma-ray shielding analysis | QAD-CGGP | S5 |
| HTAS1 | R-Z steady-state and transient analyses of a transportation package | OCULAR<br>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:<br>• zone-weighting of cross sections<br>• eigenvalue calculations for neutron multiplication<br>• fixed-source calculation for shielding analysis<br>• 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 |
| KENO-VI | Monte Carlo code for calculation of neutron multiplication factors for complex geometries | F17 |

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Computational Physics and Engineering Division

# SAS1: A ONE-DIMENSIONAL SHIELDING ANALYSIS MODULE

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## 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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## 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 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:

$$\text{Dose (rem)} = \text{total fission} * \text{dose rate}\left(\frac{\text{rem/h}}{\text{neutrons/s}}\right) * \frac{\text{1 neutron/s}}{\text{fission rate (fissions/s)}} * \frac{\text{1 h}}{\text{3600 s}}$$

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:

$$\text{Dose rate (rem/h)} = \text{dose rate}\left(\frac{\text{rem/h}}{\text{neutrons/s}}\right) * \text{power (watts)} *$$

$$\frac{\text{1 neutron/s}}{\text{fission rate(fissons/s)}} * \frac{1}{\text{energy per fission}\left(\frac{\text{watt-s}}{\text{fission}}\right)}$$

where energy per fission is typically on the order of $3 \times 10^{-11}$ 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

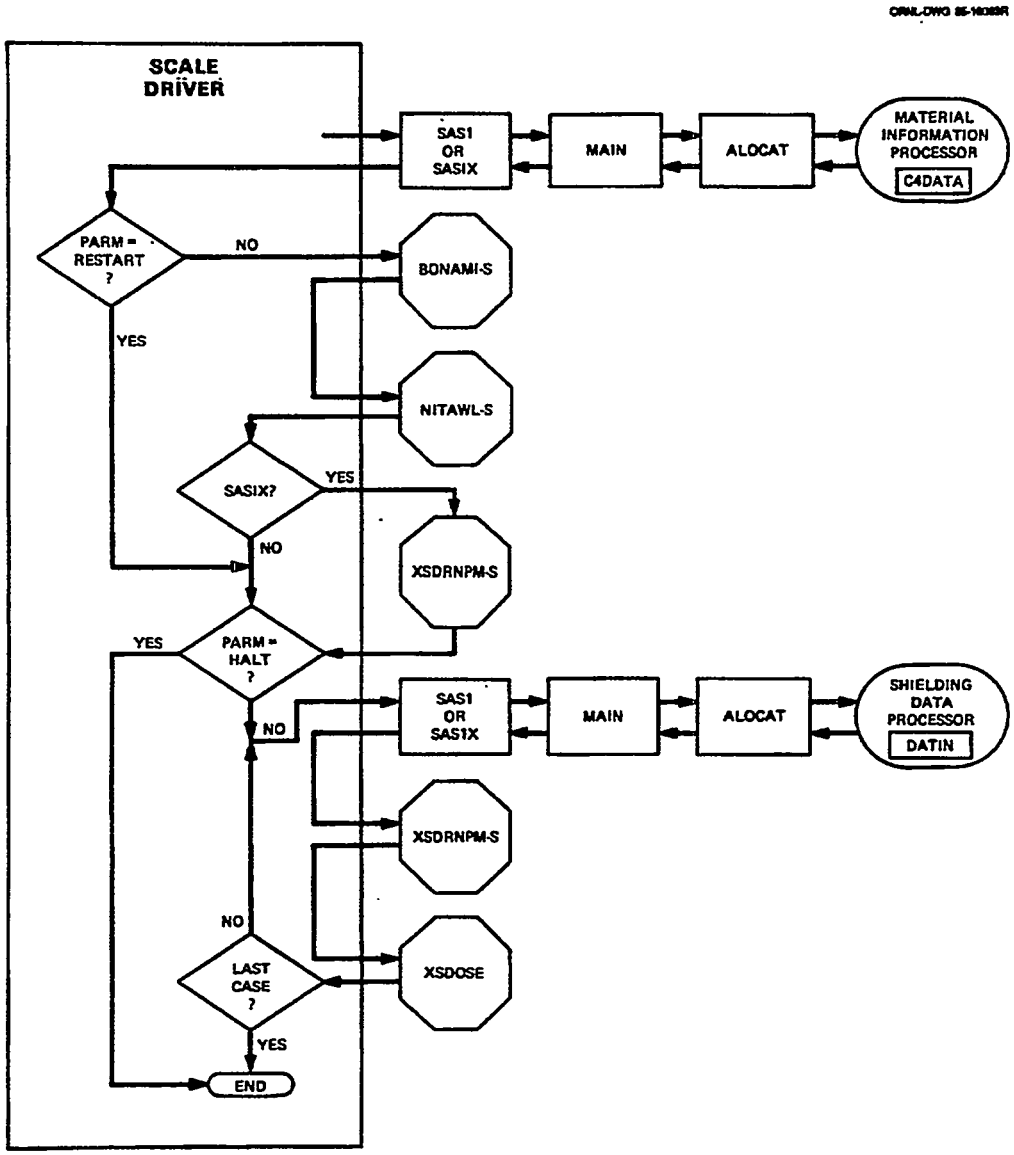



Figure S1.3.1 General SAS1 flow diagram

to MAIN following 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<br>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:

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**<br>**22N-18COUPLE**<br>**18GROUPGAMMA**<br>**27BURNUPLIB** | These are the commonly used cross-section libraries available in SCALE for shielding analyses. See Sect. M4 |
| 4 | Type of calculation | **INFHOMMEDIUM**<br>**LATTICECELL**<br>**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.**<br>See Table S1.4.3 for **LATTICECELL.**<br>See Table S1.4.4 for **MULTIREGION.**<br>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. Repeat entries 9, 10, and 11 for additional shielding problems |

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<br>or<br>ROTH | Specific gravity of the solution<br>or<br>Density of the basic standard composition | Optional | If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR<br>or<br>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 data | Terminate LATTICECELL | 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 | This provides isotopic return at the boundary |
| | | | | WHITE | |
| | | | | | 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<br>SZF<1.0 gives a finer mesh<br>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= | Buckling factor | 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. Optionally enter the inner radius (cm) to specify an annular cylinder or sphere. |
| 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<br><br>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<br>CYLINDRICAL<br>SLAB<br>DISC | For spherical geometry<br>For cylindrical geometry<br>For slab geometry<br>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<br>REFLECTED | No return condition at boundary<br>Mirror reflection at boundary |
| 4 | MXZ | Mixture number in zone | Always | Valid mixture number for zone | Repeat items 4-15 for each zone<br>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;<br>N, source from ORIGEN-S file or from XSDRNPM criticality case;<br>-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<br>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<br>>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<br>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<br>Enter inverse of value for conversion to per cm³ of zone (see Sect. S1.2.1).<br>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)<br>Set to 1 if not used<br>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<br>Disc radius for DISC<br>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<br>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.

```
=SAS1       PARM=(CHECK,SIZE=120000)
            =SAS1       PARM=(SIZE=120000,CHECK)
            =SAS1       PARM=`CHECK,SIZE=120000'
            =SAS1       PARM=`SIZE=120000,CHECK'
```

### 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:<br>-1 no flux print,<br>0 scalar flux print,<br>1 scalar flux and angular flux print |
| SCT= | 3 | Order of Legendre expansion to be used |
| PRT= | -2 | Cross-section print option:<br>-2 no cross-section print,<br>-1 print 1-D cross sections,<br>O/N print $P^L$ arrays through order N |
| PBT= | 0 | Balance table print option:<br>-1 no balance table print,<br>0 fine group balance table print,<br>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 SAS1 sample problems 1–2, 5–8, and 22–25 are not included in the distribution version of SCALE to reduce the amount of CPU time required for users to verify their installation of SAS1.

*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.

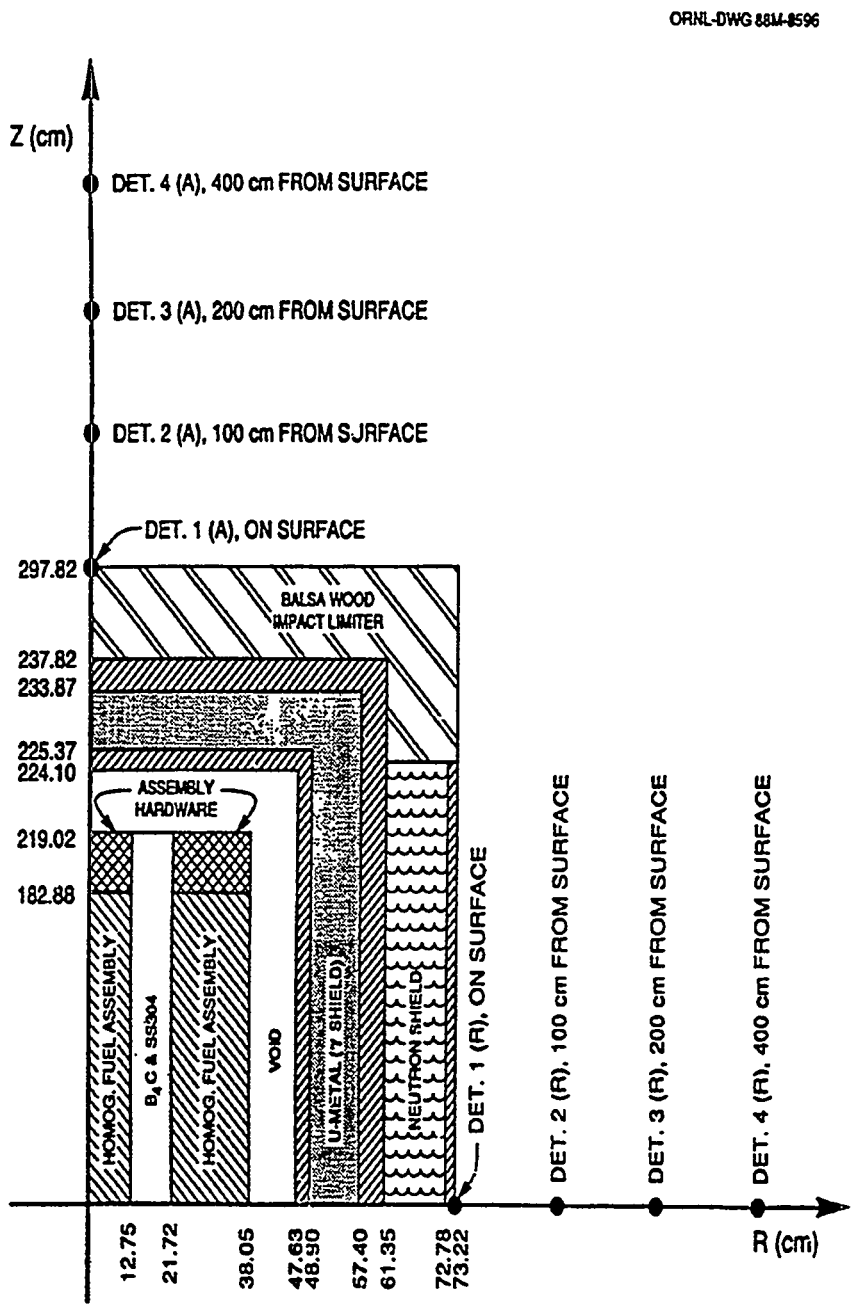



Figure S1.5.1 Seven assembly, depleted uranium metal, spent fuel shipping casks described by SAS1 sample problems

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=8 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]<br>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
```

Table S1.5.4 (continued)

```
' NOTE: THE KEYWORDS "END ZONE" MUST NOT BEGIN IN COLUMN 1:
 END ZONE
'
' 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:
```

Table S1.5.5 (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.
'
' 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
```

Table S1.5.5 (continued)

```
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):
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
```

Table S1.5.5 (continued)

```
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):
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
```

Table S1.5.6 (continued)

```
'    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
'
' 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
```

Table S1.5.6 (continued)

```
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, 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
```

Table S1.5.6 (continued)

```
' 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 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.
```

Table S1.5.6 (continued)

```
' 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-18$\gamma$, 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 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-18$\gamma$ 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-18$\gamma$ calculations ran 2.9 times longer than the collapsed 15n-18$\gamma$ 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 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).

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
'
```

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
```

Table S1.5.7 (continued)

```
'
'  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 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.
'
```

Table S1.5.7 (continued)

```
'  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
'  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.)
```

Table S1.5.7 (continued)

```
'
' 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
' 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
'
```

Table S1.5.7 (continued)

```
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
'
' 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].
```

Table S1.5.7 (continued)

```
'
' 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
```

Table S1.5.8 (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.  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
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.
```

Table S1.5.8 (continued)

```
' (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
```

Table S1.5.9 (continued)

```
'  (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
'  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):
```

Table S1.5.9 (continued)

```
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.
' 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:
```

Table S1.5.9 (continued)

```
 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 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
```

Table S1.5.9 (continued)

```
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
'  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
```

## 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'
CASE 26--HOMOGENEOUS SPHERE OF FUEL/CLAD/MOD SURROUNDED BY 15 FT OF H2O
'
' THE SIZE PARAMETER MUST BE SPECIFIED BECAUSE OF THE LARGE NUMBER OF ZONES
' NECESSARY TO MODEL 15 FEET OF H2O REFLECTOR.
'
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
AL       1  0  3.00340-2   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
LAST
STORAGE POOL DOSE
'
' THE SHIELDING CALCULATION INPUT
'
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 3 and 4 is shown in Table S1.5.11, while the SAS1 output for cases 9 through 14 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 3 and 4 with PARM=CHK

```
      PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - 95/03/29 - 09:06:37 )
 MODULE SAS1X    WILL BE CALLED
  CASES 3 & 4 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=YES
  27N-18COUPLE  LATTICECELL
  U02  1  0.90172   560   92234 0.029  92235 3.2  92236 0.016  92238 96.755  END
  ZIRCALLOY  2  1  560  END
  SS304   3  2.1712E-2  END
  B4C     3  7.7066E-2  END
  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
  END COMP
  SQUAREPITCH  1.2598  0.8357  1  8  0.94996  2  END
  MORE DATA  COLLAPSE  END.

  CASE 3 -- LATTICECELL X-SECT PROC, COLLAPSE=YES, SOURCE SPEC ENTERED BELOW
  CYLINDRICAL
  500  12.75  20 -1     7  0.17994     6.02E+02   2.65E+10
  3    21.72   8  0
  500  38.05  30 -1     7  0.17994     6.02E+02   2.65E+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
   END ZONE
  ' SOURCE FOR ZONE 1
  1.10E+01  1.26E+02  1.41E+02  7.89E+01  1.06E+02  1.16E+02  2.26E+01
  8Z
  3.39E-01  1.60E+00  8.15E+00  2.03E+01  4.68E+04  3.78E+05  1.24E+07
  5.07E+06  3.08E+08  1.20E+09  1.32E+09  1.00E+10  2.97E+09  2.98E+08
  4.38E+08  1.60E+09  1.92E+09  6.50E+09
  ' SOURCE FOR ZONE 2
  1.10E+01  1.26E+02  1.41E+02  7.89E+01  1.06E+02  1.16E+02  2.26E+01
  8Z
  3.39E-01  1.60E+00  8.15E+00  2.03E+01  4.68E+04  3.78E+05  1.24E+07
  5.07E+06  3.08E+08  1.20E+09  1.32E+09  1.00E+10  2.97E+09  2.98E+08
  4.38E+08  1.60E+09  1.92E+09  6.50E+09
  READ XSDOSE
  595.64

  CASE 4 - LATTICECELL X-SECT PROC, COLLAPSE=YES, SOURCE SPEC FROM ORIGEN-S FILE
  CYLINDRICAL
  500  12.75  20 +1     7  0.17994     60  2  1.8679E+5  1
  3    21.72   8  0
  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
   END ZONE
  READ XSDOSE
  595.64

 MODULE SAS1X    IS FINISHED. COMPLETION CODE     0. CPU TIME USED    12.03 (SECONDS).
```

Table S1.5.11 (continued)

```
CASES 3 & 4 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=YES


**** PROBLEM PARAMETERS ****

LIB 27N-18COUPLE LIBRARY
MXX            8 MIXTURES
MSC            9 COMPOSITION SPECIFICATIONS
IZM            3 MATERIAL ZONES
GE  LATTICECELL  GEOMETRY
MORE           1 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
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       560.0 DEG KELVIN
           92000      1.00 ATOM/MOLECULE
                         92234     0.029 WT%
                         92235     3.200 WT%
                         92236     0.016 WT%
                         92238    96.755 WT%
            8016      2.00 ATOMS/MOLECULE
END

SC  ZIRCALLOY    STANDARD COMPOSITION
MX             2 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH      6.5600 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       560.0 DEG KELVIN
           40302      1.00 ATOM/MOLECULE
END

SC  SS304        STANDARD COMPOSITION
MX             3 MIXTURE NO.
VF        0.0217 VOLUME FRACTION
ROTH      7.9200 THEORETICAL DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           24304    19.000 WT%
           25055     2.000 WT%
           26304    69.500 WT%
           28304     9.500 WT%
END

SC  B4C          STANDARD COMPOSITION
MX             3 MIXTURE NO.
VF        0.0771 VOLUME FRACTION
ROTH      2.5400 THEORETICAL DENSITY
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
            5000      4.00 ATOMS/MOLECULE
                         5010    18.431 WT%
                         5011    81.569 WT%
            6012      1.00 ATOM/MOLECULE
END
```

Table S1.5.11 (continued)

```
SC  SS304          STANDARD COMPOSITION
MX              4 MIXTURE NO.
VF         1.0000 VOLUME FRACTION
ROTH       7.9200 THEORETICAL DENSITY
NEL             4 NO. ELEMENTS
ICP             0 0/1 MIXTURE/COMPOUND
            24304     19.000 WT%
            25055      2.000 WT%
            26304     69.500 WT%
            28304      9.500 WT%
END

SC  U(.27)METAL  STANDARD COMPOSITION
MX              5 MIXTURE NO.
VF         1.0000 VOLUME FRACTION
ROTH      19.0500 THEORETICAL DENSITY
NEL             2 NO. ELEMENTS
ICP             0 0/1 MIXTURE/COMPOUND
            92235      0.270 WT%
            92238     99.730 WT%
END

SC  H2O            STANDARD COMPOSITION
MX              6 MIXTURE NO.
VF         0.9440 VOLUME FRACTION
ROTH       0.9982 THEORETICAL DENSITY
NEL             2 NO. ELEMENTS
ICP             1 0/1 MIXTURE/COMPOUND
             1001       2.00 ATOMS/MOLECULE
             8016       1.00 ATOM/MOLECULE
END

SC  SS304          STANDARD COMPOSITION
MX              7 MIXTURE NO.
VF         0.1188 VOLUME FRACTION
ROTH       7.9200 THEORETICAL DENSITY
NEL             4 NO. ELEMENTS
ICP             0 0/1 MIXTURE/COMPOUND
TEMP        560.0 DEG KELVIN
            24304     19.000 WT%
            25055      2.000 WT%
            26304     69.500 WT%
            28304      9.500 WT%
END

SC  N              STANDARD COMPOSITION
MX              8 MIXTURE NO.
VF         0.0012 VOLUME FRACTION
ROTH       1.0000 THEORETICAL DENSITY
NEL             1 NO. ELEMENTS
ICP             1 0/1 MIXTURE/COMPOUND
TEMP        560.0 DEG KELVIN
             7014       1.00 ATOM/MOLECULE
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
```

Table S1.5.11 (continued)

```
MCLAD          2 MIXTURE NO. OF CLAD


**** SPECIAL PARAMETERS ****

ISN            8 ORDER OF ANGULAR QUADRATURE
IIM           20 INNER ITERATION MAXIMUM
ICM           25 OUTER ITERATION MAXIMUM
SZF  1.00000E+00 SIZE FACTOR FOR SPATIAL MESH
EPS  1.00000E-04 OVERALL PROBLEM CONVERGENCE
PTC  1.00000E-04 SCALAR FLUX CONVERGENCE
BKL  1.42089E+00 BUCKLING FACTOR
IUS            0 THERMAL UPSCATTER SCALING
BAL         FINE BALANCE TABLE PRINT FLAG
DY   0.00000E+00 BUCKLING HEIGHT
DZ   0.00000E+00 BUCKLING DEPTH
IPN            0 DIFFUSION COEFFICIENT OPTION
FRD            0 LOGICAL UNIT NUMBER TO READ FLUX GUESS
FWR           -1 LOGICAL UNIT NUMBER TO WRITE FLUX GUESS
MSH         2001 NUMBER OF INTERVALS FOR RES. INTGRTNS
MLV            2 MAX LVALUE FOR RES. INTGRTNS
AXS            0 LOGICAL UNIT NUMBER TO WRITE ANISN LIB
COLL             COLLAPSE ALL THERMAL NEUTRON GROUPS TO ONE GROUP

ZONE SPECIFICATIONS FOR LATTICECELL GEOMETRY

                ZONE  1 IS FUEL
                ZONE  2 IS CLAD
                ZONE  3 IS MOD
```

Table S1.5.11 (continued)

```
*****************************************************************************************************************
***                                                                                                           ***
***                        CASES 3 & 4 (PREP) -- LATTICECELL USED FOR X-SECT PROCESSING, COLLAPSE=YES         ***
***                                                                                                           ***
*****************************************************************************************************************
*****************************************************************************************************************
***                                                                                                           ***
***                          ********** DATA LIBRARY INFORMATION **********                                  ***
***                                                                                                           ***
***      UNIT                                                VOLUME                                           ***
***     NUMBER              DATA SET NAME                    NAME        UNIT FUNCTION                        ***
***     ------              -------------                    ----        -------------                        ***
***                                                                                                           ***
***       89       C:\scale43\DATALIB\FT89F001                          STANDARD COMPOSITION LIBRARY         ***
***                                                                                                           ***
***       88       C:\scale43\DATALIB\FT88F001                          CROSS SECTION LIBRARY                ***
***                                                                                                           ***
***       11       C:\scale43\work\FT11F001                             SHORT CROSS SECTION LIBRARY          ***
***                                                                                                           ***
***       90       C:\scale43\work\FT90F001                             INPUT DATA DIRECT ACCESS             ***
***                                                                                                           ***
*****************************************************************************************************************
*****************************************************************************************************************
***                                                                                                           ***
***                                                                                                           ***
***                                 STANDARD COMPOSITION LIBRARY DATA                                         ***
***                                 ---------------------------------                                         ***
***                                                                                                           ***
***      UNIT NUMBER  :  89                                                                                   ***
***                                                                                                           ***
***      DATASET NAME :  C:\scale43\DATALIB\FT89F001                                                          ***
***                                                                                                           ***
***      LIBRARY TITLE:  SCALE-4 STANDARD COMPOSITION LIBRARY                                                 ***
***                      637 STANDARD COMPOSITIONS, 490 NUCLIDES                                              ***
***                      90 ELEMENTS WITH VARIABLE ISOTOPIC DISTRBUTIONS.                                     ***
***                                                                                                           ***
***      CREATION DATE:   6/30/95                                                                             ***
***                                                                                                           ***
***                                                                                                           ***
***                                                                                                           ***
***                                  CROSS SECTION LIBRARY DATA                                               ***
***                                  --------------------------                                               ***
***                                                                                                           ***
***      UNIT NUMBER  :  88                                                                                   ***
***                                                                                                           ***
***      DATASET NAME :  C:\scale43\DATALIB\FT88F001                                                          ***
***                                                                                                           ***
***      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                                                 08/12/94         ***
***                              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
```

Table S1.5.11 (continued)

**** ADDITIONAL DATA ****

MIXING TABLE FROM STANDARD COMPOSITIONS DATA

| MIXTURE NO. | NUCLIDE NO. | ATOM DENSITY | N.I.T. POINTER |
|---|---|---|---|
| 1 | 1092234 | 6.50089E-06 | 454 |
| 1 | 1092235 | 7.14277E-04 | 455 |
| 5 | 5092235 | 1.31783E-04 | 455 |
| 1 | 1092236 | 3.55623E-06 | 456 |
| 1 | 1092238 | 2.13240E-02 | 458 |
| 5 | 5092238 | 4.80620E-02 | 458 |
| 1 | 1008016 | 4.40967E-02 | 33 |
| 6 | 6008016 | 3.15151E-02 | 33 |
| 2 | 2040302 | 4.33078E-02 | 179 |
| 3 | 3024304 | 3.78409E-04 | 96 |
| 4 | 4024304 | 1.74286E-02 | 96 |
| 7 | 7024304 | 2.07034E-03 | 96 |
| 3 | 3025055 | 3.76992E-05 | 98 |
| 4 | 4025055 | 1.73633E-03 | 98 |
| 7 | 7025055 | 2.06259E-04 | 98 |
| 3 | 3026304 | 1.28878E-03 | 106+ |
| 4 | 4026304 | 5.93579E-02 | 106 |
| 7 | 7026304 | 7.05113E-03 | 106 |
| 3 | 3028304 | 1.67632E-04 | 117 |
| 4 | 4028304 | 7.72070E-03 | 117 |
| 7 | 7028304 | 9.17142E-04 | 117 |
| 3 | 3005010 | 1.69854E-03 | 23 |
| 3 | 3005011 | 6.83682E-03 | 24 |
| 3 | 3006012 | 2.13384E-03 | 26 |
| 6 | 6001001 | 6.30301E-02 | 6 |
| 8 | 8007014 | 5.24670E-05 | 30 |

COMPLETE MIXING TABLE

| MIXTURE NO. | NUCLIDE NO. | ATOM DENSITY |
|---|---|---|
| 1 | 1092234 | 6.50089E-06 |
| 9 | 1092234 | 2.24678E-06 |
| 1 | 1092235 | 7.14277E-04 |
| 9 | 1092235 | 2.46862E-04 |
| 5 | 5092235 | 1.31783E-04 |
| 1 | 1092236 | 3.55623E-06 |
| 9 | 1092236 | 1.22907E-06 |
| 1 | 1092238 | 2.13240E-02 |
| 9 | 1092238 | 7.36982E-03 |
| 5 | 5092238 | 4.80620E-02 |
| 1 | 1008016 | 4.40967E-02 |
| 9 | 1008016 | 1.52403E-02 |
| 6 | 6008016 | 3.15151E-02 |
| 2 | 2040302 | 4.33078E-02 |
| 9 | 2040302 | 4.37266E-03 |
| 3 | 3024304 | 3.78409E-04 |
| 4 | 4024304 | 1.74286E-02 |
| 7 | 7024304 | 2.07034E-03 |
| 3 | 3025055 | 3.76992E-05 |
| 4 | 4025055 | 1.73633E-03 |
| 7 | 7025055 | 2.06259E-04 |
| 3 | 3026304 | 1.28878E-03 |
| 4 | 4026304 | 5.93579E-02 |
| 7 | 7026304 | 7.05113E-03 |

Table S1.5.11 (continued)

```
  3      3028304   1.67632E-04
  4      4028304   7.72070E-03
  7      7028304   9.17142E-04
  3      3005010   1.69854E-03
  3      3005011   6.83682E-03
  3      3006012   2.13384E-03
  6      6001001   6.30301E-02
  8      8007014   5.24670E-05
  9      8007014   2.90364E-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 | ABAR | DANCOFF | INNER RAD. | NSUBO | ITA | M1 | SIGMA1 | IT1 | M2 | SIGMA2 | IT2 | LUMP VOL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1092234 | 560.00 | 2 | 4.17850E-01 | 9.59610E-01 | 0.00000E+00 | 6.50089E-06 | 1 | 15.991 | 2.63660E+04 | 1 | 237.955 | 4.17470E+04 | 1 | 1.0000 |
| 1092235 | 560.00 | 2 | 4.17850E-01 | 9.59610E-01 | 0.00000E+00 | 7.14277E-04 | 1 | 15.991 | 2.39966E+02 | 1 | 238.049 | 3.68163E+02 | 1 | 1.0000 |
| 5092235 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.31783E-04 | 1 | 238.051 | 4.49548E+03 | 1 | 0.000 | 0.00000E+00 | 0 | 1.0000 |
| 1092236 | 560.00 | 2 | 4.17850E-01 | 9.59610E-01 | 0.00000E+00 | 3.55623E-06 | 1 | 15.991 | 4.81978E+04 | 1 | 237.954 | 7.63248E+04 | 1 | 1.0000 |
| 1092238 | 560.00 | 2 | 4.17850E-01 | 9.59610E-01 | 0.00000E+00 | 2.13240E-02 | 1 | 15.991 | 8.03798E+00 | 1 | 235.040 | 4.04452E-01 | 1 | 1.0000 |
| 5092238 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 4.80620E-02 | 1 | 235.044 | 3.26360E-02 | 1 | 0.000 | 0.00000E+00 | 0 | 1.0000 |
| 2040302 | 560.00 | 2 | 4.74980E-01 | 8.43998E-01 | 4.17850E-01 | 4.33078E-02 | 1 | 0.000 | 0.00000E+00 | 0 | 0.000 | 0.00000E+00 | 0 | 1.0000 |
| 3025055 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3.76992E-05 | 1 | 11.009 | 9.12983E+02 | 1 | 21.192 | 8.31474E+02 | 1 | 1.0000 |
| 4025055 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.73633E-03 | 1 | 55.845 | 3.46630E+02 | 1 | 55.925 | 1.25576E+02 | 1 | 1.0000 |
| 7025055 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 2.06259E-04 | 1 | 55.845 | 3.46630E+02 | 1 | 55.925 | 1.25576E+02 | 1 | 1.0000 |

Table S1.5.11 (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 | 1092234 | 5.60000E+02 | 0 | 1 | 3 | 4.90122E-02 | 0 |
| 2 | 1092235 | 5.60000E+02 | 4.17850E-01 | 2 | 3 | 1.44256E+00 | 0 |
| 3 | 5092235 | 2.93000E+02 | 4.74980E-01 | 8 | 3 | 0 | 0 |
| 4 | 1092236 | 5.60000E+02 | 7.10766E-01 | | | 0 | 0 |
| 5 | 1092238 | 5.60000E+02 | | | | 0 | 0 |
| 6 | 5092238 | 2.93000E+02 | | | | 0 | 0 |
| 7 | 1008016 | 5.60000E+02 | | | | 0 | 0 |
| 8 | 6008016 | 2.93000E+02 | | | | 0 | 0 |
| 9 | 2040302 | 5.60000E+02 | | | | | |
| 10 | 3024304 | 2.93000E+02 | | | | | |
| 11 | 4024304 | 2.93000E+02 | | | | | |
| 12 | 7024304 | 5.60000E+02 | | | | | |
| 13 | 3025055 | 2.93000E+02 | | | | | |
| 14 | 4025055 | 2.93000E+02 | | | | | |
| 15 | 7025055 | 5.60000E+02 | | | | | |
| 16 | 3026304 | 2.93000E+02 | | | | | |
| 17 | 4026304 | 2.93000E+02 | | | | | |
| 18 | 7026304 | 5.60000E+02 | | | | | |
| 19 | 3028304 | 2.93000E+02 | | | | | |
| 20 | 4028304 | 2.93000E+02 | | | | | |
| 21 | 7028304 | 5.60000E+02 | | | | | |
| 22 | 3005010 | 2.93000E+02 | | | | | |
| 23 | 3005011 | 2.93000E+02 | | | | | |
| 24 | 3006012 | 2.93000E+02 | | | | | |
| 25 | 6001001 | 2.93000E+02 | | | | | |
| 26 | 8007014 | 5.60000E+02 | | | | | |

Table S1.5.11 (continued)

```
**** SYSTEM GEOMETRY ****

CASE 3 -- LATTICECELL X-SECT PROC, COLLAPSE=YES, 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    6.0200E+02 NEUTRON SOURCE NORMALIZATION
XNG    2.6500E+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    6.0200E+02 NEUTRON SOURCE NORMALIZATION
XNG    2.6500E+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
```

Table S1.5.11 (continued)

```
    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
    R= 2.7322E+02  Z= 2.9782E+02

    DETECTOR NO.  4
    R= 4.7322E+02  Z= 2.9782E+02


    **** SYSTEM GEOMETRY ****

    CASE 4 - LATTICECELL X-SECT PROC, COLLAPSE=YES, 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
```

Table S1.5.11 (continued)

```
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 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 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
```

Table S1.5.12 SAS1 output for cases 9-14 with PARM=CHK

```
      PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - 95/03/29 - 09:06:37 )
MODULE SAS1     WILL BE CALLED
  CASES 9-14 (PREP) -- INFHOMMEDIUM USED FOR X-SECT PROCESSING, COLLAPSE=YES
  27N-18COUPLE  INFHOMMEDIUM
  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
  SS304   2  2.1712E-2  END
  B4C     2  7.7066E-2  END
  HE          3  END
  SS304       4  END
  U(.27)METAL  5  END
  H2O         6  0.944  END
  END COMP
  MORE DATA  COLLAPSE  END

  CASE 9 -- INFHOMMEDIUM X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; ISN,ICM=DEFAULTS
  CYLINDRICAL
  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
  6  72.78  16  0
  4  73.22   1  0
   END ZONE
  READ XSDOSE
  595.64

  CASE 10 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; ISN=8,ICM=DEFAULT
  CYLINDRICAL
  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
  6  72.78  16  0
  4  73.22   1  0
   END ZONE
  ISN=8
  READ XSDOSE
  595.64

  CASE 11 - SAME AS CASE 10, WITH AXIAL BUCKLING OF 595.64 CM USED IN XSDRN CALC
  CYLINDRICAL
  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
  6  72.78  16  0
  4  73.22   1  0
   END ZONE
  ISN=8  DY=595.64
  READ XSDOSE
  595.64
```

Table S1.5.12 (continued)

```
    CASE 12 - SAME AS CASE 10, WITH OUTER FUEL ZONE SMEARED WITH ADJACENT VOID
    CYLINDRICAL
    1  12.75  20 +1      0  0.0      60  2  1.8679E+5  1
    2  21.72   8  0
    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
    6  72.78  16  0
    4  73.22   1  0
     END ZONE
    ISN=8
    READ XSDOSE
    595.64

    CASE 13 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; NO N-SHIELD USED; ISN,ICM=DEFAULTS
    CYLINDRICAL
    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
    0  72.78  16  0
    4  73.22   1  0
     END ZONE
    READ XSDOSE
    595.64

    CASE 14 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; NO N-SHIELD USED; ISN=8,ICM=DEFAULT
    CYLINDRICAL
    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
    0  72.78  16  0
    4  73.22   1  0
     END ZONE
    ISN=8
    READ XSDOSE
    595.64

  MODULE SAS1     IS FINISHED. COMPLETION CODE     0. CPU TIME USED    16.20 (SECONDS).
```

Table S1.5.12 (continued)

```
CASES 9-14 (PREP) -- INFHOMMEDIUM USED FOR X-SECT PROCESSING, COLLAPSE=YES
**** PROBLEM PARAMETERS ****

LIB 27N-18COUPLE LIBRARY
MXX            6 MIXTURES
MSC            9 COMPOSITION SPECIFICATIONS
IZM            1 MATERIAL ZONES
GE  INFHOMMEDIUM GEOMETRY
MORE           1 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
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       560.0 DEG KELVIN
           92000      1.00 ATOM/MOLECULE
                         92234     0.029 WT%
                         92235     3.200 WT%
                         92236     0.016 WT%
                         92238    96.755 WT%
            8016      2.00 ATOMS/MOLECULE
END

SC  ZIRCALLOY    STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0828 VOLUME FRACTION
ROTH      6.5600 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       560.0 DEG KELVIN
           40302      1.00 ATOM/MOLECULE
END

SC  SS304        STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0214 VOLUME FRACTION
ROTH      7.9200 THEORETICAL DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
TEMP       560.0 DEG KELVIN
           24304    19.000 WT%
           25055     2.000 WT%
           26304    69.500 WT%
           28304     9.500 WT%
END

SC  SS304        STANDARD COMPOSITION
MX             2 MIXTURE NO.
VF        0.0217 VOLUME FRACTION
ROTH      7.9200 THEORETICAL DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           24304    19.000 WT%
           25055     2.000 WT%
           26304    69.500 WT%
           28304     9.500 WT%
END
```

Table S1.5.12 (continued)

```
SC  B4C          STANDARD COMPOSITION
MX             2 MIXTURE NO.
VF        0.0771 VOLUME FRACTION
ROTH      2.5400 THEORETICAL DENSITY
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
             5000      4.00 ATOMS/MOLECULE
                          5010    18.431 WT%
                          5011    81.569 WT%
             6012      1.00 ATOM/MOLECULE
END

SC  HE           STANDARD COMPOSITION
MX             3 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH      1.0000 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
             2004      1.00 ATOM/MOLECULE
END

SC  SS304        STANDARD COMPOSITION
MX             4 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH      7.9200 THEORETICAL DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
            24304    19.000 WT%
            25055     2.000 WT%
            26304    69.500 WT%
            28304     9.500 WT%
END

SC  U(.27)METAL  STANDARD COMPOSITION
MX             5 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH     19.0500 THEORETICAL DENSITY
NEL            2 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
            92235     0.270 WT%
            92238    99.730 WT%
END

SC  H2O          STANDARD COMPOSITION
MX             6 MIXTURE NO.
VF        0.9440 VOLUME FRACTION
ROTH      0.9982 THEORETICAL DENSITY
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
             1001      2.00 ATOMS/MOLECULE
             8016      1.00 ATOM/MOLECULE
END


**** PROBLEM GEOMETRY ****


**** INFINITE HOMOGENEOUS MEDIUM ****
MFUEL          1 MIXTURE NO. OF THE INFINITE HOMOGENEOUS MEDIUM

**** SPECIAL PARAMETERS ****

ISN            8 ORDER OF ANGULAR QUADRATURE
IIM           20 INNER ITERATION MAXIMUM
```

Table S1.5.12 (continued)

```
ICM           25 OUTER ITERATION MAXIMUM
SZF  1.00000E+00 SIZE FACTOR FOR SPATIAL MESH
EPS  1.00000E-04 OVERALL PROBLEM CONVERGENCE
PTC  1.00000E-04 SCALAR FLUX CONVERGENCE
BKL  1.42089E+00 BUCKLING FACTOR
IUS            0 THERMAL UPSCATTER SCALING
BAL         FINE BALANCE TABLE PRINT FLAG
DY   0.00000E+00 BUCKLING HEIGHT
DZ   0.00000E+00 BUCKLING DEPTH
IPN            0 DIFFUSION COEFFICIENT OPTION
FRD            0 LOGICAL UNIT NUMBER TO READ FLUX GUESS
FWR           -1 LOGICAL UNIT NUMBER TO WRITE FLUX GUESS
MSH         2001 NUMBER OF INTERVALS FOR RES. INTGRTNS
MLV            2 MAX LVALUE FOR RES. INTGRTNS
AXS            0 LOGICAL UNIT NUMBER TO WRITE ANISN LIB
COLL             COLLAPSE ALL THERMAL NEUTRON GROUPS TO ONE GROUP
```

Table S1.5.12 (continued)

```
*********************************************************************************************************************
***                                                                                                               ***
***                        CASES 9-14 (PREP) -- INFHOMMEDIUM USED FOR X-SECT PROCESSING, COLLAPSE=YES             ***
***                                                                                                               ***
*********************************************************************************************************************
*********************************************************************************************************************
***                                                                                                               ***
***                          ********** DATA LIBRARY INFORMATION **********                                      ***
***                                                                                                               ***
***     UNIT                                                    VOLUME                                            ***
***    NUMBER              DATA SET NAME                         NAME        UNIT FUNCTION                         ***
***    ------              -------------                         ----        -------------                         ***
***                                                                                                               ***
***      89     C:\scale43\DATALIB\FT89F001                                  STANDARD COMPOSITION LIBRARY          ***
***                                                                                                               ***
***      88     C:\scale43\DATALIB\FT88F001                                  CROSS SECTION LIBRARY                 ***
***                                                                                                               ***
***      11     C:\scale43\work\FT11F001                                     SHORT CROSS SECTION LIBRARY           ***
***                                                                                                               ***
***      90     C:\scale43\work\FT90F001                                     INPUT DATA DIRECT ACCESS              ***
***                                                                                                               ***
*********************************************************************************************************************
*********************************************************************************************************************
***                                                                                                               ***
***                                                                                                               ***
***                              STANDARD COMPOSITION LIBRARY DATA                                                ***
***                              ---------------------------------                                                ***
***                                                                                                               ***
***       UNIT NUMBER  :  89                                                                                      ***
***                                                                                                               ***
***       DATASET NAME :  C:\scale43\DATALIB\FT89F001                                                             ***
***                                                                                                               ***
***       LIBRARY TITLE:  SCALE-4 STANDARD COMPOSITION LIBRARY                                                    ***
***                       637 STANDARD COMPOSITIONS, 490 NUCLIDES                                                 ***
***                       90 ELEMENTS WITH VARIABLE ISOTOPIC DISTRBUTIONS.                                        ***
***                                                                                                               ***
***       CREATION DATE:   6/30/95                                                                                ***
***                                                                                                               ***
***                                                                                                               ***
***                                                                                                               ***
***                                  CROSS SECTION LIBRARY DATA                                                   ***
***                                 ---------------------------                                                   ***
***                                                                                                               ***
***       UNIT NUMBER  :  88                                                                                      ***
***                                                                                                               ***
***       DATASET NAME :  C:\scale43\DATALIB\FT88F001                                                             ***
***                                                                                                               ***
***       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                                                    08/12/94          ***
***                               L.M.PETRIE        ORNL                                                        ***
***                                                                                                               ***
***                                                                                                               ***
***                                                                                                               ***
***                                                                                                               ***
*********************************************************************************************************************
*********************************************************************************************************************
```

Table S1.5.12 (continued)

**** ADDITIONAL DATA ****

MIXING TABLE FROM STANDARD COMPOSITIONS DATA

| MIXTURE NO. | NUCLIDE NO. | ATOM DENSITY | N.I.T. POINTER |
|---|---|---|---|
| 1 | 1092234 | 1.84223E-06 | 454 |
| 1 | 1092235 | 2.02412E-04 | 455 |
| 5 | 5092235 | 1.31783E-04 | 455 |
| 1 | 1092236 | 1.00777E-06 | 456 |
| 1 | 1092238 | 6.04282E-03 | 458 |
| 5 | 5092238 | 4.80620E-02 | 458 |
| 1 | 1008016 | 1.24962E-02 | 33 |
| 6 | 6008016 | 3.15151E-02 | 33 |
| 1 | 1040302 | 3.58675E-03 | 179 |
| 1 | 1024304 | 3.72536E-04 | 96 |
| 2 | 2024304 | 3.78409E-04 | 96 |
| 4 | 4024304 | 1.74286E-02 | 96 |
| 1 | 1025055 | 3.71140E-05 | 98 |
| 2 | 2025055 | 3.76992E-05 | 98 |
| 4 | 4025055 | 1.73633E-03 | 98 |
| 1 | 1026304 | 1.26878E-03 | 106 |
| 2 | 2026304 | 1.28878E-03 | 106 |
| 4 | 4026304 | 5.93579E-02 | 106 |
| 1 | 1028304 | 1.65030E-04 | 117 |
| 2 | 2028304 | 1.67632E-04 | 117 |
| 4 | 4028304 | 7.72070E-03 | 117 |
| 2 | 2005010 | 1.69854E-03 | 23 |
| 2 | 2005011 | 6.83682E-03 | 24 |
| 2 | 2006012 | 2.13384E-03 | 26 |
| 3 | 3002004 | 1.50456E-01 | 15 |
| 6 | 6001001 | 6.30301E-02 | 6 |

COMPLETE MIXING TABLE

| MIXTURE NO. | NUCLIDE NO. | ATOM DENSITY |
|---|---|---|
| 1 | 1092234 | 1.84223E-06 |
| 1 | 1092235 | 2.02412E-04 |
| 5 | 5092235 | 1.31783E-04 |
| 1 | 1092236 | 1.00777E-06 |
| 1 | 1092238 | 6.04282E-03 |
| 5 | 5092238 | 4.80620E-02 |
| 1 | 1008016 | 1.24962E-02 |
| 6 | 6008016 | 3.15151E-02 |
| 1 | 1040302 | 3.58675E-03 |
| 1 | 1024304 | 3.72536E-04 |
| 2 | 2024304 | 3.78409E-04 |
| 4 | 4024304 | 1.74286E-02 |
| 1 | 1025055 | 3.71140E-05 |
| 2 | 2025055 | 3.76992E-05 |
| 4 | 4025055 | 1.73633E-03 |
| 1 | 1026304 | 1.26878E-03 |
| 2 | 2026304 | 1.28878E-03 |
| 4 | 4026304 | 5.93579E-02 |
| 1 | 1028304 | 1.65030E-04 |
| 2 | 2028304 | 1.67632E-04 |
| 4 | 4028304 | 7.72070E-03 |
| 2 | 2005010 | 1.69854E-03 |
| 2 | 2005011 | 6.83682E-03 |
| 2 | 2006012 | 2.13384E-03 |

Table S1.5.12 (continued)

```
  3     3002004   1.50456E-01
  6     6001001   6.30301E-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
```

Table S1.5.11 (continued)

RESONANCE DATA (3* ARRAY)

| ID | TEMP | GEOM | ABAR | DANCOFF | INNER RAD. | NSUBO | ITA | M1 | SIGMA1 | IT1 | M2 | SIGMA2 | IT2 | LUMP VOL |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 1092234 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.84223E-06 | 1 | 15.991 | 2.63660E+04 | 1 | 131.863 | 6.41355E+04 | 1 | 1.0000 |
| 1092235 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 2.02412E-04 | 1 | 15.991 | 2.39966E+02 | 1 | 130.677 | 5.71928E+02 | 1 | 1.0000 |
| 5092235 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.31783E-04 | 1 | 238.051 | 4.49548E+03 | 1 | 0.000 | 0.00000E+00 | 0 | 1.0000 |
| 1092236 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.00777E-06 | 1 | 15.991 | 4.81978E+04 | 1 | 131.868 | 1.17252E+05 | 1 | 1.0000 |
| 1092238 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 6.04282E-03 | 1 | 15.991 | 8.03798E+00 | 1 | 74.712 | 7.22985E+00 | 1 | 1.0000 |
| 5092238 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 4.80620E-02 | 1 | 235.044 | 3.26360E-02 | 1 | 0.000 | 0.00000E+00 | 0 | 1.0000 |
| 1040302 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3.58675E-03 | 1 | 15.991 | 1.35421E+01 | 1 | 148.290 | 2.63771E+01 | 1 | 1.0000 |
| 1025055 | 560.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3.71140E-05 | 1 | 15.991 | 1.30873E+03 | 1 | 132.112 | 3.17998E+03 | 1 | 1.0000 |
| 2025055 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3.76992E-05 | 1 | 11.009 | 9.12983E+02 | 1 | 21.192 | 8.31474E+02 | 1 | 1.0000 |
| 4025055 | 293.00 | 0 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 1.73633E-03 | 1 | 55.845 | 3.46630E+02 | 1 | 55.925 | 1.25576E+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 | 1092234 | 5.60000E+02 | 0 | 1 | 3 | 0 | 0 |
| 2 | 1092235 | 5.60000E+02 | 1.00000E+00 | | | 0 | 0 |
| 3 | 5092235 | 2.93000E+02 | | | | 0 | 0 |
| 4 | 1092236 | 5.60000E+02 | | | | 0 | 0 |
| 5 | 1092238 | 5.60000E+02 | | | | 0 | 0 |
| 6 | 5092238 | 2.93000E+02 | | | | 0 | 0 |
| 7 | 1008016 | 5.60000E+02 | | | | | |
| 8 | 6008016 | 2.93000E+02 | | | | | |
| 9 | 1040302 | 5.60000E+02 | | | | | |
| 10 | 1024304 | 5.60000E+02 | | | | | |
| 11 | 2024304 | 2.93000E+02 | | | | | |
| 12 | 4024304 | 2.93000E+02 | | | | | |
| 13 | 1025055 | 5.60000E+02 | | | | | |
| 14 | 2025055 | 2.93000E+02 | | | | | |
| 15 | 4025055 | 2.93000E+02 | | | | | |
| 16 | 1026304 | 5.60000E+02 | | | | | |
| 17 | 2026304 | 2.93000E+02 | | | | | |
| 18 | 4026304 | 2.93000E+02 | | | | | |
| 19 | 1028304 | 5.60000E+02 | | | | | |
| 20 | 2028304 | 2.93000E+02 | | | | | |
| 21 | 4028304 | 2.93000E+02 | | | | | |
| 22 | 2005010 | 2.93000E+02 | | | | | |
| 23 | 2005011 | 2.93000E+02 | | | | | |
| 24 | 2006012 | 2.93000E+02 | | | | | |
| 25 | 3002004 | 2.93000E+02 | | | | | |
| 26 | 6001001 | 2.93000E+02 | | | | | |

Table S1.5.12 (continued)

```
**** SYSTEM GEOMETRY ****

CASE 9 -- INFHOMMEDIUM X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; 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             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
```

Table S1.5.12 (continued)

```
IMZ             1 MESH INTERVALS

SOURCE SPECTRUM NO.  1 FROM ORIGEN-S
POSITION  2 FOR 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 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 10 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; N-SHIELD PRESENT; ISN=8,ICM=DEFAULT

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.
```

Table S1.5.12 (continued)

```
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 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 DAYS

OPTIONAL PARAMETERS

ISN             8 ORDER OF ANGULAR QUADRATURE


**** 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
```

Table S1.5.12 (continued)

```
DETECTOR NO.  4
R= 4.7322E+02  Z= 2.9782E+02


**** SYSTEM GEOMETRY ****

CASE 11 - SAME AS CASE 10, WITH AXIAL BUCKLING OF 595.64 CM USED IN XSDRN CALC

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
```

Table S1.5.12 (continued)

```
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 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 DAYS

OPTIONAL PARAMETERS

ISN              8 ORDER OF ANGULAR QUADRATURE
DY  5.95640E+02 BUCKLING HEIGHT OF SLAB OR CYLINDER


**** 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 12 - SAME AS CASE 10, WITH OUTER FUEL ZONE SMEARED WITH ADJACENT VOID

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
```

Table S1.5.12 (continued)

```
ZONE NUMBER     3
MXZ             1 MIXTURE NO.
RZ          47.63 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS
ISZ             2 SOURCE SPECTRUM NO.
MIXC            0 MIXTURE NUMBER FOR HOMOGENIZED CORE
VFC        0.4568 VOLUME FRACTION FOR MIXC MATERIAL
NSOU           60 ORIGEN-S SOURCE UNIT NO.
NPOS            2 ORIGEN-S SOURCE POSITION
ZVOL   2.0647E+06 ZONE VOLUME
NASS            6 NO OF FUEL ASSEMBLIES IN ZONE

ZONE NUMBER     4
MXZ             4 MIXTURE NO.
RZ          48.90 CM RIGHT BOUNDARY LOCATION
IMZ             2 MESH INTERVALS

ZONE NUMBER     5
MXZ             5 MIXTURE NO.
RZ          57.40 CM RIGHT BOUNDARY LOCATION
IMZ            30 MESH INTERVALS

ZONE NUMBER     6
MXZ             4 MIXTURE NO.
RZ          61.35 CM RIGHT BOUNDARY LOCATION
IMZ             6 MESH INTERVALS

ZONE NUMBER     7
MXZ             6 MIXTURE NO.
RZ          72.78 CM RIGHT BOUNDARY LOCATION
IMZ            16 MESH INTERVALS

ZONE NUMBER     8
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 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 DAYS

OPTIONAL PARAMETERS

ISN             8 ORDER OF ANGULAR QUADRATURE


**** 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
```

Table S1.5.12 (continued)

```
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 13 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; 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
```

Table S1.5.12 (continued)

```
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 1826.3 DAYS

 SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
 POSITION  2 FOR 1826.3 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 14 - INFHOMMEDIUM X-SECTS; COLLAPSE=Y; NO N-SHIELD USED; ISN=8,ICM=DEFAULT

 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
```

Table S1.5.12 (continued)

```
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 1826.3 DAYS

SOURCE SPECTRUM NO.  2 FROM ORIGEN-S
POSITION  2 FOR 1826.3 DAYS

OPTIONAL PARAMETERS

ISN              8 ORDER OF ANGULAR QUADRATURE


**** 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 S1.5.12 (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
```

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# 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 lattice-cell calculations are performed, determining the neutron spectrum and, subsequently, the nuclide cross sections. 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.

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. 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 (α,n) reactions with oxygen 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, 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, to 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 the computer time limitations. The SAS2 control module provides an automated sequence to generate the radiation source, performs a 1-D radiation transport analysis through the side of a cask, and evaluates 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 through 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

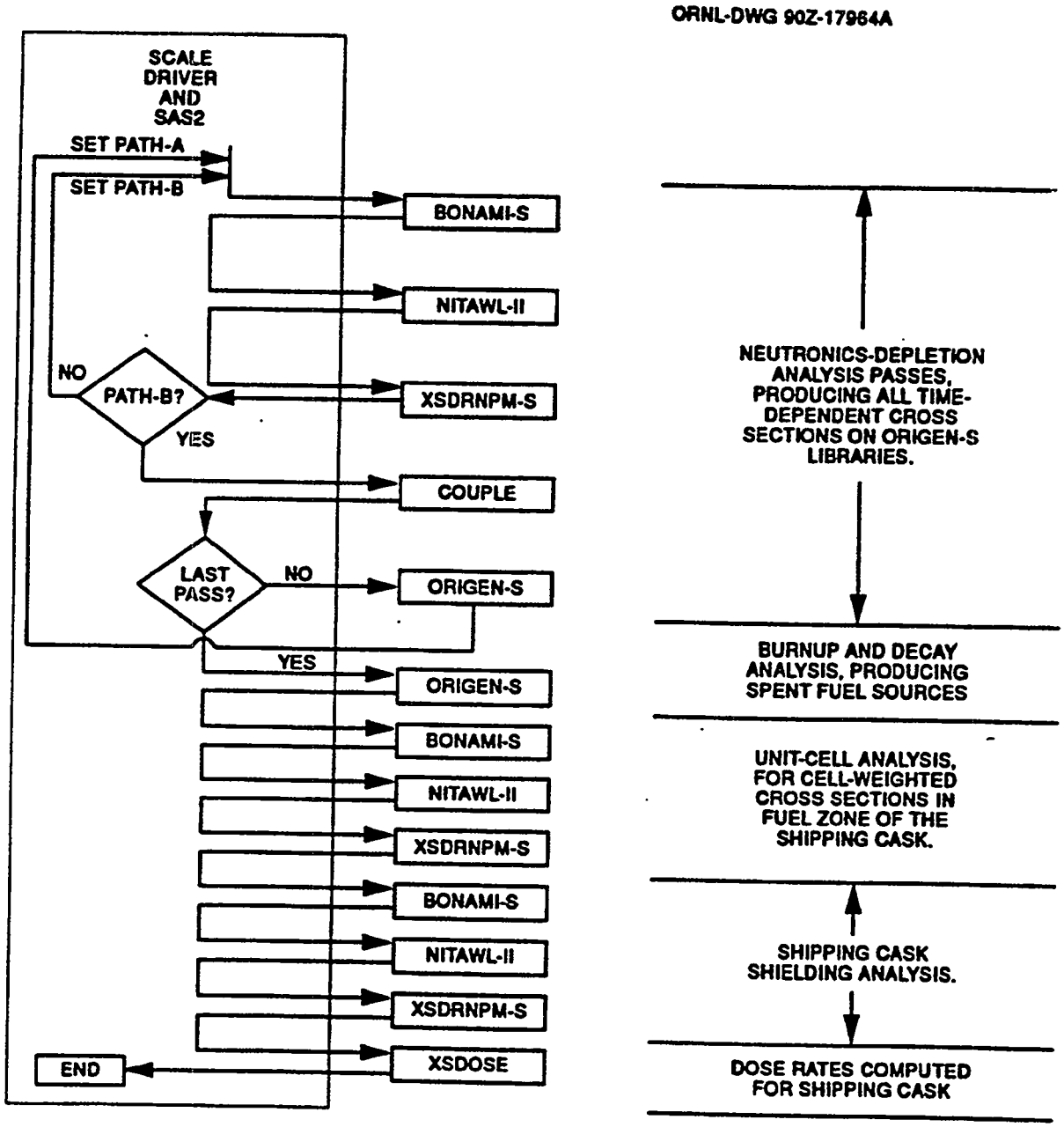



Figure S2.2.1 Computational flow chart for the SAS2H procedure

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 (see Sect. S2.6.7 for an example). Also, the fuel assembly housing material, or casing, and channel moderator between assemblies may be added by conserving volumes. A fuel assembly in which only part of the guide tubes contain burnable poison rods during a specified operating cycle is analyzed by an approximate effective mock-up, conserving material mass. Assembly rod spacers and other hardware that may be present are usually ignored. However, if their effects are estimated to be significant, they may be input by using zone average or effective densities. Reactor types, other than PWRs and BWRs, in which the path-B models require more than one fuel zone may also be represented within certain conditions or limitations.

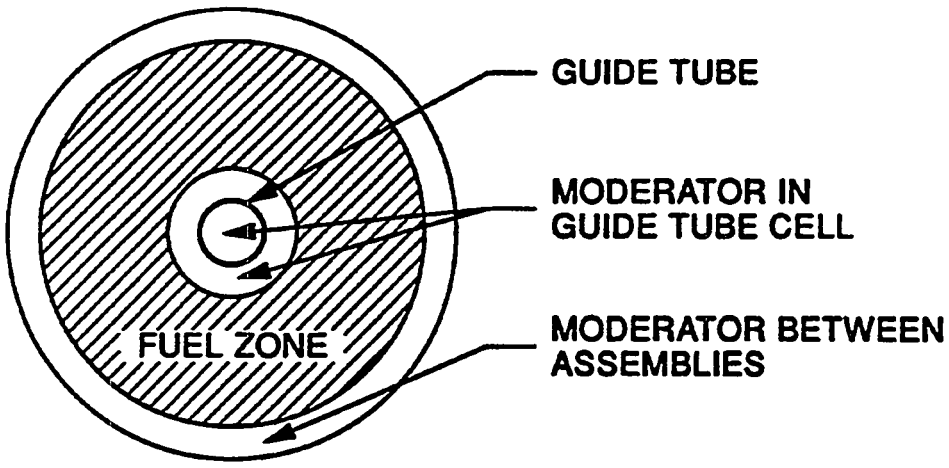
Although there is a distinct improvement in the geometry applied by SAS2H over that of earlier versions, there still remain geometrical approximations. In designing assemblies there appears to be an attempt to have control rods or burnable poison pins separated at equal distances. But, in practice, these 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

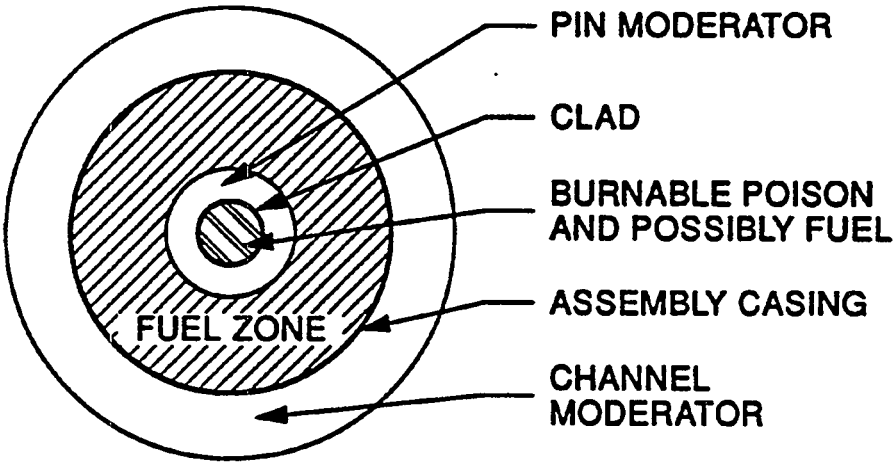
To prepare the fuel cross-section library for ORIGEN-S, the SAS2H sequence uses several SCALE functional modules. Fundamentally, the chief function of the SAS2 control module is to convert user input data, plus data available within the SCALE system into the input required by these functional modules 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; 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

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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

ets 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 ($1 \times 10^{-20}$ atoms/b-cm) of those actinides that are both on the specified neutron cross-section library and in the Block Data list for the OMMON/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.

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).

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) 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

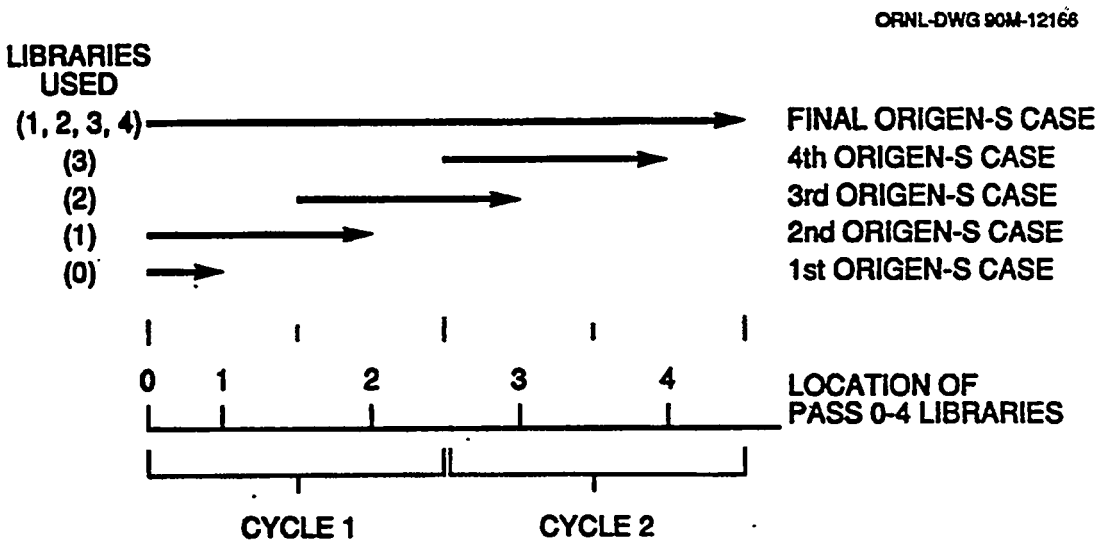



Figure S2.2.3 Schematic of successive ORIGEN-S cases used to produce the burnup-dependent number densities

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 multiburnup-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 in the fuel. In the case where the fission-product nuclide is input in both the clad and the fuel, the computation for production and depletion in the fuel is calculated for the nuclide as an FP isotope, and the depletion and activation product calculation in the clad is treated for the nuclide as an LE isotope. 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 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 ($k_\infty$) 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 multiburnup-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, $\nu_{sf}$, 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 $\nu_{sf}$ data are taken from Ref. 8. Measured values are available for 21 nuclides, including the most significant. An equation, derived[8] to compute $\nu_{sf}$, produces values that 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 $(\alpha,n)$ 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 small percentage of the spontaneous fission and $(\alpha,n)$ neutron source in spent PWR fuel over a 10-year decay time. The next largest contribution is usually from the $(\alpha,n)$ reaction of alphas from $^{238}Pu$, which is approximately 1 to 2% of the source. Neutron energy spectra of both the spontaneous fission and $(\alpha,n)$ reactions have been determined for the curium isotopes[14,15] and $^{238}Pu$ (Ref. 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 $(\alpha,n)$ neutron spectra were determined by extrapolating the neutron spectrum from Po-$\alpha$-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 $(\alpha,n)$ 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 $(\alpha,n)$ 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-d cooling time, approximately 0.01% at 90 d, 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 kg 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-d 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 $\nu_{sf}$ 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-d half-life of $^{242}Cm$. By considering the uncertainty of the thick target $(\alpha,n)$ 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 $(\alpha,n)$ 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 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, NITAWL-II, and XSDRNPM 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 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.

The XSDRNPM 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 $(n,\gamma)$ 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, $\Sigma_T$, 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 $i$,
$\Sigma_a$ = macroscopic absorption cross section of zone $i$,
$\Sigma_t$ = 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
$Y_2 = [1+9/(10^b - 1)]_{\text{truncated}}$
$Y = \max(Y_1, Y_2)$ (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 (BPRs), 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 d 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 calculations 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 d 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 ($\alpha$,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 ($\alpha$,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 d 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 $1\sigma$.

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 $\Sigma$ be the linear attenuation coefficient or total cross section, $I_o$ and $I$ be the incident and transmitted intensities, $\sigma$ 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 $\Sigma$ 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 affect 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 $\Sigma x$, 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 $1\sigma$ of the source spectrum is 10 to 15%; other $1\sigma$ 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 $1\sigma$ 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 $(n,\gamma)$ 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 that 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, MIPID, 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:** BPMOCK, RD1S2H, RD2S2H, SETGEO, MTAB2H, S2HBON, S2HNIT, S2HXSD, S2HOUT

**Utility Routines:** BALNCE, 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 BPMOCK, 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 optional call to MPMOCK is triggered if the input (BPRNUM) specified that only part of the guide tubes contain burnable poison rods (BPRs). Then the mock-up geometry is derived by conserving mass, and a material balance table of BPRs is printed by BALNCE. 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.

### S.2.4.6 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, WRFT33

**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. ORIGEN-S libraries produced in the previous pass through COUPLE are consolidated into a final library by WRFT33.

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 ($1 \times 10^{-20}$ 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 the 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 ≤ 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.

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: 44GROUPNDF5 (recommended); 27BURNUPLIB (next alternative); 27GROUPNDF4; 238GROUPNDF5; HANSEN-ROACH; or for any other name the code uses library on unit number 70. See Sect. M4 for more information on available libraries |
| | GE | Reactor lattice type. SAS2 always requires LATTICECELL<br>Example: 44GROUPNDF5 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<br>Examples: UO2 1 0.94 1000 92235 3.1 92238 96.9 END<br>FE 4 0 4.2-3 END<br>SS304 6 END |
| | END COMP* | Ends entire material data input. See Data Note A and Table M7.4.5 for more information |

Table S2.5.1 (continued)

| Data block | Name or keyword | Definitions, comments, and examples |
|---|---|---|
| | CPT | Type of fuel lattice: SQUAREPITCH, TRIANGPITCH, or SYMMSLABCELL only allowed in SAS2 |
| | PITCH | Center-to-center spacing between fuel pins or fuel slabs, cm |
| | FUELOD | Outside diameter of fuel in pin or fuel thickness in slab, cm |
| | MFUEL | Mixture number of fuel. Always enter 1 in SAS2 |
| | MMOD | Moderator mixture number. Always 3 in SAS2 |
| 5 | CLADOD | Clad outside diameter of rod or distance between outer clad surfaces of slab, cm. There must be SC for clad. |
| | MCLAD | Clad mixture number. Always 2 in SAS2 |
| | CLADID | Clad inside diameter of rod or distance between inner clad surfaces of slab, 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<br>Example: SQUAREPITCH 1.5 0.94 1 3 1.06 2 END |
| | 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<br>Example: MORE DATA ISN=16 SZF=0.9 END |

Table S2.5.1 (continued)

| Data block | Name or keyword | Definitions, comments, and examples |
|---|---|---|
| | | (The first seven 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.) |
| | VOLFUELTOT=* | Total volume of the fuel (MX=1) in the entire assembly or quantity to which POWER applies, $cm^3$. Always applied if non-zero. Do not enter for cylindrical fuel rods. Always enter for slab-lattice. See Data Note B for discussion of slab. (0.0) |
| | INPLEVEL=* | Input level of data below (0) |
| | 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 |
| 7 | 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 |
| | BPRNUM=* | Array data of number of burnable poison rods (BPRs) per assembly for each library segment of the NCYCLES*NLIB/CYC libraries. (First entry applies to first segment of first cycle, etc.) Not required if no BPRs or if all guide tubes contain BPRs. May omit final zeroes in the array. See next entry. Never required unless INPLEVEL=2 or 3. See Data Note F for discussion of BPRs. |
| | GTHOLENUM=* | Number of guide tubes without BPRs per assembly in first cycle of case. The number of guide tubes without BPRs for the remaining cycles is known implicitly by the total number of guide tubes minus BPRNUM. May include if BPRNUM is input or let code compute it. Never required unless INPLEVEL=2 or 3. See Data Note F. |
| | FACMESH=* | Mesh size factor: Interval size = (default size)(FACMESH) is applied (1.0). Required if INPLEVEL=2 or 3 |
| | LIMINTGEO=* | Upper limit to the number of geometry intervals, after the default interval sizes and FACMESH are applied. If this value is exceeded, FACMESH is increased to where LIMINTGEO is not exceeded (200). Required only 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<br>(Enter NCYCLES* NLIB/CYC times if MXREPEATS=0) | | (Repeat the following, as pairs of data, NUMZTOTAL times.) |
| | MIXES | Mixture number of path-B zone, inner zone first. The next pair of data applies to the adjacent zone, etc. Use 500 for the fuel zone, composed of densities of the homogenized path-A unit cell computed by code. Use mixture numbers 50 to 59, inclusive, for additional fuel zones. Required if INPLEVEL = 2 or 3 |
| | RADIUS | Outer radius of zone; ascending order, cm<br>Example: 3 1.3 2 1.4 3 1.7 500 5.197<br>5 6.1 7 8.2 50 12.6 7 16.1 500 22.2 6 30.1 |
| 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 power (megawatts) of either the assembly, an extended assembly increased to FUELNGTH, or the total fuel volume (if VOLFUELTOT > 0.0) |
| | BURN=* | Fuel irradiation period of reactor, d |
| | DOWN=* | Downtime, d, 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<br>Example: POWER=15.2 BURN=330 DOWN=35.25 END |
| 10<br>(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<br>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 | | (Repeat pair of entries NUMZONES times. See Data |
| (Enter NUMZONES times) | MXZ | 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 |

Table S2.5.1 (continued)

| Data block | Name or keyword | Definitions, comments, and examples |
|---|---|---|
| 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<br>Example: ZONE=1 FUELBNDL=1 ZONE=3 FUELBNDL=5 |
| 15 | | (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<br>(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) |
| | 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.

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.

#### 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. The recommended library to use for most LWR cases is denoted by 44GROUPNDF5. 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≤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≥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 $4 \le MX \le 10$ 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 $MX \ge 4$ 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.

Table S2.5.2 Density of subcooled water (g/cm³) 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 | 1.0018 | 1.0004 | 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)

| Temperature (°C) | Temperature (°F) | Pressure, psia ≤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 | 0.9467 | 0.9276 | 0.9035 | 0.8858 | 0.8717 |
| | (T-sat, °F) | (115.6) | (138.3) | (163.9) | (181.1) | (193.9) |

### 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 1. The boron change over the reactor history can then be approximated using the BFRAC entry. Note that if H2OFRAC and BFRAC are equal, the boron concentration remains constant. Where important shutdowns or power magnitudes change within the refueling cycle, it may be logical to increase the number of cycles.

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 or 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;
NUMHOLES = $(\sqrt{\text{NPIN/ASSM}}|_{\text{trunc}} + 1)^2 - (\text{NPIN/ASSM}) - 1$;
NUMINSTR = 1;
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.

Although the primary application of SAS2 is to the depletion analysis of PWR or BWR fuel assemblies, the SAS2 procedure may adequately apply to other types of reactors. These reactors include the Canadian deuterium-uranium reactor (CANDU), the High Flux Isotope Reactor (HFIR), the materials testing reactor (MTR), the Molten Salt Reactor Experient (MSRE), and possibly other types. SAS2 accepts either the cylindrical fuel rod geometry of PWRs and BWRs, or fuel plates (slab geometry) of MTRs and the HFIR. Also, the use of multiple fuel zones (e.g., as in the HFIR) may be included in the input by using mixture numbers 50 to 59, inclusive. Then, additional standard composition data may specify other material additions to these fuel zones by using the same mixture numbers (i.e., MIXES=MX). The code computes the total fuel volume for cylindrical geometry from the fuel pin input and NPIN/ASSM. However, the total fuel volume, VOLFUELTOT, is required if specifying a slab geometry. Then, POWER must be the power (megawatts) for the volume of fuel equaling VOLFUELTOT. Although some reactors or their fuel assemblies are not adequately described by the limited features of SAS2, it is possible to sufficiently model the entire core of other reactors.

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.

Burnable poison rods (BPRs) in current PWR designs typically contain borosilicate glass and clad located within all or part of the guide tubes of the fuel assembly. The Level-2 input described above applies to the case in which BPRs are coupled into all of the guide tubes. However, in normal reactor operations, the BPRs are frequently contained in only part of the guide tubes. An option is provided in SAS2 that uses an approximate

mockup to effectively analyze the fuel assembly during cycles in which the guide tubes are partially filled with BPRs.[42] The number of BPRs is entered in BPRNUM and the number of guide tubes without BPRs in the starting cycle may be entered in GTHOLENUM. As a default, GTHOLENUM is

$$\text{GTHOLENUM} = (\sqrt{\text{NPIN/ASSM}}|_{\text{trunc}} + 1)^2 - (\text{NPIN/ASSM}) - \text{NUMINS} - \text{BPRNUM(1)} .$$

The input to BPRNUM is array data for the number of library segments, NCYCLES*NLIB/CYC (or the number of cycles if NLIB/CYC = 1). The later data entries to BPRNUM may be omitted if all remaining data are zeroes (usually the case after the first cycle). Note that Data Bock 8 does not need to be repeated if MXREPEAT=1, which is permitted when using BPRNUM data. Also, the user's labrious precalculation of effective mock-up BPR input data is unnecessary in applying this option.

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. Different methods are used to obtain "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

## 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 $k_\infty$, Final Case | |
| 1. Neutron production, absorption and $k_\infty$ | 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 | L≥1 |
| value of L in the above tests. | 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.

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.

### 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. Second, 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, 43, and 44 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,

$\sigma_a$ = 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-d 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 corner 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

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 multiburnup binary library |
| 60 | 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.

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))

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≤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≥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≥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). This option requires INPLEVEL=0 in Data Block 7.

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 xxxxxxxx.

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. Four libraries 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. Note 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 guide tubes per fuel 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 = $1.55 \times 10^7$ 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. 43. 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 = $1.032 \times 10^5$ 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$^3$
$\rho$(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
$\rho_{H2O}$ (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 |

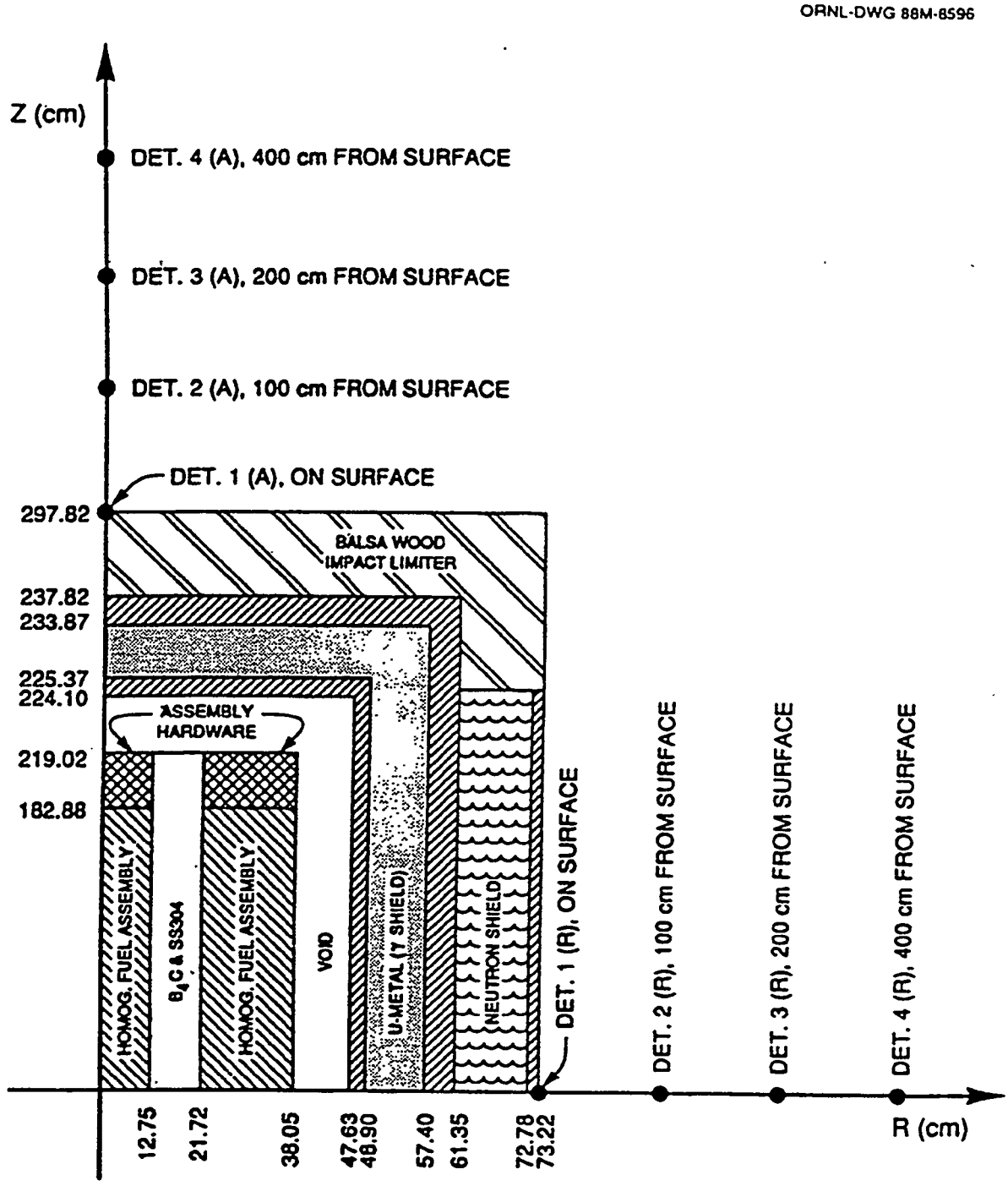



Figure S2.6.1 Model of shipping cask for PWR fuel assemblies

## 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  0  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
```

**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 with SCALE 4.3. Subsequent updates to SCALE 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 | 1.38 |
| 2 | 5 | 4.79 | 1.54 |
| 3A | 5 | 4.61 | 1.55 |
| 3B | 10 | 1.86 | 1.29 |

## 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 0 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
```

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 0 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
```

## 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[45,46] at various positions on the surface of the cask. Note: the assembly design and reactor moderator density data[46] used in this case are different than that for the assemblies in the measurements because the readily available data[45,46] 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[45,46] 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. 47. 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 48 and Sect. M6.7 by similarly applying data from Tables 3.7, 4.3, and 4.4 of Ref. 43. Gadolinium content is computed from data in Table S2.6.4. The $^{59}Co$ contents in Ref. 43 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. 45 and Table 4.1 of Ref. 46) 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 % $Gd_2O_3$ |

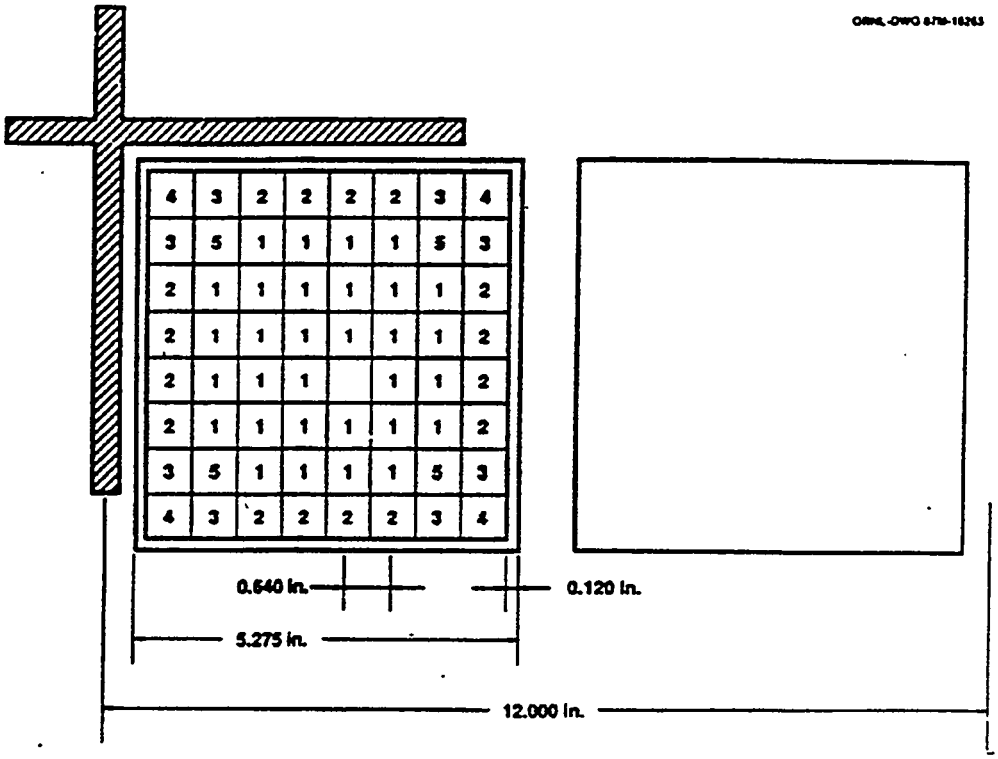



Figure S2.6.2 BWR assembly schematic for sample case 4

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. 45 and 46 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[49] 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
```

## 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 2-m detector. Even though none of the output from sample cases 2 and 3 are shown, the dose rates computed at the 2-m detector are listed in Table S2.6.3. Note that the output of all of these cases 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
```

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     1.4696E+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 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 | 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

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 | MIXING TABLE MIXTURE | COMPONENT | ATOM DENSITY | EXTRA XSECT ID'S |
|---|---|---|---|---|---|---|
| 1 | 999 | | 1 | 92234 | 6.27728E-06 | |
| 2 | 1001 | | 1 | 92235 | 7.14337E-04 | |
| 3 | 5010 | | 1 | 92236 | 3.33426E-06 | |
| 4 | 5011 | | 1 | 92238 | 2.13264E-02 | |
| 5 | 8016 | | 1 | 8016 | 4.41006E-02 | |
| 6 | 6 | | 3 | 6 | 2.45150E-02 | |
| 7 | 27059 | | 2 | 40302 | 4.33078E-02 | |
| 8 | 40302 | | 3 | 1001 | 4.90301E-02 | |
| 9 | 54135 | | 3 | 5010 | 6.47995E-06 | |
| 10 | 55133 | | 3 | 5011 | 2.60826E-05 | |
| 11 | 92234 | | 3 | 27059 | 1.02186E-22 | |
| 12 | 92235 | | 1 | 54135 | 1.00000E-20 | |
| 13 | 92236 | | 1 | 55133 | 1.00000E-20 | |
| 14 | 92238 | | 1 | 93237 | 1.00000E-20 | |
| 15 | 93237 | | 1 | 94238 | 1.00000E-20 | |
| 16 | 94238 | | 1 | 94239 | 1.00000E-20 | |
| 17 | 94239 | | 1 | 94240 | 1.00000E-20 | |
| 18 | 94240 | | 1 | 94241 | 1.00000E-20 | |
| 19 | 94241 | | 1 | 94242 | 1.00000E-20 | |
| 20 | 94242 | | 1 | 95241 | 1.00000E-20 | |
| 21 | 95241 | | 1 | 95243 | 1.00000E-20 | |
| 22 | 95243 | | 1 | 96244 | 1.00000E-20 | |
| 23 | 96244 | | 1 | 999 | 1.00000E-20 | |

15507 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     2.45150E-02              201
   2        3        1001     4.90301E-02              202
   3        3        5010     6.47995E-06              203
   4        3        5011     2.60826E-05              204
   5        3       27059     1.02186E-22              205
   6        2       40302     4.33078E-02              206
   7        1       92234     2.16915E-06           200007
   8        1       92235     2.46843E-04           200008
   9        1       92236     1.15217E-06           200009
  10        1       92238     7.36945E-03           200010
  11        1        8016     1.52392E-02           200011
  12        1        8016     1.35679E-02           200012
  13        1       40302     4.37381E-03           200013
  14        1        1001     2.71357E-02           200014
  15        1        5010     3.58633E-06           200015
  16        1        5011     1.44354E-05           200016
  17        1       27059     5.65548E-23           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
```

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 | EXTRA XSECT ID'S |
|---|---|---|---|---|---|---|
| 1 | 202 | | 3 | 201 | 2.45150E-02 | |
| 2 | 203 | | 3 | 202 | 4.90301E-02 | |
| 3 | 204 | | 3 | 203 | 6.47995E-06 | |
| 4 | 201 | | 3 | 204 | 2.60826E-05 | |
| 5 | 205 | | 3 | 205 | 1.02186E-22 | |
| 6 | 206 | | 2 | 206 | 4.33078E-02 | |
| 7 | 999 | | 1 | 92234 | 2.16915E-06 | |
| 8 | 1001 | | 1 | 92235 | 2.46843E-04 | |
| 9 | 5010 | | 1 | 92236 | 1.15217E-06 | |
| 10 | 5011 | | 1 | 92238 | 7.36945E-03 | |
| 11 | 8016 | | 1 | 8016 | 1.52392E-02 | |
| 12 | 6 | | 1 | 6 | 1.35679E-02 | |
| 13 | 27059 | | 1 | 40302 | 4.37381E-03 | |
| 14 | 40302 | | 1 | 1001 | 2.71357E-02 | |
| 15 | 54135 | | 1 | 5010 | 3.58633E-06 | |
| 16 | 55133 | | 1 | 5011 | 1.44354E-05 | |
| 17 | 92234 | | 1 | 27059 | 5.65548E-23 | |
| 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 | |

19939 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 ACTINIDES PAGE 1
POWER= 1.968E-04MW, BURNUP=8.6574E-02MWD, FLUX= 4.01E+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 | 2.61E-10 | 1.57E-09 | 6.67E-09 | 2.19E-08 |
| U230 | 0.00E+00 | 8.76E-22 | 2.58E-21 | 5.78E-21 | 1.16E-20 |
| U231 | 0.00E+00 | 2.74E-20 | 6.64E-20 | 1.35E-19 | 2.54E-19 |
| U232 | 0.00E+00 | 1.65E-13 | 4.29E-13 | 9.05E-13 | 1.71E-12 |
| U233 | 0.00E+00 | 1.37E-11 | 2.41E-11 | 3.20E-11 | 3.79E-11 |
| U234 | 6.28E-06 | 5.93E-06 | 5.61E-06 | 5.29E-06 | 4.98E-06 |
| U235 | 7.14E-04 | 6.11E-04 | 5.22E-04 | 4.44E-04 | 3.76E-04 |
| U236 | 3.33E-06 | 2.20E-05 | 3.75E-05 | 5.06E-05 | 6.17E-05 |
| U237 | 0.00E+00 | 7.71E-08 | 1.09E-07 | 1.40E-07 | 1.68E-07 |
| U238 | 2.13E-02 | 2.13E-02 | 2.12E-02 | 2.11E-02 | 2.11E-02 |
| U239 | 0.00E+00 | 1.12E-08 | 1.12E-08 | 1.15E-08 | 1.18E-08 |
| U240 | 0.00E+00 | 6.98E-39 | 1.11E-35 | 8.09E-34 | 1.69E-32 |
| U241 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| NP235 | 0.00E+00 | 3.64E-15 | 1.76E-14 | 4.47E-14 | 8.70E-14 |
| NP236M | 0.00E+00 | 2.04E-14 | 5.36E-14 | 9.85E-14 | 1.54E-13 |
| NP236 | 0.00E+00 | 2.62E-13 | 1.34E-12 | 3.57E-12 | 7.28E-12 |
| NP237 | 0.00E+00 | 5.79E-07 | 1.52E-06 | 2.72E-06 | 4.13E-06 |
| NP238 | 0.00E+00 | 1.47E-09 | 3.88E-09 | 7.12E-09 | 1.12E-08 |
| NP239 | 0.00E+00 | 1.62E-06 | 1.62E-06 | 1.66E-06 | 1.71E-06 |
| NP240M | 0.00E+00 | 5.96E-41 | 9.45E-38 | 6.90E-36 | 1.44E-34 |
| NP240 | 0.00E+00 | 5.45E-11 | 5.46E-11 | 5.72E-11 | 6.10E-11 |
| NP241 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| PU236 | 0.00E+00 | 3.43E-13 | 1.71E-12 | 4.43E-12 | 8.81E-12 |
| PU237 | 0.00E+00 | 7.61E-14 | 1.93E-13 | 3.17E-13 | 4.64E-13 |
| PU238 | 0.00E+00 | 2.26E-08 | 1.14E-07 | 2.98E-07 | 5.99E-07 |
| PU239 | 0.00E+00 | 4.00E-05 | 6.52E-05 | 8.06E-05 | 9.00E-05 |
| PU240 | 0.00E+00 | 3.20E-06 | 8.97E-06 | 1.45E-05 | 1.89E-05 |
| PU241 | 0.00E+00 | 7.30E-07 | 3.96E-06 | 9.32E-06 | 1.56E-05 |
| PU242 | 0.00E+00 | 2.17E-08 | 2.48E-07 | 9.38E-07 | 2.25E-06 |
| PU243 | 0.00E+00 | 5.45E-12 | 6.24E-11 | 2.42E-10 | 6.01E-10 |
| PU244 | 0.00E+00 | 3.48E-28 | 5.52E-25 | 4.03E-23 | 8.43E-22 |
| PU245 | 0.00E+00 | 6.19E-34 | 9.84E-31 | 7.37E-29 | 1.59E-27 |
| PU246 | 0.00E+00 | 6.42E-36 | 1.02E-32 | 7.86E-31 | 1.76E-29 |
| AM239 | 0.00E+00 | 7.96E-20 | 8.59E-19 | 3.07E-18 | 6.95E-18 |
| AM240 | 0.00E+00 | 3.42E-17 | 3.70E-16 | 1.33E-15 | 3.01E-15 |
| AM241 | 0.00E+00 | 2.70E-09 | 2.91E-08 | 1.01E-07 | 2.22E-07 |
| AM242M | 0.00E+00 | 2.54E-11 | 4.50E-10 | 2.01E-09 | 5.11E-09 |
| AM242 | 0.00E+00 | 7.05E-12 | 7.60E-11 | 2.72E-10 | 6.15E-10 |
| AM243 | 0.00E+00 | 4.22E-10 | 9.91E-09 | 5.86E-08 | 1.96E-07 |
| AM244M | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| AM244 | 0.00E+00 | 2.86E-13 | 6.73E-12 | 4.08E-11 | 1.41E-10 |
| AM245 | 0.00E+00 | 4.61E-32 | 6.94E-29 | 4.93E-27 | 1.01E-25 |
| AM246 | 0.00E+00 | 1.60E-38 | 2.56E-35 | 1.96E-33 | 4.39E-32 |
| CM241 | 0.00E+00 | 2.48E-21 | 1.72E-19 | 1.76E-18 | 8.29E-18 |
| CM242 | 0.00E+00 | 1.31E-10 | 2.76E-09 | 1.44E-08 | 4.23E-08 |
| CM243 | 0.00E+00 | 4.72E-13 | 1.98E-11 | 1.56E-10 | 6.16E-10 |
| CM244 | 0.00E+00 | 8.98E-12 | 4.35E-10 | 4.02E-09 | 1.88E-08 |
| CM245 | 0.00E+00 | 4.97E-14 | 4.61E-12 | 6.16E-11 | 3.72E-10 |
| CM246 | 0.00E+00 | 5.72E-16 | 1.09E-13 | 2.28E-12 | 1.91E-11 |
| CM247 | 0.00E+00 | 9.19E-19 | 3.52E-16 | 1.11E-14 | 1.26E-13 |

Figure S2.6.10 Part of ORIGEN-S actinide table of PASS 0

POWER= 1.968E-04MW, BURNUP=8.6574E-02MWD, FLUX= 4.01E+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 |
|---|---|---|---|---|---|
| CM248 | 0.00E+00 | 6.59E-21 | 5.15E-18 | 2.50E-16 | 3.93E-15 |
| CM248 | 0.00E+00 | 6.59E-21 | 5.15E-18 | 2.50E-16 | 3.93E-15 |
| CM249 | 0.00E+00 | 7.83E-26 | 6.14E-23 | 3.06E-21 | 4.96E-20 |
| CM250 | 0.00E+00 | 3.98E-30 | 6.35E-27 | 4.87E-25 | 1.09E-23 |
| CM251 | 0.00E+00 | 2.36E-37 | 3.77E-34 | 2.97E-32 | 6.85E-31 |
| TOTALS | 2.21E-02 | 2.20E-02 | 2.19E-02 | 2.18E-02 | 2.17E-02 |
| FLUX | | 3.92E+13 | 3.93E+13 | 4.03E+13 | 4.16E+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 (continued)

13Q ARRAY HAS 23 ENTRIES.

14Q ARRAY HAS 23 ENTRIES.

15Q ARRAY HAS 23 ENTRIES.

DATA BLOCK 2 (MIXING TABLE, ETC.)

| NUCLIDES | CCCC | MIXING TABLE | | | EXTRA |
|---|---|---|---|---|---|
| ON TAPE | IDENTIFICATION | MIXTURE | COMPONENT | ATOM DENSITY | XSECT ID'S |
| 1 999 | | 1 | 92234 | 4.98491E-06 | |
| 2 1001 | | 1 | 92235 | 3.76136E-04 | |
| 3 5010 | | 1 | 92236 | 6.16618E-05 | |
| 4 5011 | | 1 | 92238 | 2.10881E-02 | |
| 5 8016 | | 1 | 8016 | 4.41006E-02 | |
| 6 6 | | 3 | 6 | 2.45150E-02 | |
| 7 27059 | | 2 | 40302 | 4.33078E-02 | |
| 8 40302 | | 3 | 1001 | 4.90301E-02 | |
| 9 54135 | | 3 | 5010 | 4.46893E-06 | |
| 10 55133 | | 3 | 5011 | 1.79880E-05 | |
| 11 92234 | | 3 | 27059 | 1.02186E-22 | |
| 12 92235 | | 1 | 54135 | 8.24237E-09 | |
| 13 92236 | | 1 | 55133 | 2.40421E-05 | |
| 14 92238 | | 1 | 93237 | 4.12985E-06 | |
| 15 93237 | | 1 | 94238 | 5.98876E-07 | |
| 16 94238 | | 1 | 94239 | 8.99544E-05 | |
| 17 94239 | | 1 | 94240 | 1.88569E-05 | |
| 18 94240 | | 1 | 94241 | 1.56412E-05 | |
| 19 94241 | | 1 | 94242 | 2.25334E-06 | |
| 20 94242 | | 1 | 95241 | 2.22100E-07 | |
| 21 95241 | | 1 | 95243 | 1.95977E-07 | |
| 22 95243 | | 1 | 96244 | 1.88089E-08 | |
| 23 96244 | | 1 | 999 | 1.00000E-20 | |

15507 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

POWER= 17.30MW, BURNUP= 15226.MWD, FLUX= 4.17E+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 | 1.54E-03 | 8.47E-03 | 2.73E-02 |
| PB206 | 0.00E+00 | 1.33E-18 | 2.73E-17 | 1.71E-16 | 6.81E-16 |
| PB207 | 0.00E+00 | 2.80E-15 | 3.49E-14 | 1.53E-13 | 4.28E-13 |
| PB208 | 0.00E+00 | 6.85E-12 | 7.10E-11 | 3.34E-10 | 1.09E-09 |
| PB209 | 0.00E+00 | 2.44E-18 | 1.47E-17 | 5.46E-17 | 1.54E-16 |
| PB210 | 0.00E+00 | 1.14E-15 | 7.79E-15 | 2.92E-14 | 8.16E-14 |
| PB211 | 0.00E+00 | 2.00E-18 | 1.18E-17 | 3.27E-17 | 6.58E-17 |
| PB212 | 0.00E+00 | 6.45E-14 | 3.79E-13 | 1.31E-12 | 3.40E-12 |
| PB214 | 0.00E+00 | 7.31E-20 | 2.58E-19 | 5.12E-19 | 7.99E-19 |
| RA222 | 0.00E+00 | 7.32E-21 | 2.98E-20 | 8.84E-20 | 2.06E-19 |
| RA223 | 0.00E+00 | 9.12E-16 | 5.37E-15 | 1.49E-14 | 3.00E-14 |
| RA224 | 0.00E+00 | 5.32E-13 | 3.13E-12 | 1.08E-11 | 2.80E-11 |
| RA225 | 0.00E+00 | 2.66E-16 | 1.60E-15 | 5.97E-15 | 1.68E-14 |
| RA226 | 0.00E+00 | 2.30E-12 | 8.12E-12 | 1.61E-11 | 2.51E-11 |
| RA228 | 0.00E+00 | 3.67E-19 | 2.39E-18 | 7.04E-18 | 1.48E-17 |
| TH226 | 0.00E+00 | 3.57E-19 | 1.45E-18 | 4.31E-18 | 1.00E-17 |
| TH227 | 0.00E+00 | 1.47E-15 | 8.67E-15 | 2.41E-14 | 4.84E-14 |
| TH228 | 0.00E+00 | 1.02E-10 | 5.97E-10 | 2.06E-09 | 5.34E-09 |
| TH229 | 0.00E+00 | 4.99E-12 | 2.75E-11 | 1.01E-10 | 3.07E-10 |
| TH230 | 0.00E+00 | 7.79E-07 | 1.29E-06 | 1.57E-06 | 1.67E-06 |
| TH231 | 0.00E+00 | 1.57E-09 | 2.50E-09 | 3.20E-09 | 3.64E-09 |
| TH232 | 0.00E+00 | 3.43E-08 | 1.14E-07 | 2.25E-07 | 3.54E-07 |
| TH233 | 0.00E+00 | 5.91E-14 | 2.03E-13 | 4.31E-13 | 7.34E-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 | 6.83E-07 | 9.93E-07 |
| PA232 | 0.00E+00 | 2.13E-10 | 6.52E-10 | 1.28E-09 | 2.01E-09 |
| PA233 | 0.00E+00 | 3.72E-09 | 1.10E-08 | 2.03E-08 | 3.04E-08 |
| PA234M | 0.00E+00 | 9.29E-13 | 9.28E-13 | 9.27E-13 | 9.26E-13 |
| PA234 | 0.00E+00 | 9.04E-13 | 1.91E-12 | 3.38E-12 | 5.21E-12 |
| PA235 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| U230 | 0.00E+00 | 3.46E-16 | 1.41E-15 | 4.18E-15 | 9.73E-15 |
| U231 | 0.00E+00 | 7.20E-15 | 2.64E-14 | 7.49E-14 | 1.71E-13 |
| U232 | 0.00E+00 | 4.32E-08 | 1.69E-07 | 4.64E-07 | 9.96E-07 |
| U233 | 0.00E+00 | 2.44E-06 | 3.79E-06 | 4.46E-06 | 4.68E-06 |
| U234 | 5.52E-01 | 4.90E-01 | 4.33E-01 | 3.80E-01 | 3.29E-01 |
| U235 | 6.28E+01 | 4.57E+01 | 3.29E+01 | 2.31E+01 | 1.58E+01 |
| U236 | 2.93E-01 | 3.38E+00 | 5.55E+00 | 7.06E+00 | 8.03E+00 |
| U237 | 0.00E+00 | 9.60E-03 | 1.41E-02 | 1.83E-02 | 2.20E-02 |
| U238 | 1.88E+03 | 1.86E+03 | 1.85E+03 | 1.84E+03 | 1.83E+03 |
| U239 | 0.00E+00 | 1.04E-03 | 1.07E-03 | 1.15E-03 | 1.23E-03 |
| U240 | 0.00E+00 | 8.62E-31 | 1.31E-27 | 9.56E-26 | 1.99E-24 |
| U241 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| NP235 | 0.00E+00 | 1.85E-09 | 8.79E-09 | 2.21E-08 | 4.22E-08 |
| NP236M | 0.00E+00 | 5.61E-09 | 1.51E-08 | 2.86E-08 | 4.51E-08 |
| NP236 | 0.00E+00 | 1.41E-07 | 7.39E-07 | 2.03E-06 | 4.22E-06 |
| NP237 | 0.00E+00 | 1.37E-01 | 3.59E-01 | 6.29E-01 | 9.17E-01 |
| NP238 | 0.00E+00 | 3.62E-04 | 9.78E-04 | 1.85E-03 | 2.91E-03 |
| NP239 | 0.00E+00 | 1.51E-01 | 1.54E-01 | 1.66E-01 | 1.78E-01 |
| NP240M | 0.00E+00 | 7.36E-33 | 1.12E-29 | 8.16E-28 | 1.70E-26 |
| NP240 | 0.00E+00 | 5.33E-06 | 5.63E-06 | 6.51E-06 | 7.54E-06 |
| NP241 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 | 0.00E+00 |
| PU236 | 0.00E+00 | 1.80E-07 | 8.93E-07 | 2.33E-06 | 4.57E-06 |
| PU237 | 0.00E+00 | 2.13E-08 | 4.99E-08 | 9.53E-08 | 1.70E-07 |
| PU238 | 0.00E+00 | 1.07E-02 | 5.38E-02 | 1.43E-01 | 2.84E-01 |
| PU239 | 0.00E+00 | 6.26E+00 | 8.80E+00 | 9.77E+00 | 1.01E+01 |
| PU240 | 0.00E+00 | 8.97E-01 | 2.12E+00 | 2.97E+00 | 3.43E+00 |
| PU241 | 0.00E+00 | 2.56E-01 | 1.12E+00 | 2.15E+00 | 2.97E+00 |
| PU242 | 0.00E+00 | 1.51E-02 | 1.46E-01 | 4.75E-01 | 9.75E-01 |
| PU243 | 0.00E+00 | 4.01E-06 | 4.00E-05 | 1.40E-04 | 3.10E-04 |
| PU244 | 0.00E+00 | 4.29E-20 | 6.53E-17 | 4.76E-15 | 9.92E-14 |
| PU245 | 0.00E+00 | 7.65E-26 | 1.20E-22 | 9.44E-21 | 2.12E-19 |
| PU246 | 0.00E+00 | 8.08E-28 | 1.31E-24 | 1.11E-22 | 2.69E-21 |
| AM239 | 0.00E+00 | 5.93E-14 | 5.13E-13 | 1.49E-12 | 2.70E-12 |
| AM240 | 0.00E+00 | 2.55E-11 | 2.22E-10 | 6.45E-10 | 1.17E-09 |
| AM241 | 0.00E+00 | 1.86E-03 | 1.56E-02 | 4.20E-02 | 7.06E-02 |
| AM242M | 0.00E+00 | 2.71E-05 | 3.33E-04 | 1.06E-03 | 1.94E-03 |
| AM242 | 0.00E+00 | 4.64E-06 | 4.02E-05 | 1.17E-04 | 2.12E-04 |
| AM243 | 0.00E+00 | 6.29E-04 | 1.29E-02 | 6.73E-02 | 1.97E-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 PAGE 13
DECAY, FOLLOWING REACTOR IRRADIATION IDENTIFIED BY: POWER= 17.30MW, BURNUP= 15226.MWD, FLUX= 4.17E+13N/CM**2-SEC

NUCLIDE CONCENTRATIONS, GRAM ATOMS
BASIS = SINGLE REACTOR ASSEMBLY

| | INITIAL | 304.4 D | 608.8 D | 913.1 D | 1217.5 D | 1521.9 D | 1826.3 D |
|---|---|---|---|---|---|---|---|
| HE 4 | 2.73E-02 | 4.98E-02 | 5.92E-02 | 6.50E-02 | 6.99E-02 | 7.47E-02 | 7.94E-02 |
| TH230 | 1.67E-06 | 2.45E-06 | 3.23E-06 | 4.01E-06 | 4.80E-06 | 5.60E-06 | 6.40E-06 |
| TH232 | 3.54E-07 | 5.52E-07 | 7.50E-07 | 9.48E-07 | 1.15E-06 | 1.34E-06 | 1.54E-06 |
| PA231 | 9.93E-07 | 1.01E-06 | 1.02E-06 | 1.04E-06 | 1.05E-06 | 1.06E-06 | 1.07E-06 |
| U232 | 9.96E-07 | 1.82E-06 | 2.48E-06 | 3.01E-06 | 3.44E-06 | 3.79E-06 | 4.06E-06 |
| U233 | 4.68E-06 | 4.96E-06 | 5.25E-06 | 5.53E-06 | 5.82E-06 | 6.11E-06 | 6.39E-06 |
| U234 | 3.29E-01 | 3.31E-01 | 3.33E-01 | 3.35E-01 | 3.37E-01 | 3.39E-01 | 3.41E-01 |
| U235 | 1.58E+01 | 1.58E+01 | 1.58E+01 | 1.58E+01 | 1.58E+01 | 1.58E+01 | 1.58E+01 |
| U236 | 8.03E+00 | 8.03E+00 | 8.03E+00 | 8.03E+00 | 8.03E+00 | 8.03E+00 | 8.03E+00 |
| U238 | 1.83E+03 | 1.83E+03 | 1.83E+03 | 1.83E+03 | 1.83E+03 | 1.83E+03 | 1.83E+03 |
| NP236 | 4.22E-06 | 4.22E-06 | 4.22E-06 | 4.22E-06 | 4.22E-06 | 4.22E-06 | 4.22E-06 |
| NP237 | 9.17E-01 | 9.39E-01 | 9.39E-01 | 9.40E-01 | 9.40E-01 | 9.41E-01 | 9.42E-01 |
| PU236 | 4.57E-06 | 3.77E-06 | 3.09E-06 | 2.53E-06 | 2.07E-06 | 1.70E-06 | 1.39E-06 |
| PU238 | 2.84E-01 | 3.03E-01 | 3.06E-01 | 3.06E-01 | 3.04E-01 | 3.02E-01 | 3.00E-01 |
| PU239 | 1.01E+01 | 1.03E+01 | 1.03E+01 | 1.03E+01 | 1.03E+01 | 1.03E+01 | 1.03E+01 |
| PU240 | 3.43E+00 | 3.43E+00 | 3.43E+00 | 3.43E+00 | 3.43E+00 | 3.43E+00 | 3.43E+00 |
| PU241 | 2.97E+00 | 2.85E+00 | 2.74E+00 | 2.63E+00 | 2.53E+00 | 2.43E+00 | 2.33E+00 |
| PU242 | 9.75E-01 | 9.75E-01 | 9.75E-01 | 9.75E-01 | 9.75E-01 | 9.75E-01 | 9.75E-01 |
| AM241 | 7.06E-02 | 1.88E-01 | 3.00E-01 | 4.08E-01 | 5.11E-01 | 6.10E-01 | 7.05E-01 |
| AM242M | 1.94E-03 | 1.94E-03 | 1.93E-03 | 1.92E-03 | 1.91E-03 | 1.91E-03 | 1.90E-03 |
| AM243 | 1.97E-01 | 1.97E-01 | 1.97E-01 | 1.97E-01 | 1.97E-01 | 1.97E-01 | 1.97E-01 |
| CM242 | 2.51E-02 | 6.93E-03 | 1.90E-03 | 5.25E-04 | 1.47E-04 | 4.40E-05 | 1.56E-05 |
| CM243 | 7.35E-04 | 7.20E-04 | 7.06E-04 | 6.91E-04 | 6.78E-04 | 6.64E-04 | 6.51E-04 |
| CM244 | 4.66E-02 | 4.53E-02 | 4.39E-02 | 4.25E-02 | 4.12E-02 | 3.99E-02 | 3.86E-02 |
| CM245 | 1.70E-03 | 1.70E-03 | 1.70E-03 | 1.70E-03 | 1.70E-03 | 1.70E-03 | 1.70E-03 |
| CM246 | 2.10E-04 | 2.09E-04 | 2.09E-04 | 2.09E-04 | 2.09E-04 | 2.09E-04 | 2.09E-04 |
| CM247 | 3.03E-06 | 3.03E-06 | 3.03E-06 | 3.03E-06 | 3.03E-06 | 3.03E-06 | 3.03E-06 |
| TOTAL | 1.87E+03 | 1.87E+03 | 1.87E+03 | 1.87E+03 | 1.87E+03 | 1.87E+03 | 1.87E+03 |

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 | 1.2481E+15 | 3.7443E+13 |
| 5.0000E-02 TO | 1.0000E-01 | 3.6968E+14 | 2.7726E+13 |
| 1.0000E-01 TO | 2.0000E-01 | 3.0824E+14 | 4.6236E+13 |
| 2.0000E-01 TO | 3.0000E-01 | 8.4463E+13 | 2.1116E+13 |
| 3.0000E-01 TO | 4.0000E-01 | 5.7983E+13 | 2.0294E+13 |
| 4.0000E-01 TO | 6.0000E-01 | 5.7129E+14 | 2.8565E+14 |
| 6.0000E-01 TO | 8.0000E-01 | 1.8986E+15 | 1.3290E+15 |
| 8.0000E-01 TO | 1.0000E+00 | 2.5066E+14 | 2.2559E+14 |
| 1.0000E+00 TO | 1.3300E+00 | 2.2467E+14 | 2.6174E+14 |
| 1.3300E+00 TO | 1.6600E+00 | 5.8644E+13 | 8.7672E+13 |
| 1.6600E+00 TO | 2.0000E+00 | 1.0093E+12 | 1.8471E+12 |
| 2.0000E+00 TO | 2.5000E+00 | 2.5303E+12 | 5.6931E+12 |
| 2.5000E+00 TO | 3.0000E+00 | 7.5170E+10 | 2.0672E+11 |
| 3.0000E+00 TO | 4.0000E+00 | 9.3162E+09 | 3.2607E+10 |
| 4.0000E+00 TO | 5.0000E+00 | 3.7096E+06 | 1.6693E+07 |
| 5.0000E+00 TO | 6.5000E+00 | 1.4886E+06 | 8.5593E+06 |
| 6.5000E+00 TO | 8.0000E+00 | 2.9197E+05 | 2.1168E+06 |
| 8.0000E+00 TO | 1.0000E+01 | 6.1984E+04 | 5.5786E+05 |
| TOTALS | | 5.0760E+15 | 2.3503E+15 |

TOTAL ENERGY FROM NUCLIDES WITH SPECTRUM DATA = 2.3502E+15

TOTAL ENERGY FROM NUCLIDES WITH NO SPECTRUM DATA = 5.7962E+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 ORIGEN-S neutron source spectrum

M I X I N G  T A B L E

| ENTRY | MIXTURE | ISOTOPE | NUMBER DENSITY | NEW IDENTIFIER |
|---|---|---|---|---|
| 1 | 1 | 92234 | 1.10085E-06 | 92234 |
| 2 | 2 | 92234 | 1.10010E-06 | 1000002 |
| 3 | 1 | 92235 | 5.08348E-05 | 92235 |
| 4 | 2 | 92235 | 5.08000E-05 | 1000004 |
| 5 | 6 | 92235 | 1.31783E-04 | 28 |
| 6 | 1 | 92236 | 2.58815E-05 | 92236 |
| 7 | 2 | 92236 | 2.58638E-05 | 1000007 |
| 8 | 1 | 92238 | 5.89485E-03 | 92238 |
| 9 | 2 | 92238 | 5.89081E-03 | 1000009 |
| 10 | 6 | 92238 | 4.80620E-02 | 33 |
| 11 | 1 | 8016 | 1.25034E-02 | 8016 |
| 12 | 2 | 8016 | 1.24948E-02 | 1000012 |
| 13 | 9 | 8016 | 3.15151E-02 | 36 |
| 14 | 1 | 40302 | 3.58860E-03 | 40302 |
| 15 | 2 | 40302 | 3.58614E-03 | 1000015 |
| 16 | 1 | 54135 | 2.83519E-19 | 54135 |
| 17 | 2 | 54135 | 2.83325E-19 | 1000017 |
| 18 | 1 | 55133 | 1.28740E-05 | 55133 |
| 19 | 2 | 55133 | 1.28652E-05 | 1000019 |
| 20 | 1 | 93237 | 3.03707E-06 | 93237 |
| 21 | 2 | 93237 | 3.03499E-06 | 1000021 |
| 22 | 1 | 94238 | 9.67482E-07 | 94238 |
| 23 | 2 | 94238 | 9.66819E-07 | 1000023 |
| 24 | 1 | 94239 | 3.31291E-05 | 94239 |
| 25 | 2 | 94239 | 3.31064E-05 | 1000025 |
| 26 | 1 | 94240 | 1.10648E-05 | 94240 |
| 27 | 2 | 94240 | 1.10573E-05 | 1000027 |
| 28 | 1 | 94241 | 7.52311E-06 | 94241 |
| 29 | 2 | 94241 | 7.51795E-06 | 1000029 |
| 30 | 1 | 94242 | 3.14259E-06 | 94242 |
| 31 | 2 | 94242 | 3.14044E-06 | 1000031 |
| 32 | 1 | 95241 | 2.27267E-06 | 95241 |
| 33 | 2 | 95241 | 2.27111E-06 | 1000033 |
| 34 | 1 | 95243 | 6.35873E-07 | 95243 |
| 35 | 2 | 95243 | 6.35437E-07 | 1000035 |
| 36 | 1 | 96244 | 1.24576E-07 | 96244 |
| 37 | 2 | 96244 | 1.24491E-07 | 1000037 |
| 38 | 9 | 1001 | 6.30301E-02 | 61 |
| 39 | 3 | 5010 | 1.69854E-03 | 62 |
| 40 | 3 | 5011 | 6.83682E-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 | 3.71140E-05 | 25055 |
| 46 | 2 | 25055 | 3.71140E-05 | 69 |
| 47 | 3 | 25055 | 3.76992E-05 | 70 |
| 48 | 5 | 25055 | 1.73633E-03 | 71 |
| 49 | 1 | 26304 | 1.26878E-03 | 26304 |
| 50 | 2 | 26304 | 1.26878E-03 | 73 |
| 51 | 3 | 26304 | 1.28878E-03 | 74 |
| 52 | 5 | 26304 | 5.93579E-02 | 75 |
| 53 | 1 | 28304 | 1.65030E-04 | 28304 |
| 54 | 2 | 28304 | 1.65030E-04 | 77 |
| 55 | 3 | 28304 | 1.67632E-04 | 78 |
| 56 | 5 | 28304 | 7.72070E-03 | 79 |
| 57 | 1 | 7014 | 2.90142E-05 | 7014 |
| 58 | 2 | 7014 | 2.90142E-05 | 81 |
| 59 | 4 | 7014 | 4.30057E-22 | 82 |
| 60 | 3 | 6012 | 2.13384E-03 | 6012 |

Figure S2.6.16 BONAMI mixing table of cell-weighted case

```
THIS XSDRN WORKING TAPE WAS CREATED 09/07/95 AT 04:30:00
THE TITLE OF THE PARENT CASE IS AS FOLLOWS
THIS XSDRN WORKING TAPE WAS CREATED 09/07/95 AT 04:30:00
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 08/12/94        ID       61
   BORON-10        ENDF/B-IV MAT 1273                       UPDATED 08/12/94        ID       62
   BORON-11        ENDF/B-IV MAT 1160                       UPDATED 08/12/94        ID       63
   CARBON-12       ENDF/B-IV MAT 1274/THRM1065              UPDATED 08/12/94        ID     6012
   NITROGEN-14     ENDF/B-IV MAT 1275                       UPDATED 08/12/94        ID     7014
   NITROGEN-14     ENDF/B-IV MAT 1275                       UPDATED 08/12/94        ID       81
   NITROGEN-14     ENDF/B-IV MAT 1275                       UPDATED 08/12/94        ID       82
   OXYGEN-16       ENDF/B-IV MAT 1276                       UPDATED 08/12/94        ID       36
   CHROMIUM(SS304)ENDF/B-IV MAT 1191                        UPDATED 08/12/94        ID    24304
   CHROMIUM(SS304)ENDF/B-IV MAT 1191                        UPDATED 08/12/94        ID       65
   CHROMIUM(SS304)ENDF/B-IV MAT 1191                        UPDATED 08/12/94        ID       66
   CHROMIUM(SS304)ENDF/B-IV MAT 1191                        UPDATED 08/12/94        ID       67
   MANGANESE       ENDF/B-IV MAT 1197                       UPDATED 08/12/94        ID    25055
   MANGANESE       ENDF/B-IV MAT 1197                       UPDATED 08/12/94        ID       69
   MANGANESE       ENDF/B-IV MAT 1197                       UPDATED 08/12/94        ID       70
   MANGANESE       ENDF/B-IV MAT 1197                       UPDATED 08/12/94        ID       71
   IRON(SS304)     ENDF/B-IV MAT 1192                       UPDATED 08/12/94        ID    26304
   IRON(SS304)     ENDF/B-IV MAT 1192                       UPDATED 08/12/94        ID       73
   IRON(SS304)     ENDF/B-IV MAT 1192                       UPDATED 08/12/94        ID       74
   IRON(SS304)     ENDF/B-IV MAT 1192                       UPDATED 08/12/94        ID       75
   NICKEL(SS304)   ENDF/B-IV MAT 1190                       UPDATED 08/12/94        ID    28304
   NICKEL(SS304)   ENDF/B-IV MAT 1190                       UPDATED 08/12/94        ID       77
   NICKEL(SS304)   ENDF/B-IV MAT 1190                       UPDATED 08/12/94        ID       78
   NICKEL(SS304)   ENDF/B-IV MAT 1190                       UPDATED 08/12/94        ID       79
   URANIUM-235     ENDF/B-IV MAT 1261                       UPDATED 08/12/94        ID       28
   URANIUM-238     ENDF/B-IV MAT 1262                       UPDATED 08/12/94        ID       33
   OXYGEN-16       ENDF/B-IV MAT 1276                       UPDATED 08/12/94        ID     8016
   ZIRCALLOY       ENDF/B-IV MAT 1284                       UPDATED 08/12/94        ID    40302
   XENON-135       ENDF/B-IV MAT 1294                       UPDATED 08/12/94        ID    54135
   CESIUM-133      ENDF/B-IV MAT 1141                       UPDATED 08/12/94        ID    55133
   URANIUM-234     ENDF/B-IV MAT 1043                       UPDATED 08/12/94        ID    92234
   URANIUM-235     ENDF/B-IV MAT 1261                       UPDATED 08/12/94        ID    92235
   URANIUM-235     ENDF/B-IV MAT 1163                       UPDATED 08/12/94        ID    92236
   URANIUM-238     ENDF/B-IV MAT 1262                       UPDATED 08/12/94        ID    92238
   NEPTUNIUM-237   ENDF/B-IV MAT 1263                       UPDATED 08/12/94        ID    93237
   PLUTONIUM-238   ENDF/B-IV MAT 1050                       UPDATED 08/12/94        ID    94238
   PLUTONIUM-239   ENDF/B-IV MAT 1264                       UPDATED 08/12/94        ID    94239
   PLUTONIUM-240   ENDF/B-IV MAT 1265                       UPDATED 08/12/94        ID    94240
   PLUTONIUM-241   ENDF/B-IV MAT 1266                       UPDATED 08/12/94        ID    94241
   PLUTONIUM-242   ENDF/B-IV MAT 1161                       UPDATED 08/12/94        ID    94242
  AM-241 1056 SIGP=5+4 NEWXLACS 218NGP P-3 293K             UPDATED 08/12/94        ID    95241
  AM-243 1057 218 GP WT F-1/E-M 090376 P3 293K              UPDATED 08/12/94        ID    95243
   CURIUM-244      ENDF/B-IV MAT 1162                       UPDATED 08/12/94        ID    96244

    TAPE COPY USED       0 I/O'S, AND TOOK    20.27 SECONDS
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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 WGTD) | 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 | IDEM | 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 | MIXING TABLE MIXTURE | COMPONENT | ATOM DENSITY | EXTRA XSECT ID'S |
|---|---|---|---|---|---|---|
| 1 | 900 | | 1 | 92234 | 1.10085E-06 | |
| 2 | 61 | | 2 | 92234 | 1.10010E-06 | |
| 3 | 62 | | 1 | 92235 | 5.08348E-05 | |
| 4 | 63 | | 2 | 92235 | 5.08000E-05 | |
| 5 | 6012 | | 6 | 28 | 1.31783E-04 | |
| 6 | 7014 | | 1 | 92236 | 2.58815E-05 | |
| 7 | 81 | | 2 | 92236 | 2.58638E-05 | |
| 8 | 82 | | 1 | 92238 | 5.89485E-03 | |
| 9 | 36 | | 2 | 92238 | 5.89081E-03 | |
| 10 | 24304 | | 6 | 33 | 4.80620E-02 | |
| 11 | 65 | | 1 | 8016 | 1.25034E-02 | |
| 12 | 66 | | 2 | 8016 | 1.24948E-02 | |
| 13 | 67 | | 9 | 36 | 3.15151E-02 | |
| 14 | 25055 | | 1 | 40302 | 3.58860E-03 | |
| 15 | 69 | | 2 | 40302 | 3.58614E-03 | |
| 16 | 70 | | 1 | 54135 | 2.83519E-19 | |
| 17 | 71 | | 2 | 54135 | 2.83325E-19 | |
| 18 | 26304 | | 1 | 55133 | 1.28740E-05 | |
| 19 | 73 | | 2 | 55133 | 1.28652E-05 | |
| 20 | 74 | | 1 | 93237 | 3.03707E-06 | |
| 21 | 75 | | 2 | 93237 | 3.03499E-06 | |
| 22 | 28304 | | 1 | 94238 | 9.67482E-07 | |
| 23 | 77 | | 2 | 94238 | 9.66819E-07 | |
| 24 | 78 | | 1 | 94239 | 3.31291E-05 | |
| 25 | 79 | | 2 | 94239 | 3.31064E-05 | |
| 26 | 28 | | 1 | 94240 | 1.10648E-05 | |
| 27 | 33 | | 2 | 94240 | 1.10573E-05 | |
| 28 | 8016 | | 1 | 94241 | 7.52311E-06 | |
| 29 | 40302 | | 2 | 94241 | 7.51795E-06 | |
| 30 | 54135 | | 1 | 94242 | 3.14259E-06 | |
| 31 | 55133 | | 2 | 94242 | 3.14044E-06 | |
| 32 | 92234 | | 1 | 95241 | 2.27267E-06 | |
| 33 | 92235 | | 2 | 95241 | 2.27111E-06 | |
| 34 | 92236 | | 1 | 95243 | 6.35873E-07 | |
| 35 | 92238 | | 2 | 95243 | 6.35437E-07 | |
| 36 | 93237 | | 1 | 96244 | 1.24576E-07 | |
| 37 | 94238 | | 2 | 96244 | 1.24491E-07 | |
| 38 | 94239 | | 9 | 61 | 6.30301E-02 | |
| 39 | 94240 | | 3 | 62 | 1.69854E-03 | |
| 40 | 94241 | | 3 | 63 | 6.83682E-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 | 3.71140E-05 | |
| 46 | | | 2 | 69 | 3.71140E-05 | |
| 47 | | | 3 | 70 | 3.76992E-05 | |
| 48 | | | 5 | 71 | 1.73633E-03 | |
| 49 | | | 1 | 26304 | 1.26878E-03 | |
| 50 | | | 2 | 73 | 1.26878E-03 | |
| 51 | | | 3 | 74 | 1.28878E-03 | |
| 52 | | | 5 | 75 | 5.93579E-02 | |
| 53 | | | 1 | 28304 | 1.65030E-04 | |
| 54 | | | 2 | 77 | 1.65030E-04 | |
| 55 | | | 3 | 78 | 1.67632E-04 | |
| 56 | | | 5 | 79 | 7.72070E-03 | |
| 57 | | | 1 | 7014 | 2.90142E-05 | |
| 58 | | | 2 | 81 | 2.90142E-05 | |
| 59 | | | 4 | 82 | 4.30057E-22 | |
| 60 | | | 3 | 6012 | 2.13384E-03 | |

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 | 3.56552E-01 | 1.49160E-04 | 5.31832E-05 |
| 2 | 1.35240E+00 | 1.44640E-04 | 1.95612E-04 |
| 3 | 1.66302E+00 | 1.27010E-04 | 2.11220E-04 |
| 4 | 8.91862E-01 | 1.28110E-04 | 1.14256E-04 |
| 5 | 1.23758E+00 | 1.29770E-04 | 1.60601E-04 |
| 6 | 2.85554E+00 | 1.02810E-04 | 2.93579E-04 |
| 7 | 2.53881E+00 | 5.11830E-05 | 1.29944E-04 |
| 8 | 1.69350E+00 | 1.23189E-05 | 2.08620E-05 |
| 9 | 1.18760E+00 | 3.83650E-06 | 4.55622E-06 |
| 10 | 1.21098E+00 | 3.72469E-06 | 4.51054E-06 |
| 11 | 1.27682E+00 | 4.01500E-06 | 5.12641E-06 |
| 12 | 1.01048E+00 | 4.29259E-06 | 4.33756E-06 |
| 13 | 1.00208E+00 | 4.47439E-06 | 4.48372E-06 |
| 14 | 1.17277E+00 | 4.56760E-06 | 5.35672E-06 |
| 15 | 5.97676E-01 | 4.55809E-06 | 2.72426E-06 |
| 16 | 3.60322E-01 | 4.51850E-06 | 1.62811E-06 |
| 17 | 1.68121E-01 | 4.48790E-06 | 7.54512E-07 |
| 18 | 1.48799E-01 | 4.46649E-06 | 6.64608E-07 |
| 19 | 2.78462E-01 | 4.43450E-06 | 1.23484E-06 |
| 20 | 9.41221E-01 | 4.32709E-06 | 4.07275E-06 |
| 21 | 3.34900E-01 | 4.19750E-06 | 1.40574E-06 |
| 22 | 1.11154E+00 | 4.09759E-06 | 4.55464E-06 |
| 23 | 9.47043E+00 | 3.83900E-06 | 3.63570E-05 |
| 24 | 1.57838E+01 | 3.67480E-06 | 5.80022E-05 |
| 25 | 9.47812E+00 | 3.67480E-06 | 3.48302E-05 |
| 26 | 7.25754E+00 | 3.67480E-06 | 2.66700E-05 |
| 27 | 1.10151E+00 | 3.67480E-06 | 4.04783E-06 |
| | | | 1.38458E-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 | 6.57152E+00 | 8.77160E-06 | 5.76427E-05 |
| 29 | 1.43387E+01 | 7.47849E-06 | 1.07232E-04 |
| 30 | 7.06587E+00 | 6.37479E-06 | 4.50434E-05 |
| 31 | 4.45273E+00 | 5.41360E-06 | 2.41053E-05 |
| 32 | 6.23836E+00 | 4.62209E-06 | 2.88343E-05 |
| 33 | 7.13374E+00 | 3.95960E-06 | 2.82468E-05 |
| 34 | 1.47932E+02 | 3.46860E-06 | 5.13118E-04 |
| 35 | 7.10440E+01 | 3.01920E-06 | 2.14496E-04 |
| 36 | 2.62896E+02 | 2.62759E-06 | 6.90782E-04 |
| 37 | 3.07753E+02 | 2.20510E-06 | 6.78625E-04 |
| 38 | 1.88076E+02 | 1.83260E-06 | 3.44668E-04 |
| 39 | 1.88431E+02 | 1.52280E-06 | 2.86943E-04 |
| 40 | 2.06225E+02 | 1.17250E-06 | 2.41799E-04 |
| 41 | 1.10914E+02 | 8.75940E-07 | 9.71544E-05 |
| 42 | 1.32266E+02 | 6.30610E-07 | 8.34080E-05 |
| 43 | 1.66930E+02 | 3.83380E-07 | 6.39975E-05 |
| 44 | 6.12213E+00 | 2.66930E-07 | 1.63418E-06 |
| 45 | 1.65122E-02 | 9.34720E-07 | 1.54343E-08 |
| | | | 3.50774E-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 any of the path-B derived input to the neutronics codes.

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 an immediate 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. Some of the input rules are discussed below in procedure 6.

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.

6. The array data are input either by using general SCALE free-form input rules or by using special YREAD provisions corresponding more nearly to FIDO-type input. The general rules apply to all of the BONAMI, NITAWL-II, and XSDRNPM data except for four data arrays. The X33, X35, I36, and X38 data arrays are input using the YREAD provisions. The general input rules are more direct but not as extensive as FIDO-type rules (e.g., the options for skipping data entries or filling arrays with a single value are not allowed). Also, all values in the first entries (including the normal defaults) must be read when a later entry is required. The end of the data array may be skipped when the skipped values produced by INPLEVEL=2 are correct. The end of an array is detected when starting a new data array

(e.g., I2=) or when the "END" is read at the end of the code data. The general free-form system has the provision for multiple entries of the same data vlaue. This feature requires first the number of repeats, immediately followed by an R, *, or $, and finally followed by the value (integer or floating point) to be repeated. For example, 12R25 causes the value 25 to be repeated 12 times. In contrast to the general free-form input rules, the special YREAD system has provisions for significantly more options. Similar to the FIDO system: the Aj option sets the current array position to j; the Fj option fills the remainder of the array with j; the iQj option repeats the previous j entries i times; the iIjk option linearly interpolates i entries between the j and k end points; the iRj, i*j, and i$j options repeat j for the next i entries; and the T option terminates the data reading for the array. The array input always requires the T option, unless it is the last data array for the code (requiring an "END" to be input). The four data arrays for which the YREAD provisions apply are usually large and may have greater need for options such as the Q, F, I, or R options.

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 (or reset by input entry LIMINTGEO), 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 is used in place of the FIDO input system. See the above procedure 6 and Sect. M3 for details of input rules.

```
=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     I0= 12, 17, 18, 1      END
 NIT    I0= 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  T
 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  T
   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=HALT03SKIPSHIPDATA
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  T
 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  T
 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)

```
SAS2H     PARM='HALT00,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,   T
 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,   T
  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 $(n,\gamma)$ 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 (applying initial weight)

5. BURASM: accumulated burnup at TW, MWd/assembly

6. PWMTU: specific power of cycle, kW/kg heavy metal (initial heavy metal)

7. PWASM: specific power of cycle, MW/assembly

8. WTMTU: initial metric ton heavy metal, 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 ($\alpha$,n) source, n/s-assembly

3. SPNEUT(NGRP): total neutron spectrum, n/s-assembly

4. SPECAN(NGRP): ($\alpha$,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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Computational Physics and Engineering 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,$\gamma$ 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 $\theta$ between the particle trajectory and the preferred direction of travel. It returned the cosine of this angle.

The current version of MORSE-SGC 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 $\theta$ for various values of PATH. DIREC is taken to be the cosine of $\theta$. 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

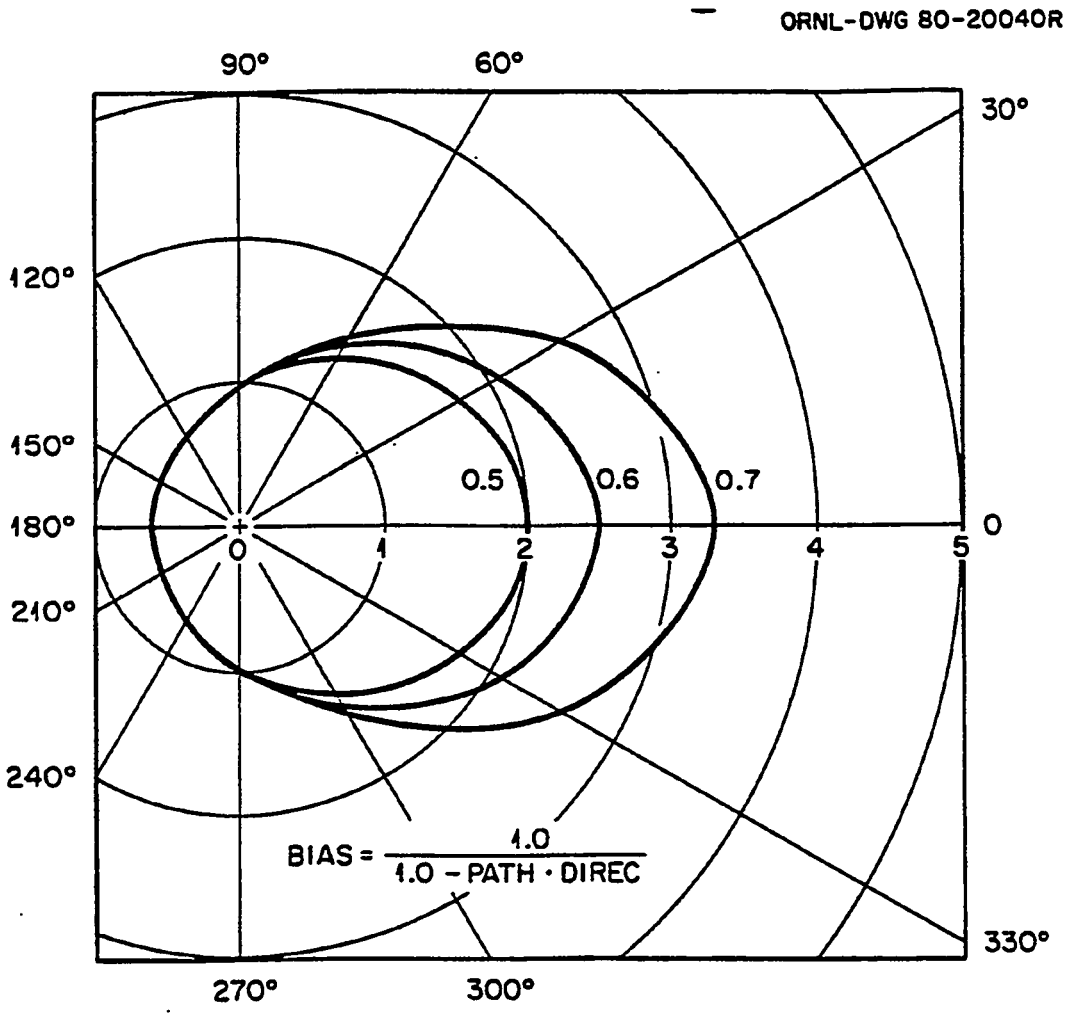



Figure S3.2.1 Polar diagram of BIAS versus θ

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 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.

## S3.3 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. The total flux response printed out by SAS3 is actually the collided 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.

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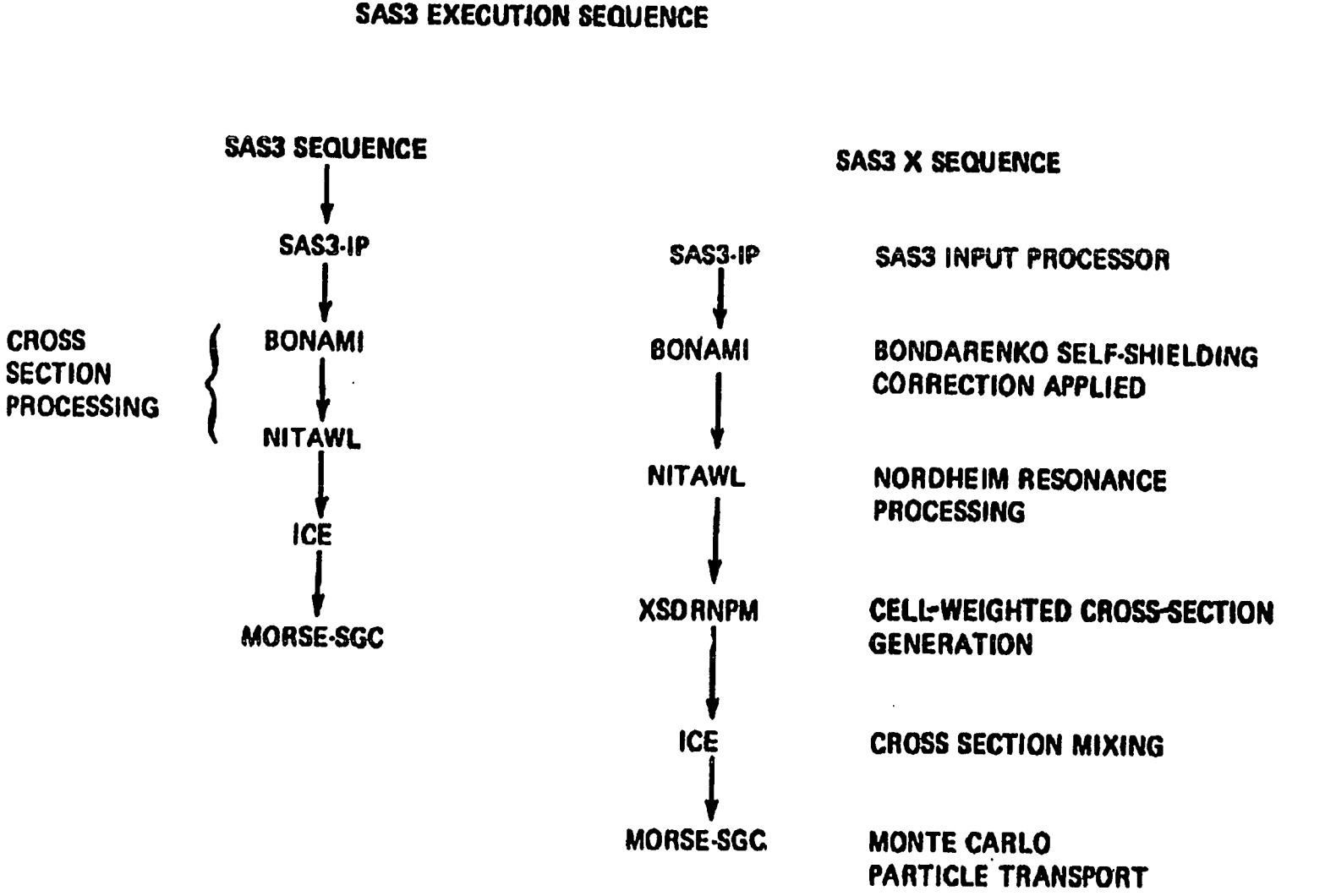



Figure S3.4.1 SAS3 and SAS3X program execution sequence

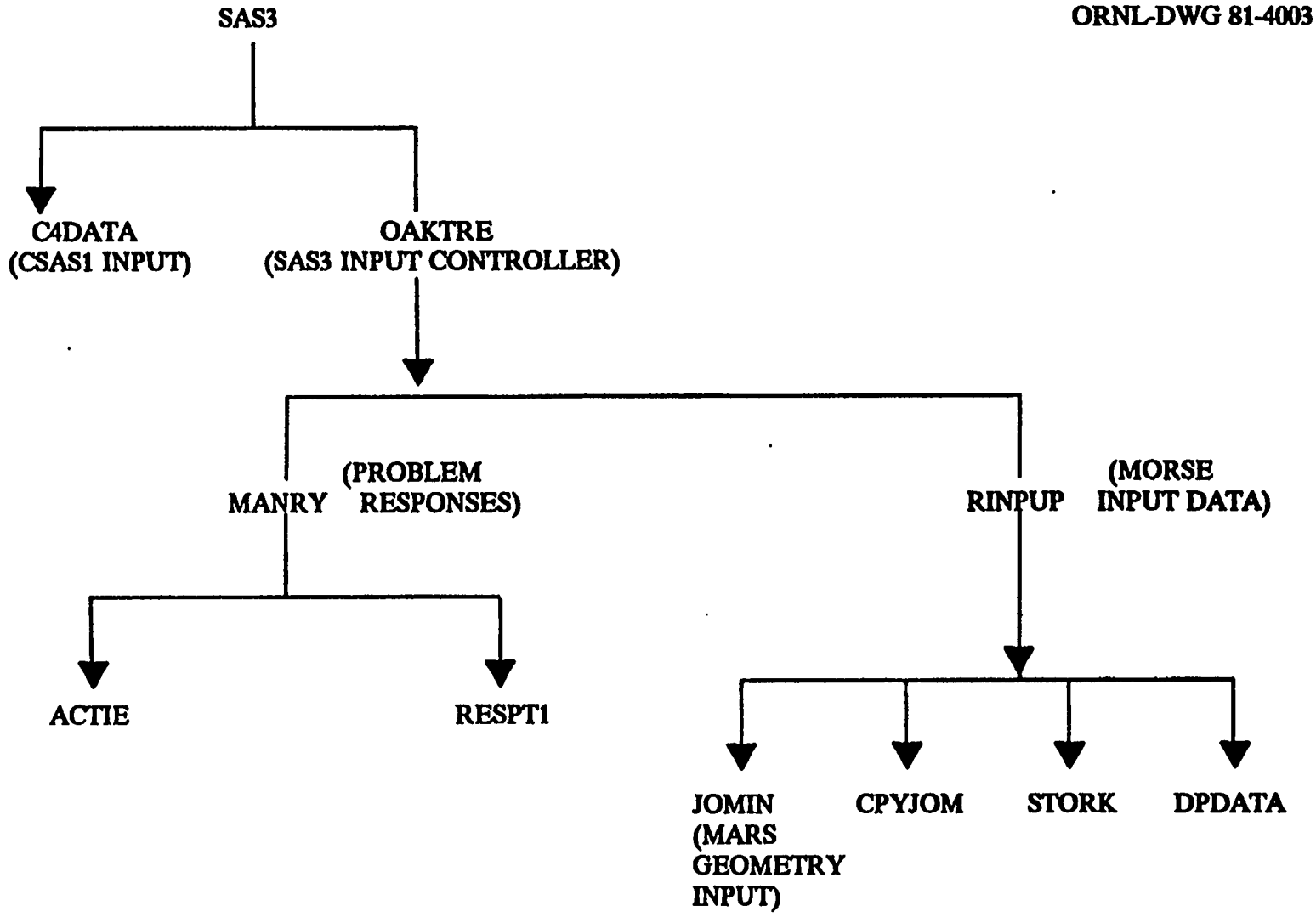



Figure S3.4.2 SAS3 input processor flow chart

## 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 300)

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<br>User must enter response ID required immediately following parameter input<br>See Table S3.3.4 for available response IDs<br>Not all SCALE libraries contain responses |
| NRE=0 | Default ID requested for standard neutron and gamma dose<br>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 (2Z8 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.)

C1 - Enter zero. If zero is not the value entered, then WTSTRT is set to the value.

C2 - Enter zero. If zero is not the value entered, AGSTRT is set to the value.

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 and source normalization.

{(FS(I), I=1, NNGA+NGGA), SRCNRM.} 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 > 0, 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 Fig. S3.6.2. 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

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 | |

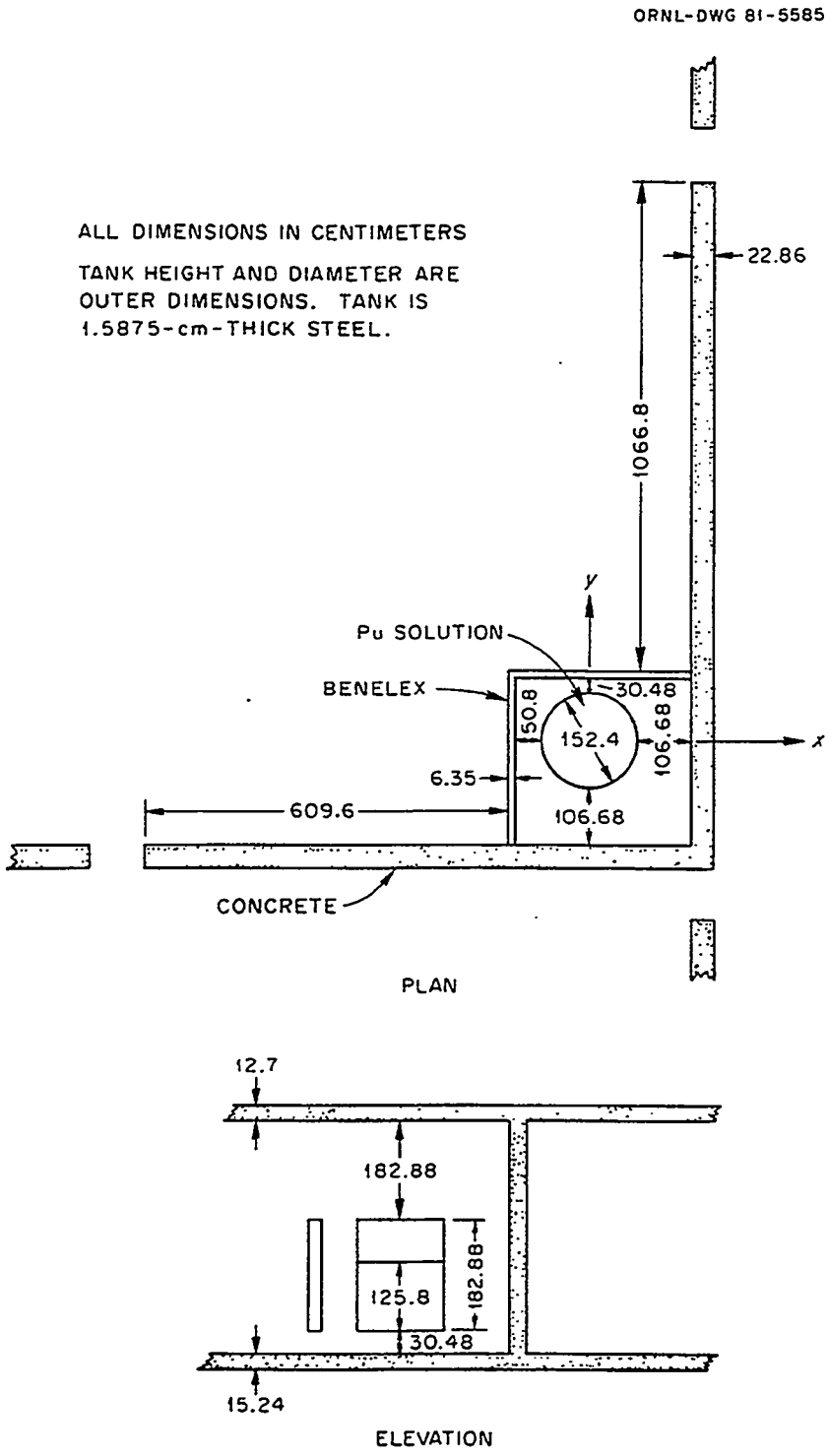



Figure S3.6.1 Geometry for the tank shielding problem

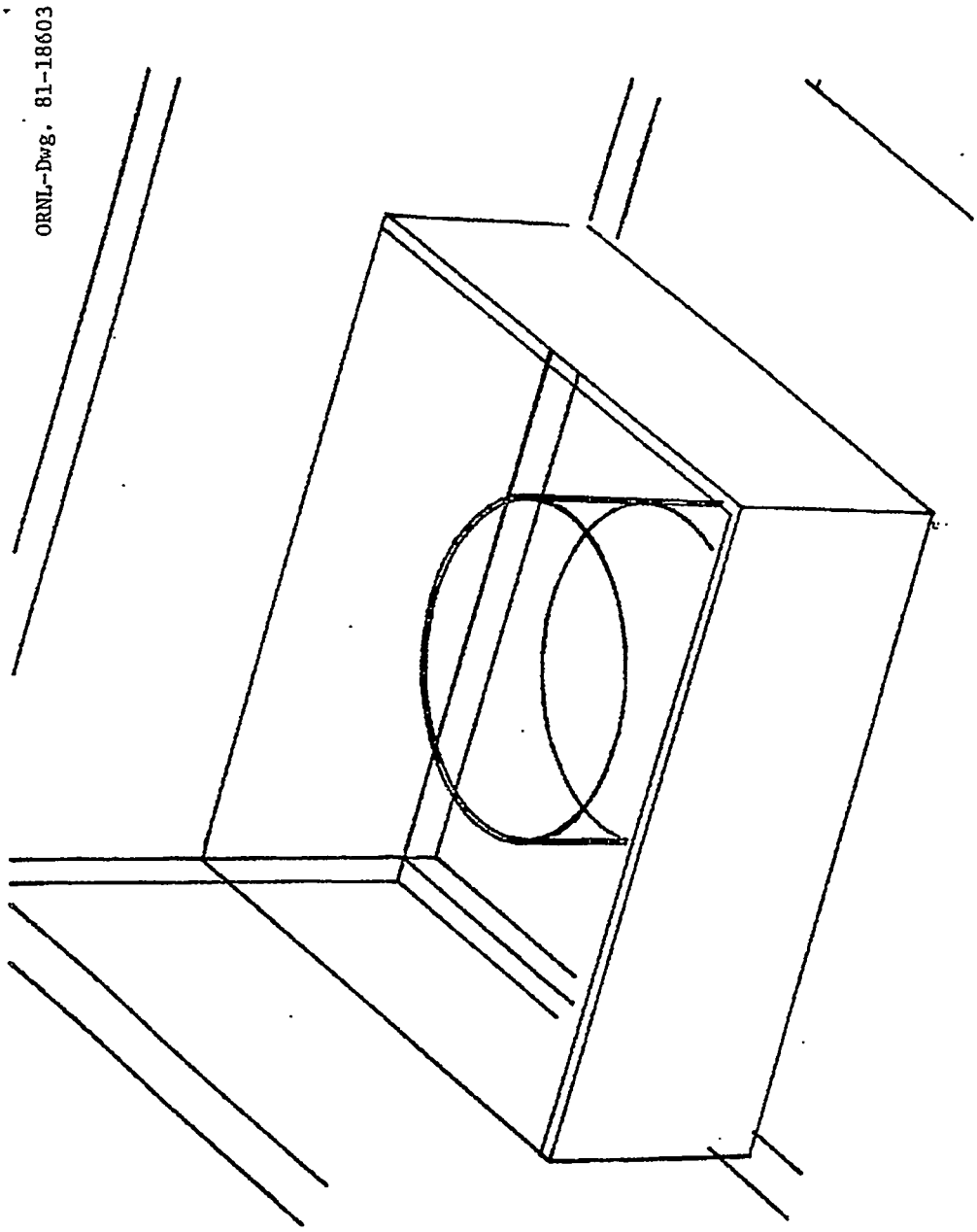



Figure S3.6.2 Tank shielding model for SAS3

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

```
=sas3
 tank shielding problem, jim west, ornl, august, 1980
27n-18couple     infhommedium
h        1 0.0 0.066522      end
n        1 0.0 9.0675e-05    end
o        1 0.0 0.033533      end
pu-240   1 0.0 1.129e-06     end
pu-239   1 0.0 2.154e-05     end
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 0.0001968     end
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-06  33*0.0  1.0
 -134.0 0.0 64.49
  0.0 113.5 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
```

to a point detector location. The closer the detector is to the scattering source, the more difficult it is to obtain satisfactory statistics with a reasonable amount of computer time.

The final results output from MORSE for the point-source neutron and gamma dose are shown in Table S3.6.5. 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)

responses(detector) shielding problem

| detector | uncoll response | fsd uncoll | total response | fsd total |
|---|---|---|---|---|
| 1 | 5.5438E-11 | 0.01121 | 1.4954E-10 | 0.30463 |
| 2 | 7.7271E-11 | 0.01121 | 2.1202E-10 | 0.23039 |
| 3 | 1.9174E-12 | 0.01869 | 3.2965E-10 | 0.89384 |
| 4 | 2.4658E-13 | 0.02651 | 1.7120E-12 | 0.32786 |
| 5 | 1.3685E-12 | 0.01869 | 3.8978E-11 | 0.33417 |
| 6 | 1.8036E-12 | 0.01121 | 1.8338E-11 | 0.06015 |
| 7 | 2.2728E-13 | 0.02059 | 5.2634E-12 | 0.10679 |
| 8 | 7.1517E-13 | 0.01121 | 7.0838E-12 | 0.07319 |
| 9 | 6.2308E-11 | 0.00415 | 2.1918E-10 | 0.11009 |

ansi standard gamma dose rate (rem per hour)

responses(detector) shielding problem

| detector | uncoll response | fsd uncoll | total response | fsd total |
|---|---|---|---|---|
| 1 | 0.0000E+00 | 0.00000 | 4.1971E-12 | 0.20912 |
| 2 | 0.0000E+00 | 0.00000 | 3.5155E-11 | 0.88572 |
| 3 | 0.0000E+00 | 0.00000 | 4.2746E-13 | 0.24693 |
| 4 | 0.0000E+00 | 0.00000 | 7.9442E-13 | 0.89965 |
| 5 | 0.0000E+00 | 0.00000 | 8.0764E-13 | 0.15459 |
| 6 | 0.0000E+00 | 0.00000 | 4.0651E-13 | 0.10226 |
| 7 | 0.0000E+00 | 0.00000 | 3.1222E-13 | 0.12298 |
| 8 | 0.0000E+00 | 0.00000 | 1.8521E-13 | 0.18254 |
| 9 | 0.0000E+00 | 0.00000 | 2.5337E-12 | 0.19426 |

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Computational Physics and Engineering Division

# 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

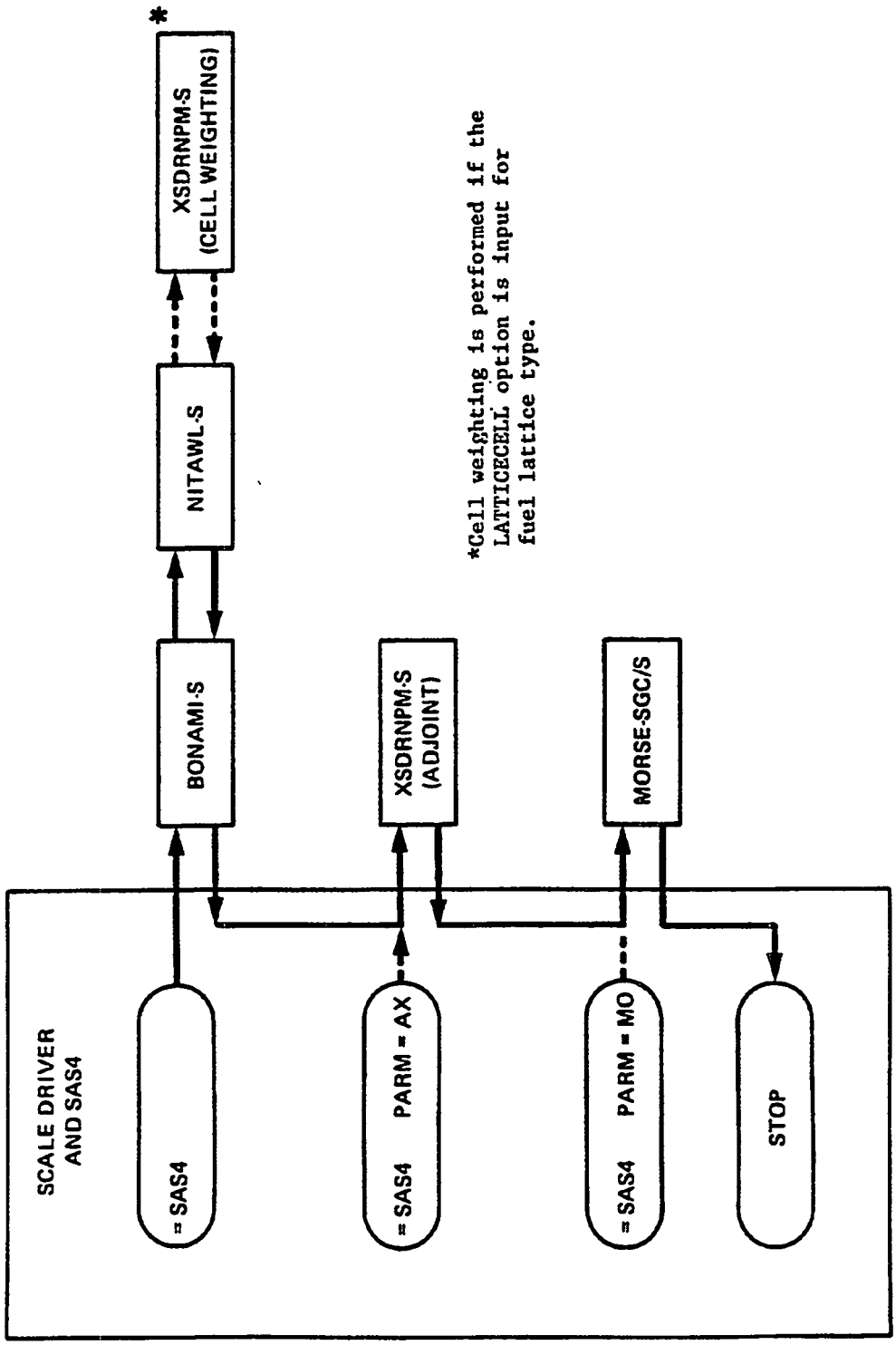



Figure S4.2.1 Outline of the SAS4 analytic sequence

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.

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 discrete ordinates 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

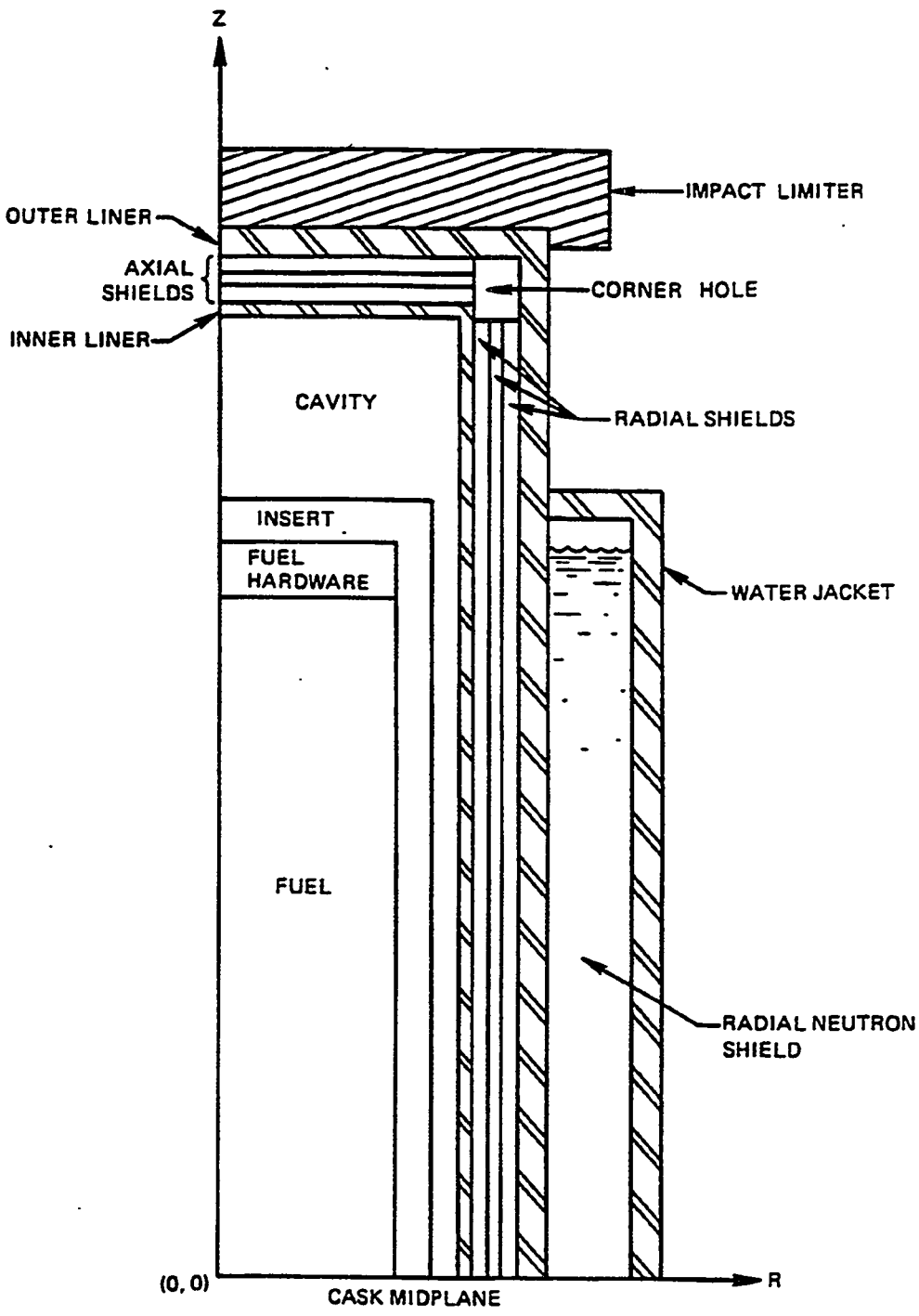



Figure S4.2.2 SAS4 cask model for IGO = 0

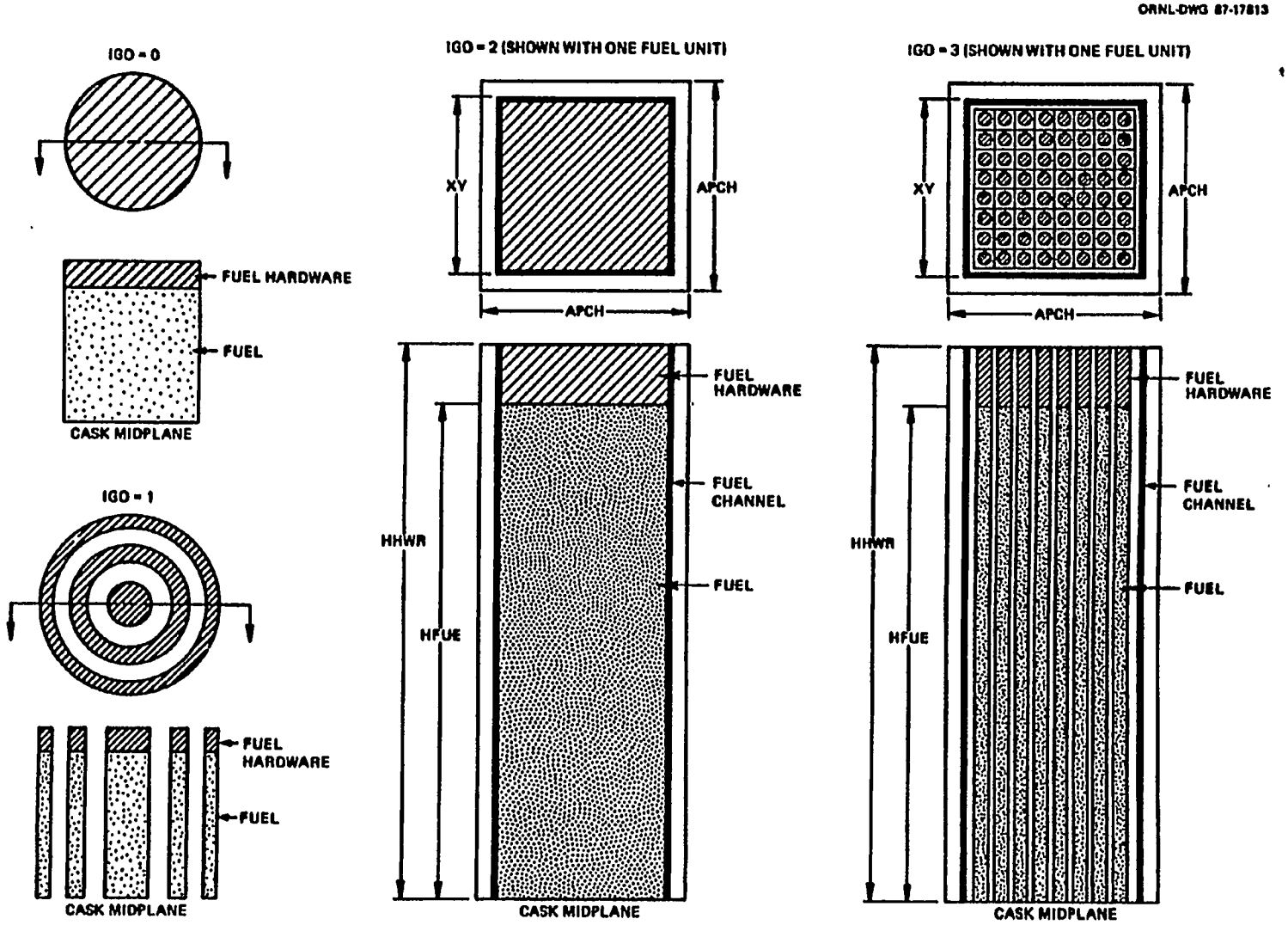



Figure S4.2.3 Geometry options of source region for simplified geometry input

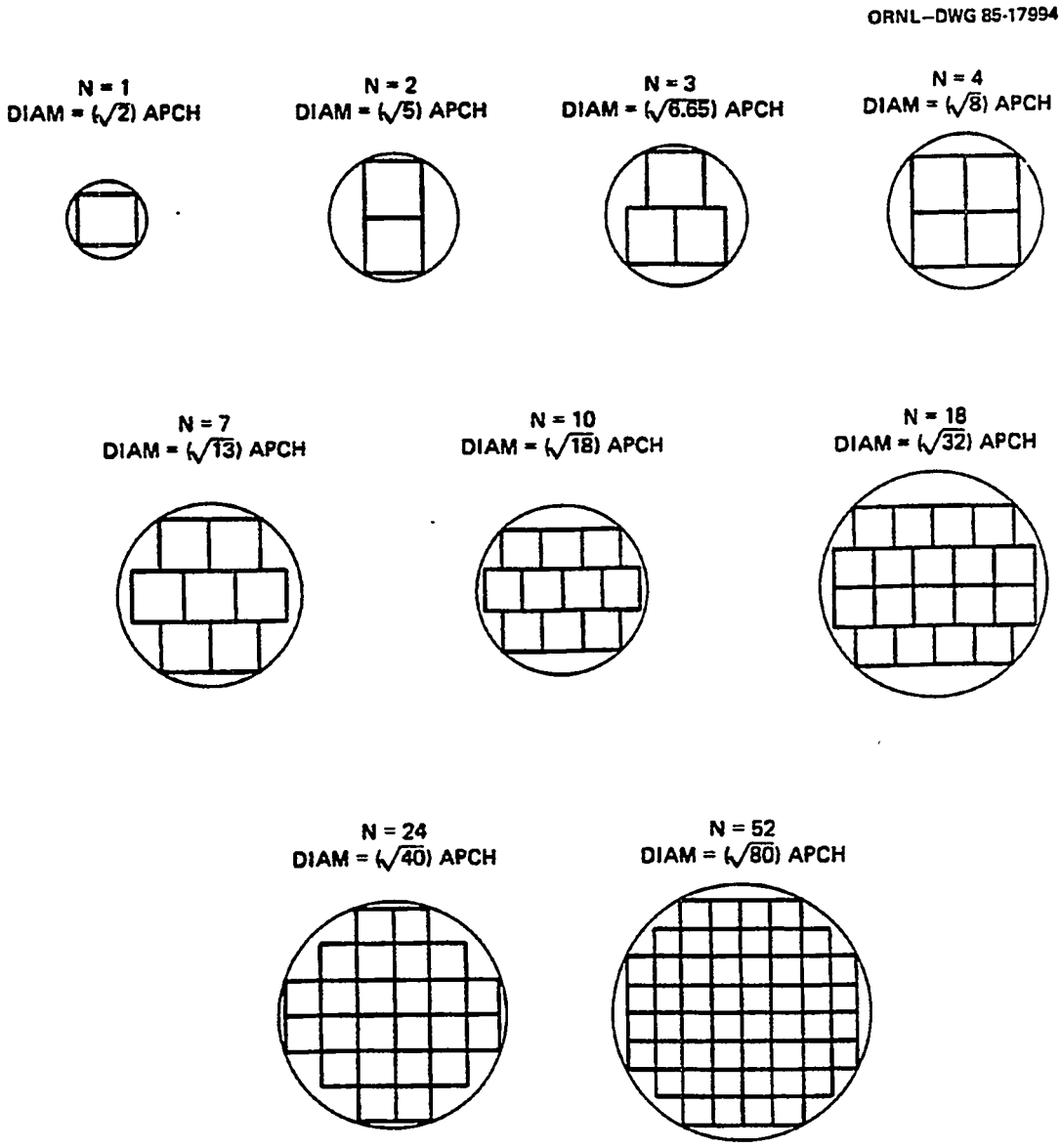



Figure S4.2.4 Packing arrangements of fuel units for geometry options IGO = 2 and 3

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 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 4 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.

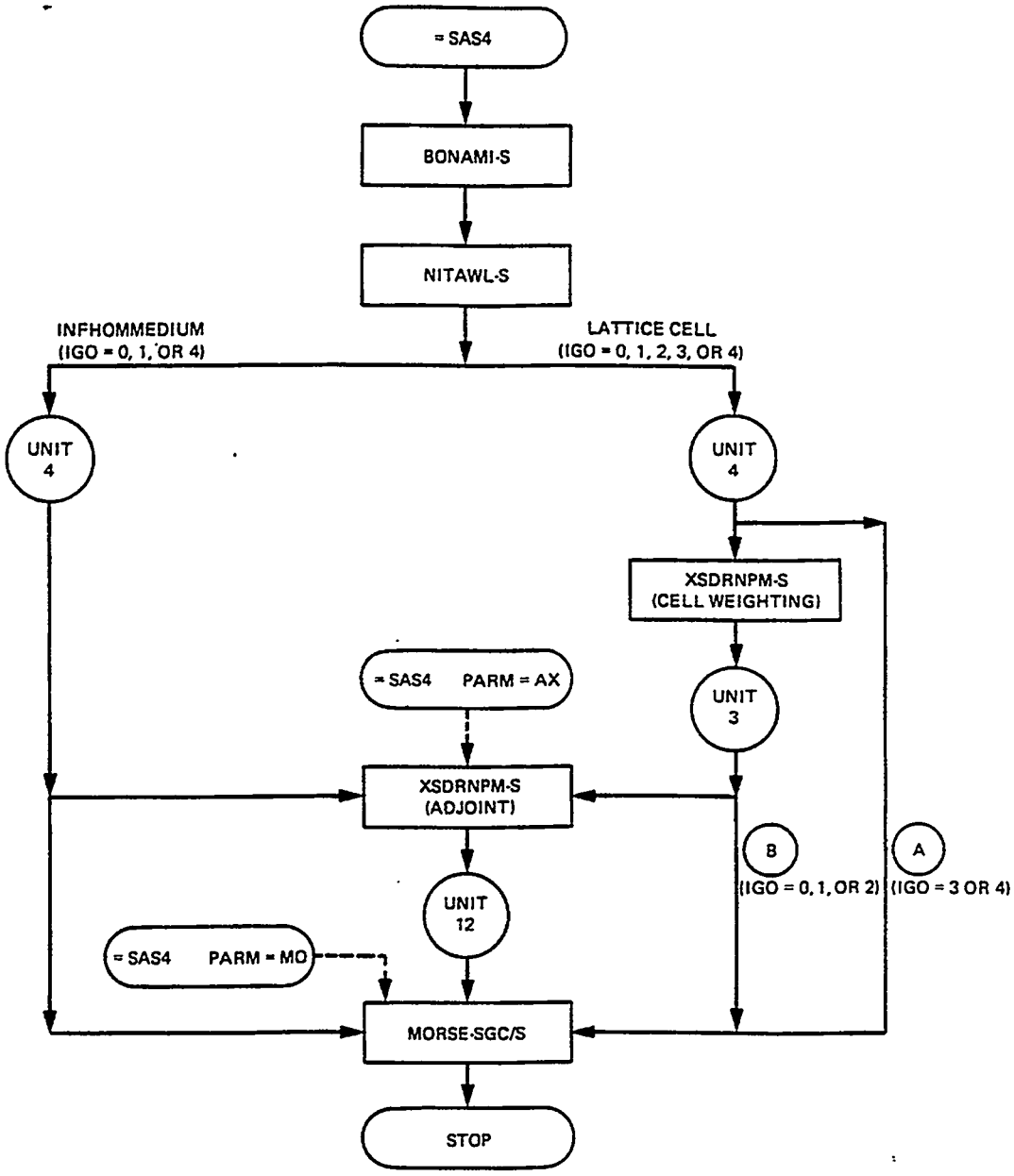
After defining the mixtures in the material information data, the user must apply them in the unit cell specification (if needed) and in the adjoint discrete-ordinates and Monte Carlo calculations. The mixtures in SAS4 can be separated into two categories: (1) fuel materials and (2) cask materials. The 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.




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 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 = ±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 ≤ 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 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,

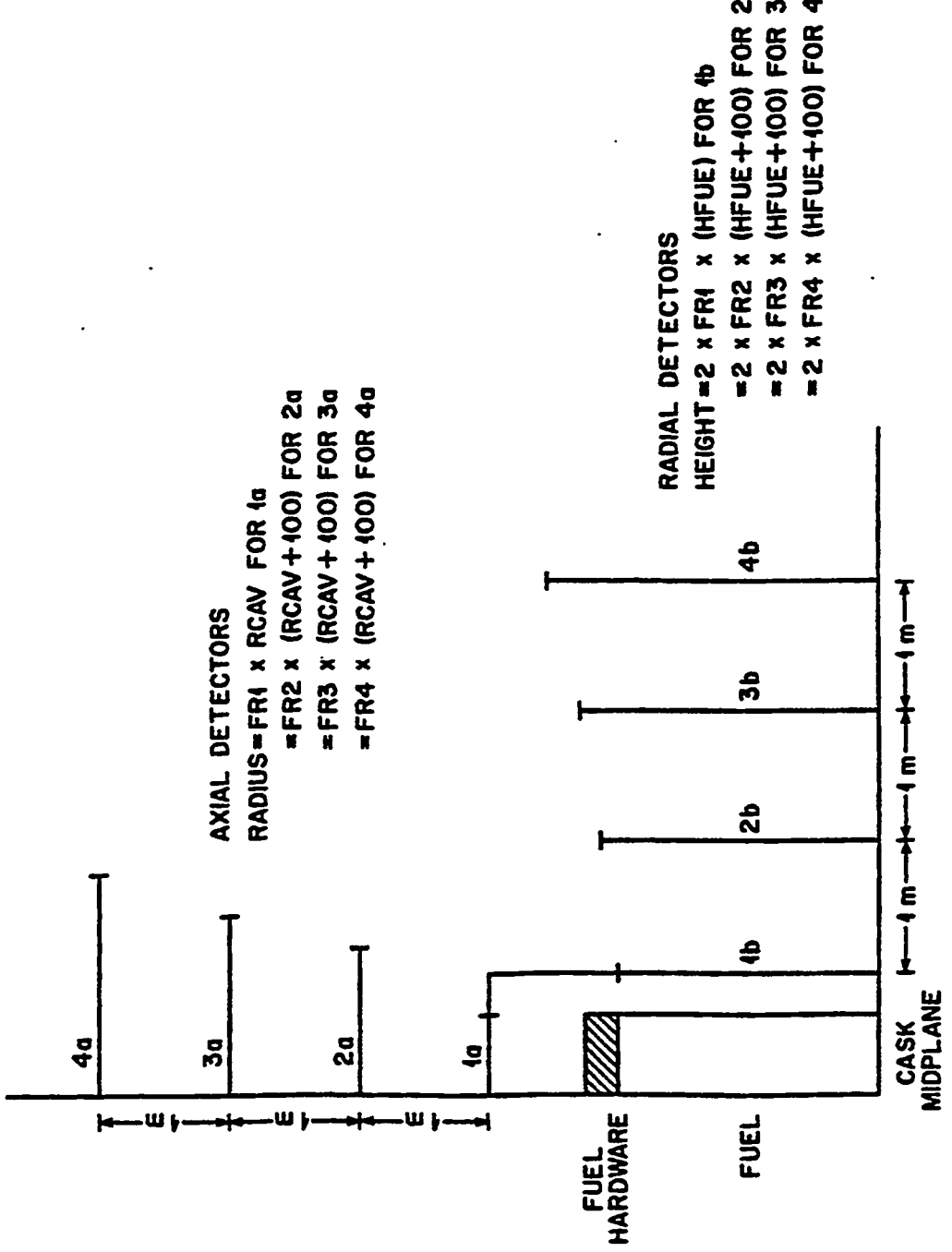



Figure S4.2.6 SAS4 default axial and radial surface detectors (only the top half is shown)

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 $\leq$ 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 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 or 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 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

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

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.[7]

## 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.

**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.

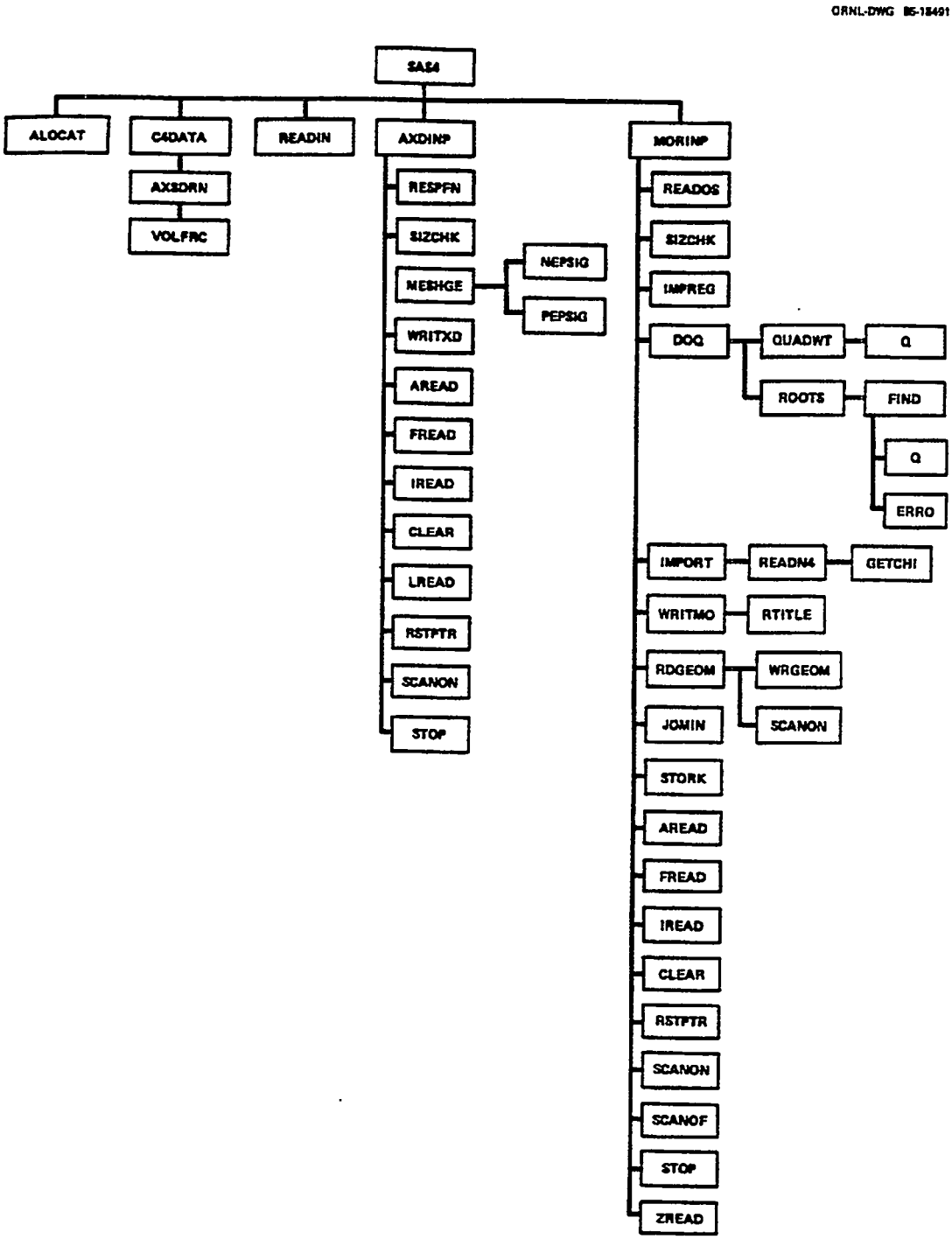



Figure S4.3.1 Flow diagram of SAS4 subroutines

**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.

**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 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≠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 | 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 option 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,<br>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,<br>RFUE,HFUE,HHWR | Written by RDGEOM |
| | If IGO=1,<br>RIN(I),ROUT(I),HFUE,HHWR,<br>I=1,3 | Written by RDGEOM |
| | If IGO=2 or 3,<br>APCH,HFUE,HHWR,MXX | Written by RDGEOM |
| | If IGO=4,<br>XMIN,XMAX,YMIN,YMAX,<br>ZMIN,ZMAX,HFUE | Written by MORINP |
| 8 | RJAC,RCAV,HIM1,SFA,FR1,FR2,<br>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 $1.0 \times 10^4$.

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[a] | End of this SC data. Repeat for all SC of case |
| | Examples: U02 1 0.94 1000 92235 3.1 92238 96.9 END<br>FE 4 0 4.2-3 END<br>SS304 6 END |
| END COMP[a] | 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<br>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[a] | End of unit cell specification |
| Optional parameter data (omit for INFHOMMEDIUM) | |
| MORE DATA[a] | (The following entries may be in any order but must be terminated by END) |
| SZF=[a] | Spatial mesh factor. SZF < 1 for finer; >1 for coarser mesh (1) |
| ISN=[a] | Order of angular quadrature (8) |
| IIM=[a] | Maximum number of inner iterations (20) |
| ICM=[a] | Maximum number of outer iterations (25) |
| EPS=[a] | Overall convergence criteria (0.0001) |
| PTC=[a] | Scalar flux point convergence (0.0001) |
| IUS=[a] | IUS = 1, upscatter scaling applied to speed convergence; 0, no scaling applied (0) |
| END[a] | End of option<br>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=[a] | 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=[a] | Type of response. ITY = 1 for neutron response; ITY = 2 for gamma-ray response (2). |
| IZM=[a] | Number of separate material zones (must be input). IZM≥2 for IDR = 0 and ≥3 for IDR > 0. |
| ISN=[a] | Order of quadrature set (8) |
| IRF=[a] | 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=[a] | 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=[a] | 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=[a] | Radius of the fuel zone (must be input). For the LATTICECELL option, ($\pi$*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)<br>FRD is the radius of the fuel zone (source region) of the Monte Carlo calculation with IGO = 0<br>For IDR = 0 (radial calculation), FRD = ZB(1) in the zone boundary array<br>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=[a] | Spatial mesh factor. SZF < L for finer mesh; SZF > L for coarser mesh (1) |
| END[a] | 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[a] | Terminates the fuel zone card<br>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[a] | - 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[a] | - 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[a] | - 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[a] | 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=[a] | RANDOM, starting random number in 2Z8, but use only 12 characters |
| TIM=[a] | TMAX, computing time allowed for MORSE run in minutes (1.0) |
| NST=[a] | NSTRT, number of source particles per batch (100). 100 is recommended for neutron response, and 1000 is recommended for gamma response |
| NMT=[a] | NMOST, maximum number of particles allowed (4*NST). NMT should be at least 2*NST |
| NIT=[a] | NITS, number of batches for this run (100) |
| NCO=[a] | NCOEF, number of Legendre coefficients for each mixture, including $P_o(4)$ |

Table S4.4.2 (continued)

| Name or keyword | Definitions, comments, and examples |
|---|---|
| | *Monte Carlo input data (continued)* |
| IST=[a] | 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=[a] | IPRIN, switch to print the discrete scattering angles and probabilities if >0 (0). Beware that large amount of output is generated when IPR > 0 |
| ISO=[a] | 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=[a] | Number of point detectors (0) |
| SFA=[a] | 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=[a] | 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=[a] | 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=[a] | Fraction multiplied to the third surface detector (1.0). Condition and recommended value are identical to those of FR2 |
| FR4=[a] | Fraction multiplied to the fourth surface detector (1.0). Condition and recommended value are identical to those of FR2 |
| IGO=[a] | Flag for geometry input option and source region geometry (0)<br>See Figs. S4.2.3 and S4.2.4 for geometries of the source region for IGO = 0, 1, 2, and 3<br>For LATTICECELL option, IGO can have a value between 0 to 4<br>For INFHOMMEDIUM option, IGO can only be 0, 1, or 4<br>**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<br>**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 cell-averaged 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 |

Table S4.4.2 (continued)

| Name or keyword | Definitions, comments, and examples |
|---|---|
| | *Monte Carlo input data (continued)* |
| | INFHOMMEDIUM option, the fuel mixture is MFU input by the user and the hardware mixture is MHW<br>**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, 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<br>**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.<br>**For IGO = 4,** detailed MARS geometry must be input by the user |
| MFU=[a] | Fuel mixture number must be input when the INFHOMMEDIUM option is used and IGO=1 |
| ISP=[a] | A flag for source energy spectrum input option (0)<br>**For ISP = 0,** the source energy spectrum is input via the SOE array<br>**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=[a] | Flag for source axial profile input option in the active fuel (0)<br>For source in the hardware (ISO > 0), IPF is irrelevant because only uniform distribution is allowed in the hardware<br>For IPF = 0, a flat axial profile is used<br>For IPF = 1, default top profiles are used<br>For IPF = −1, default bottom profiles are used<br>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.<br>**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 |

Table S4.4.2 (continued)

| Name or keyword | Definitions, comments, and examples |
|---|---|
| | *Monte Carlo input data (continued)* |
| | 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.<br>If the height of the axial profile is not equal to HFUE, execution will be terminated and an error message will be printed. |
| END[a] | Terminates the parameter card |
| Source energy spectrum array (must be skipped if ISP > 0) | |
| SOE[a],(FS(I),I=1,NGPFS), END[a] – 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[a],((XD(I),YD(I),ZD(I)),I=1,NOD), END[a] – 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[a] MSM XMIN,XMAX,YMIN,YMAX,ZMIN,ZMAX,RCAV,HFUE,RMAX,HMAX END[a] 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 | |

Table S4.4.2 (continued)

| Name or keyword | Definitions, comments, and examples |
|---|---|
| | *Monte Carlo input data (continued)* |
| Axial source profile boundary array (enter only if ISO = 0 and IPF > 1)<br>BUB[a], (BB(I),I=1,IPF), END[a] – 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 |
| Axial source profile array (enter only if ISO = 0 and IPF > 1)<br>BUF[a], (PP(I),I=1,IPF), END[a] – 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[a] | 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).<br>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[a] | SAS4 module termination card. Must start from column one |

[a] = 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.

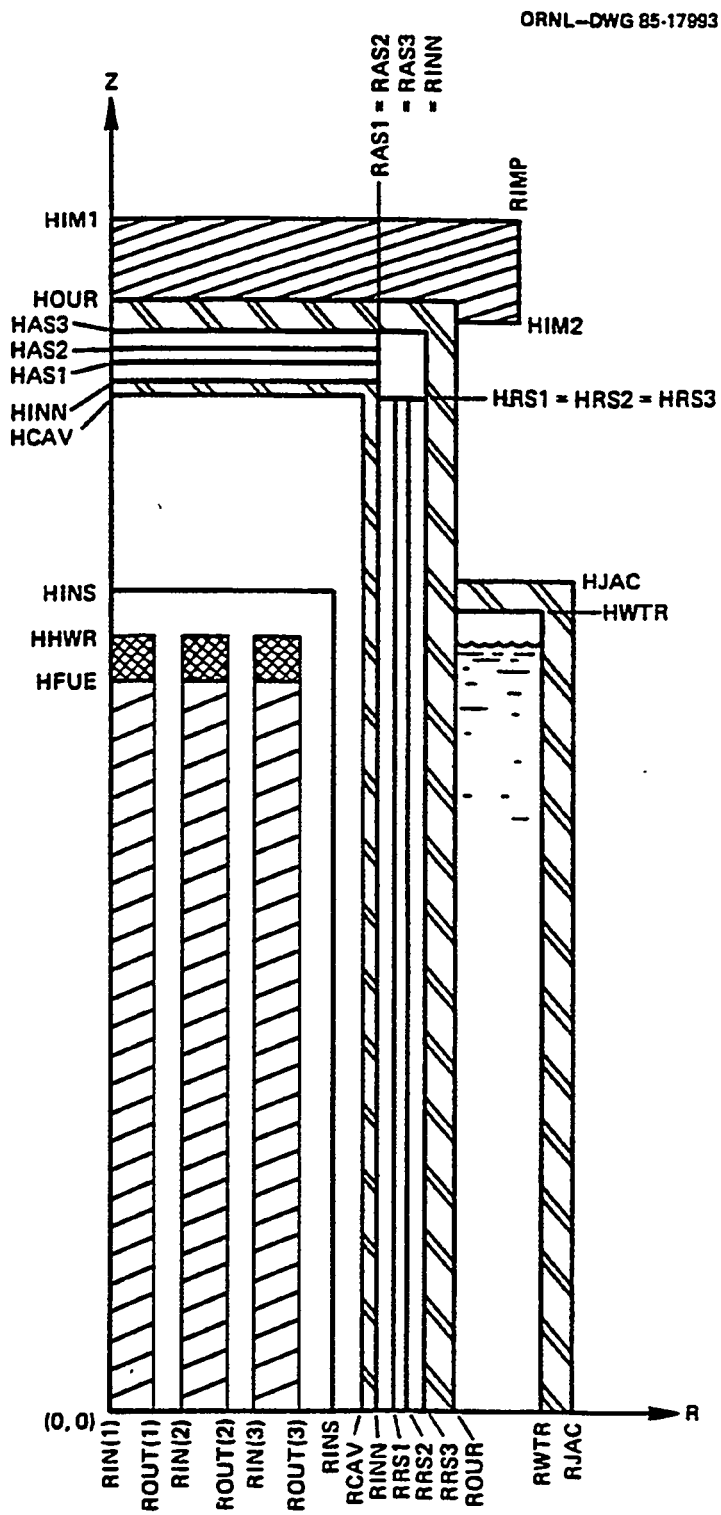



Figure S4.4.1 SAS4 cask model for IGO = 1 (dimensions of each component are shown)

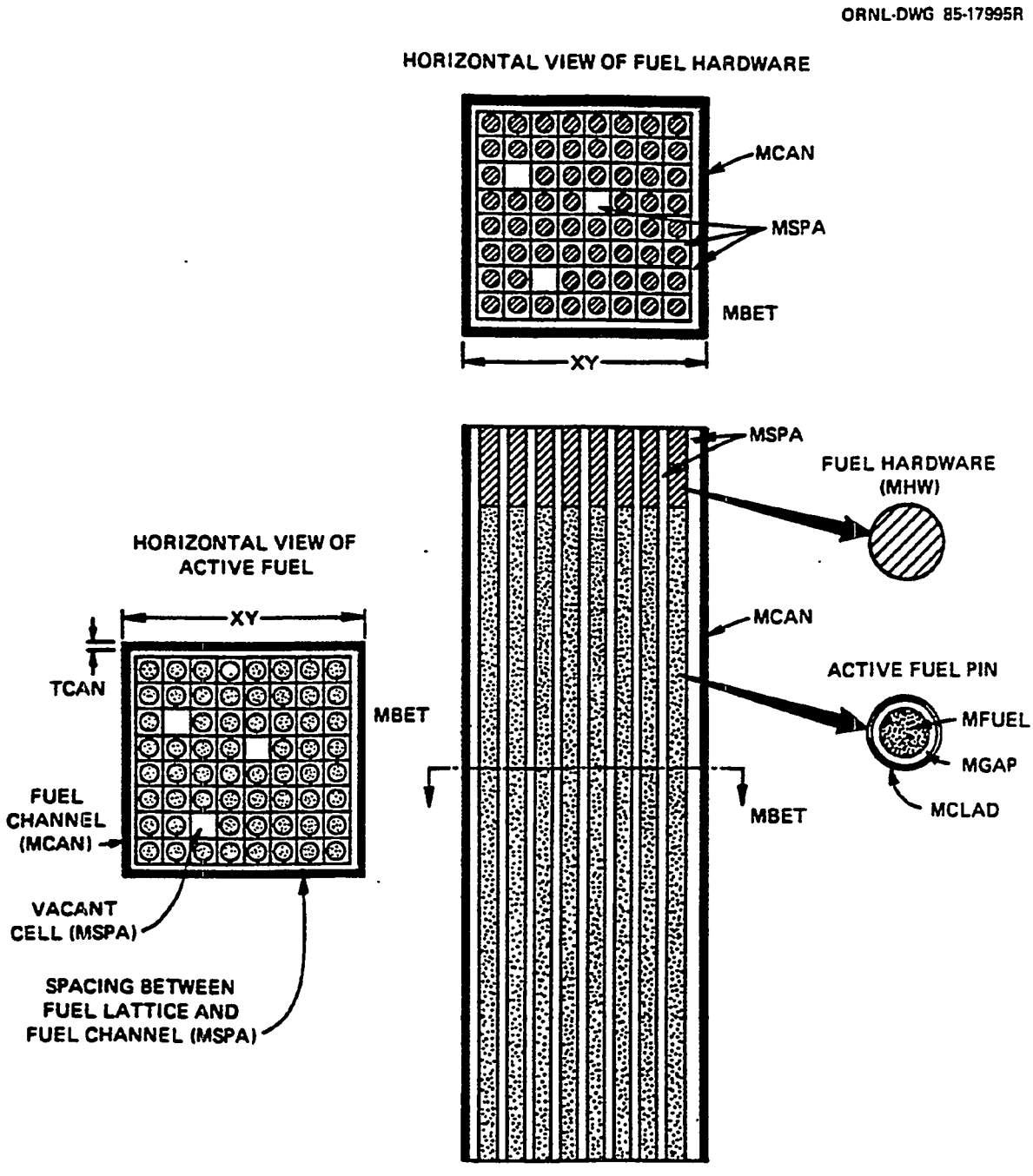



Figure S4.4.2 Fuel assembly model used in LATTICECELL option (only the top half shows)

Table S4.4.4. Mixture numbers of fuel and fuel hardware used in MORSE-SGC and adjoint XSDRNPM 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.

[b]MORSE-SGC 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 calculation only for the axial calculation with IDR > 0.

[d]Input via the parameter card of the Monte Carlo input data.

[e]MORSE-SGC 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 1.26 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. 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 and 5, 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.

Portions of the computer output of MORSE-SGC and SAS4 have 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 omitted to limit the size of this document.

Although only 10 batches of 100 histories per batch were processed in this problem, reasonable results were obtained. However, for actual analyses, it is recommended that a minimum of 30 batches be executed and the minimum size of each batch should be 500 histories for neutron problems and 2000 for gamma problems.

The results given in the MORSE-SGC output indicate that reasonable fractional standard deviations (FSDs) were obtained for detectors 1 to 6. The FSD for detector 7 is 26%, and the result is not 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 $2.614 \times 10^8$ neutrons/s (33 GWd/MTU PWR spent fuel with 120-day cooling time).

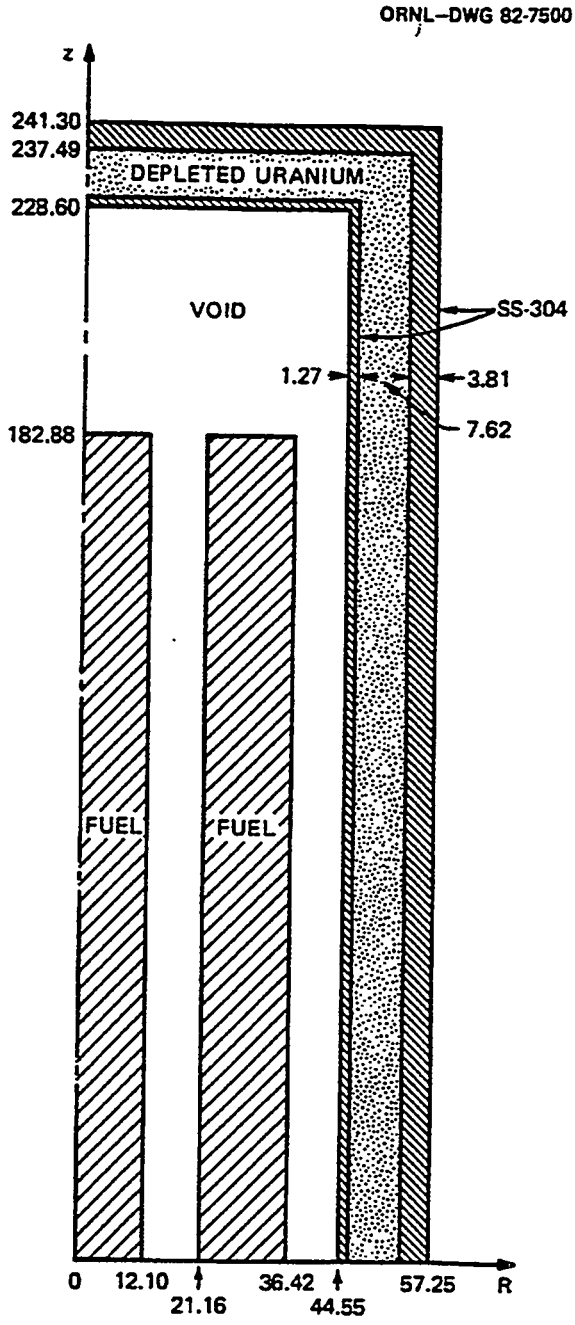



Figure S4.5.1 Upper half of depleted uranium shipping cask of sample problem 1

```
                =sas4
                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 1.000-9  end
                cr       4  0.0 1.662-2   end
Material        mn       4  0.0 1.200-3   end
information     fe       4  0.0 5.775-2   end
input data      ni       4  0.0 7.520-3   end
                mo       4  0.0 1.100-4   end      Neutron doses are calculated
                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
Adjoint         ity=1 izm=5 frd=36.42 end
discrete        7 17 25 0 0 0  0.01 21.4493 end
ordinates       36.42 44.55 45.82 53.44 57.27 end   IDR not input, radial calculation by default
input data      0 0 4 5 4 end
                xend
                tim=15.0 nst=100 nit=10 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            22 entries required
                    121.91 0.0 305.96 end
                gend
Monte Carlo     sample problem 1, 2 homogenized fuel zones
input data      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 S4.5.2 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 FSDs are quite good (less than 10%) for detectors 1 to 6, but are not acceptable (26%) for detector 7. The calculated neutron dose rates for the two axial point detectors (detectors 5 and 6) are 8.92 and 2.76 mrem/h per assembly. These dose rates are in agreement with the corrected results (9.05 and 2.85) reported in Ref. 1. 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 = $1.8298 \times 10^9$ neutrons/s was input so that results of this case are expressed per total source strength.

The FSDs of the results are quite good (much less than 10%) for detectors 1 to 6, and not acceptable (33%) 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 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

```
=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 1.000-9  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 0 0 0  0.01 21.4493 end
182.88 228.60 229.87 237.49 241.30  end   Zone boundaries of axial calculations
7 8 4 5 4 end
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          Axial detectors
    121.91 0.0 305.96 end
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  1.000-9   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 3r0 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  24.65  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

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 $8 \times 4 \times 1$.

The FSDs of the results are less than 10% for detectors 1 to 6 and are 42% 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  1.000-9   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 idr=1 end
7 17 25 3r0 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 0.00 0.00  -2.29870e+02 0.00 0.00   4.59740e+02   4.58200e+01
rcc     2 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34400e+01
rcc     3 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34410e+01
rcc     4 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   5.34420e+01
rcc     5 0.00 0.00  -2.41300e+02 0.00 0.00   4.82600e+02   5.72500e+01
rcc     6 0.00 0.00  -2.41270e+02 0.00 0.00   4.82540e+02   5.72600e+01
rcc     7 0.00 0.00  -2.41280e+02 0.00 0.00   4.82560e+02   5.72700e+01
rcc     8 0.00 0.00  -2.37490e+02 0.00 0.00   4.74980e+02   4.58200e+01
rcc     9 0.00 0.00  -2.37491e+02 0.00 0.00   4.74982e+02   4.58200e+01
rcc    10 0.00 0.00  -2.37492e+02 0.00 0.00   4.74984e+02   4.58200e+01
rcc    11 0.00 0.00  -2.41310e+02 0.00 0.00   4.82620e+02   5.72600e+01
rcc    12 0.00 0.00  -2.41290e+02 0.00 0.00   4.82580e+02   5.72600e+01
rcc    13 0.00 0.00  -2.37492e+02 0.00 0.00   4.74984e+02   5.34420e+01
rcc    14 0.00 0.00  -3.41310e+02 0.00 0.00   6.82620e+02   1.57270e+02
rcc    15 0.00 0.00  -4.41310e+02 0.00 0.00   8.82620e+02   2.57270e+02
rcc    16 0.00 0.00  -5.41310e+02 0.00 0.00   1.08262e+03   3.57270e+02
rcc    17 0.00 0.00  -2.24131e+03 0.00 0.00   4.48262e+03   2.05727e+03
rcc    18 0.00 0.00  -2.34131e+03 0.00 0.00   4.68262e+03   2.15727e+03
rcc    19 0.00 0.00  -2.28600e+02 0.00 0.00   4.57200e+02   4.45500e+01
rcc    20 0.00 0.00  -2.28599e+02 0.00 0.00   4.57198e+02   4.45490e+01
rcc    21 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   3.99349e-01
rcc    22 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   4.26660e-01
rcc    23 0.00 0.00  -1.82880e+02 0.00 0.00   3.65760e+02   4.53971e-01
rcc    24 0.00 0.00   0.00000e+00 0.00 0.00   1.82890e+02   4.53971e-01
rcc    25 0.00 0.00  -1.82890e+02 0.00 0.00   1.82890e+02   4.53971e-01
```

Figure S4.5.5 Input listing of sample problem 4

```
rpp   26 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01 -1.8288e+02
          1.8288e+02
rpp   27 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01  1.8288e+02
          1.8289e+02
rpp   28 -6.3000e-01  6.3000e-01 -6.3000e-01  6.3000e-01 -1.8289e+02
         -1.8288e+02
rpp   29 -1.0710e+01  1.0710e+01 -1.0710e+01  1.0710e+01 -1.8289e+02
          1.8289e+02
rpp   30 -1.0715e+01  1.0715e+01 -1.0715e+01  1.0715e+01 -1.8289e+02
          1.8289e+02
rpp   31 -1.0725e+01  1.0725e+01 -1.0725e+01  1.0725e+01 -1.8289e+02
          1.8289e+02
rpp   32 -1.2325e+01  1.2325e+01 -1.2325e+01  1.2325e+01 -1.8289e+02
          1.8289e+02
rpp   33 -2.4650e+01  2.4650e+01 -3.6975e+01 -1.2325e+01 -1.8289e+02
          1.8289e+02
rpp   34 -3.6975e+01  3.6975e+01 -1.2325e+01  1.2325e+01 -1.8289e+02
          1.8289e+02
rpp   35 -2.4650e+01  2.4650e+01  1.2325e+01  3.6975e+01 -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  -33  -34  -35
fue    21
gap    22  -21
cla    23  -22
fcl    26  -23
uv1    18  -26                    Universe 1
hr2    24  -23
hc2    27  -24
uv2    18  -27
hr3    25  -23
hc3    28  -25
uv3    18  -28
ar1    29                        Array 1
spa    30  -29
can    31  -30
unt    32  -31
uv4    18  -32
ar2    33
ar3    34
ar4    35
  end
```

Zones 1–18 describe the cask body. This portion is generic for the SAS4 cask mode.

Figure S4.5.5 (continued)

```
12r1 2 1 2  23r1            Region Specification
19*0  5*1 3*2 3*3 5*4 3r0          Universe Specification
    4    5 1000 1000    4 1000 1000    5 1000 1000 1000 1000  4*1000        Medium number
      0   1000   1000      1      2      2   1000  -1000   1000   1000       for each zone
  -1000   1000   1000  -1000     -1   1000   1000   1000
 -1000    -2    -3    -4
   17   17    3    2    1    1    3    1    1    2    1    1    0    0
  289*3    289*1    289*2  7*4
4r0
end
```

Figure S4.5.5 (continued)

## 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 = 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 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 1.00-9   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=10   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
```

Fuel material mixture used in Monte Carlo calculation

Material of fuel zone in adjoint discrete ordinates 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

```
=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 1.000-9  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                          Gamma doses are calculated
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 3r0 0.01 21.4493 end                  Neutron source spectrum is zero.
182.88 228.60 229.87 237.49 241.30 end        Only primary gamma doses are calculated.
2r0 4 5 4 end
xend
tim=5.0   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                              40 entries are
fu2 21.16 36.42 182.88 182.89 end                            required
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 S4.5.7 Input listing of sample problem 6

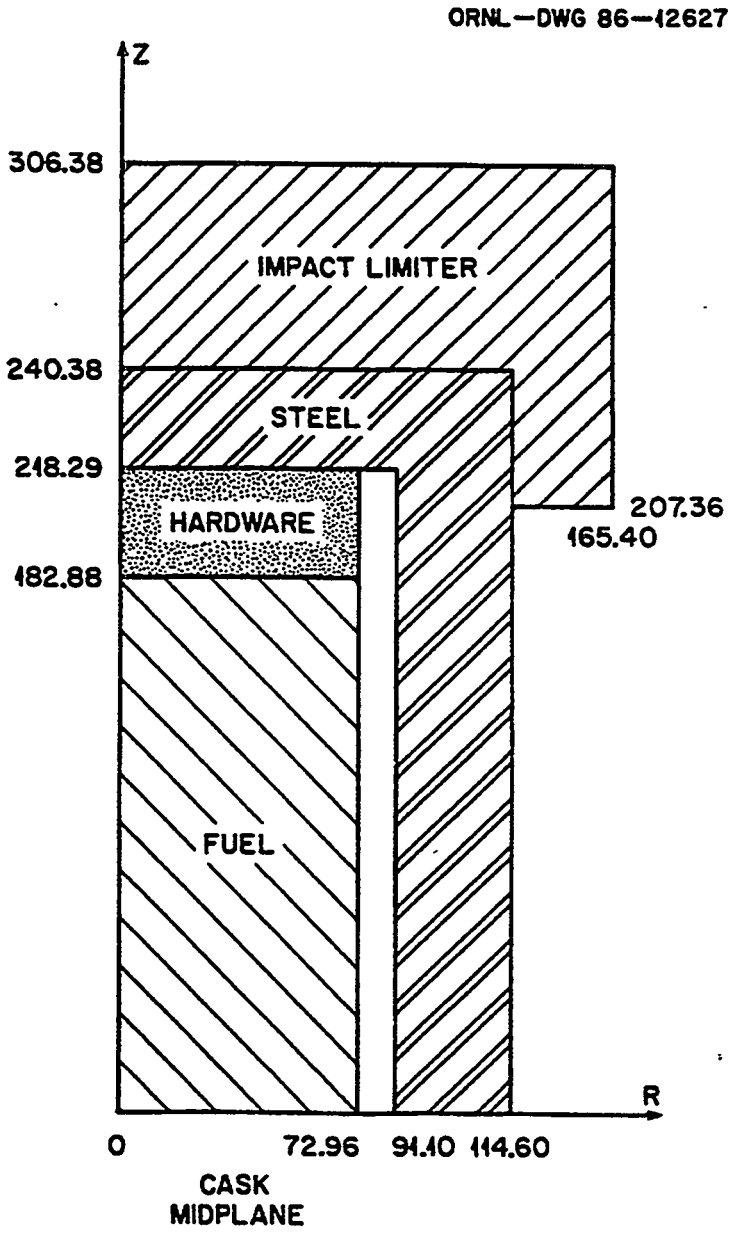



Figure S4.5.8 Upper half of steel cask of sample problem 7

```
=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
#shell
cp ft04f001 $RTNDIR/sas4g.ft04f001
cp ft12f001 $RTNDIR/sas4g.ft12f001
end
```

Figure S4.5.9 Input listing of sample problem 7

```
#shell
ln -fs $RTNDIR/sas4g.ft04f001 ft04f001
ln -fs $RTNDIR/sas4g.ft12f001 ft12f001
end
=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
```

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

```
*******************************************************************************
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                  program verification information                *****
*****                                                                     *****
*****                 code system:    scale  version:    4.3           *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*****                                                                     *****
*****                                                                     *****
*****              program:  o0o106                                       *****
*****                                                                     *****
*****        creation date:  09/13/95                                     *****
*****                                                                     *****
*****              library:  /scale4.3/bin                                *****
*****                                                                     *****
*****                                                                     *****
*****      production code:  morse                                        *****
*****                                                                     *****
*****              version:  3.0                                          *****
*****                                                                     *****
*****              jobname:  x4s                                          *****
*****                                                                     *****
*****    date of execution:  09/07/95                                     *****
*****                                                                     *****
*****    time of execution:  04:30:00                                     *****
*****                                                                     *****
*****                                                                     *****
*******************************************************************************
*******************************************************************************
*******************************************************************************
```

```
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 thursday, september 7,1995

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 | 10 | 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 | 8 |
| nmix | number of mixing operations | 19 | mfistp | fission indicator | 1 |
| medalb | albedo indicator | 0 | | | |

3 $ array

Only neutron is analyzed for neutron dose calculation

| | | | | | |
|---|---|---|---|---|---|
| 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          thursday, september 7,1995
          4 $ array
  isour   source energy group                          0      isbias   source energy bias indicator      1
  ngpfs   number of source groups                     22      nsour    fixed source indicator            0

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
 subroutine  stbtch  version     1
 subroutine  sdata   version     1
 subroutine  sgam    version     1
 subroutine  bdryx   version     1
 subroutine  relcoa  version    -1
```

Always called in a MORSE-SGC/S calculation

Always called in SAS4

SDATA, SGAM, and RELCOA are called when point detecors are input in SAS4

```
sample problem 1, radial neutron doses of dry depleted uranium cask     thursday, september 7,1995
      6q array has    10 entries.
      8q array has   704 entries.
      9q array has   176 entries.
     10q array has   184 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  thursday, september 7,1995

6 * array

| | | | | | |
|---|---|---|---|---|---|
| tmax | maximum 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 |
| wtstrt | input starting weight of particles | 0.1000E+01 | ymax | upper y limit of source volume | 0.0000E+00 |
| agstrt | starting age of source particles | 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 |



**In SAS4, these values are set internally.**

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 |

sample problem 1, radial neutron doses of dry depleted uranium cask thursday, september 7,1995
8 * array

| group | region | splitting wt | rr weight | surviving wt | stretch parameters |
|---|---|---|---|---|---|
| 1 | 1 | 0.4777E+00 | 0.3908E+00 | 0.4299E+00 | 0.2106E+00 |
| 2 | 1 | 0.5393E+00 | 0.4412E+00 | 0.4854E+00 | 0.1953E+00 |
| 3 | 1 | 0.5659E+00 | 0.4630E+00 | 0.5093E+00 | 0.1930E+00 |
| 4 | 1 | 0.6732E+00 | 0.5508E+00 | 0.6059E+00 | 0.1971E+00 |
| 5 | 1 | 0.8169E+00 | 0.6684E+00 | 0.7352E+00 | 0.1991E+00 |
| 6 | 1 | 0.8928E+00 | 0.7305E+00 | 0.8035E+00 | 0.1998E+00 |
| 7 | 1 | 0.9387E+00 | 0.7622E+00 | 0.8448E+00 | 0.1901E+00 |
| 8 | 1 | 0.9773E+00 | 0.7918E+00 | 0.8796E+00 | 0.2189E+00 |
| 9 | 1 | 0.9859E+00 | 0.8030E+00 | 0.8873E+00 | 0.2326E+00 |
| 10 | 1 | 0.1058E+01 | 0.8303E+00 | 0.9524E+00 | 0.2475E+00 |
| 11 | 1 | 0.1350E+01 | 0.1018E+01 | 0.1204E+01 | 0.2579E+00 |
| 12 | 1 | 0.1579E+01 | 0.1113E+01 | 0.1371E+01 | 0.2510E+00 |
| 13 | 1 | 0.2566E+01 | 0.1794E+01 | 0.2224E+01 | 0.1931E+00 |
| 14 | 1 | 0.1114E+02 | 0.9113E+01 | 0.1002E+02 | 0.2894E-01 |
| 15 | 1 | 0.1448E+02 | 0.1145E+02 | 0.1260E+02 | -0.6474E-01 |
| 16 | 1 | 0.2034E+02 | 0.1664E+02 | 0.1831E+02 | -0.6111E-01 |
| 17 | 1 | 0.2546E+02 | 0.2083E+02 | 0.2292E+02 | -0.4388E-01 |
| 18 | 1 | 0.1612E+02 | 0.1319E+02 | 0.1451E+02 | -0.8186E-01 |
| 19 | 1 | 0.2833E+02 | 0.2318E+02 | 0.2549E+02 | -0.4781E-01 |
| 20 | 1 | 0.3874E+01 | 0.3169E+01 | 0.3486E+01 | -0.9708E-02 |
| 21 | 1 | 0.5375E+01 | 0.3766E+01 | 0.4812E+01 | 0.1317E+00 |
| 22 | 1 | 0.8136E+00 | 0.6573E+00 | 0.7231E+00 | -0.8631E-01 |
| 1 | 2 | 0.4329E+00 | 0.3542E+00 | 0.3896E+00 | 0.3288E+00 |
| 2 | 2 | 0.4966E+00 | 0.4063E+00 | 0.4469E+00 | 0.3124E+00 |
| 3 | 2 | 0.5238E+00 | 0.4286E+00 | 0.4714E+00 | 0.3112E+00 |
| 4 | 2 | 0.6236E+00 | 0.5102E+00 | 0.5612E+00 | 0.2977E+00 |
| 5 | 2 | 0.7501E+00 | 0.6137E+00 | 0.6751E+00 | 0.2892E+00 |
| 6 | 2 | 0.8111E+00 | 0.6636E+00 | 0.7300E+00 | 0.2886E+00 |
| 7 | 2 | 0.8402E+00 | 0.6874E+00 | 0.7562E+00 | 0.2832E+00 |
| 8 | 2 | 0.8696E+00 | 0.7115E+00 | 0.7826E+00 | 0.2905E+00 |
| 9 | 2 | 0.8825E+00 | 0.7220E+00 | 0.7942E+00 | 0.2857E+00 |
| 10 | 2 | 0.9068E+00 | 0.7419E+00 | 0.8161E+00 | 0.2929E+00 |
| 11 | 2 | 0.1106E+01 | 0.9049E+00 | 0.9954E+00 | 0.3066E+00 |
| 12 | 2 | 0.1199E+01 | 0.9814E+00 | 0.1079E+01 | 0.3064E+00 |
| 13 | 2 | 0.1929E+01 | 0.1578E+01 | 0.1736E+01 | 0.2353E+00 |
| 14 | 2 | 0.1183E+02 | 0.9679E+01 | 0.1065E+02 | 0.6886E-01 |
| 15 | 2 | 0.1695E+02 | 0.1387E+02 | 0.1526E+02 | -0.3782E-01 |
| 16 | 2 | 0.2392E+02 | 0.1957E+02 | 0.2152E+02 | -0.4913E-01 |
| 17 | 2 | 0.2892E+02 | 0.2366E+02 | 0.2603E+02 | -0.3855E-01 |
| 18 | 2 | 0.1855E+02 | 0.1518E+02 | 0.1670E+02 | -0.7739E-01 |
| 19 | 2 | 0.2565E+02 | 0.2098E+02 | 0.2308E+02 | -0.6907E-01 |
| 20 | 2 | 0.3876E+01 | 0.3171E+01 | 0.3489E+01 | -0.3977E-02 |
| 21 | 2 | 0.3798E+01 | 0.3108E+01 | 0.3418E+01 | 0.1083E+00 |
| 22 | 2 | 0.1038E+01 | 0.8490E+00 | 0.9339E+00 | -0.2169E-01 |

Russian roulette, splitting, and path length stretching parameters are generated from the adjoint XSDRNPM-S results.

| | | | | | |
|---|---|---|---|---|---|
| 1 | 3 | 0.4187E+00 | 0.3426E+00 | 0.3768E+00 | 0.3398E+00 |
| 2 | 3 | 0.4848E+00 | 0.3967E+00 | 0.4363E+00 | 0.2927E+00 |
| 3 | 3 | 0.5120E+00 | 0.4189E+00 | 0.4608E+00 | 0.2683E+00 |
| 4 | 3 | 0.6097E+00 | 0.4988E+00 | 0.5487E+00 | 0.2577E+00 |
| 5 | 3 | 0.7342E+00 | 0.6007E+00 | 0.6607E+00 | 0.2508E+00 |
| 6 | 3 | 0.7915E+00 | 0.6476E+00 | 0.7123E+00 | 0.2575E+00 |
| 7 | 3 | 0.8218E+00 | 0.6724E+00 | 0.7396E+00 | 0.2568E+00 |
| 8 | 3 | 0.8448E+00 | 0.6912E+00 | 0.7603E+00 | 0.2568E+00 |
| 9 | 3 | 0.8546E+00 | 0.6992E+00 | 0.7691E+00 | 0.2701E+00 |
| 10 | 3 | 0.8735E+00 | 0.7147E+00 | 0.7861E+00 | 0.2860E+00 |
| 11 | 3 | 0.1068E+01 | 0.8740E+00 | 0.9614E+00 | 0.3186E+00 |
| 12 | 3 | 0.1157E+01 | 0.9469E+00 | 0.1042E+01 | 0.3150E+00 |

Russian roulette and splitting parameters

Path length stretching parameters

sample problem 1, radial neutron doses of dry depleted uranium cask thursday, september 7,1995
8 * array

| group | region | splitting wt | rr weight | surviving wt | stretch parameters |
|---|---|---|---|---|---|
| 13 | 3 | 0.1855E+01 | 0.1517E+01 | 0.1669E+01 | 0.2358E+00 |
| 14 | 3 | 0.1222E+02 | 0.1000E+02 | 0.1100E+02 | 0.8933E-01 |
| 15 | 3 | 0.1977E+02 | 0.1589E+02 | 0.1768E+02 | -0.4127E-02 |
| 16 | 3 | 0.3483E+02 | 0.2298E+02 | 0.2777E+02 | -0.1911E-01 |
| 17 | 3 | 0.4374E+02 | 0.2778E+02 | 0.3395E+02 | -0.2003E-01 |
| 18 | 3 | 0.3207E+02 | 0.1818E+02 | 0.2327E+02 | -0.4737E-01 |
| 19 | 3 | 0.3245E+02 | 0.2316E+02 | 0.2614E+02 | -0.5796E-01 |
| 20 | 3 | 0.3957E+01 | 0.3237E+01 | 0.3561E+01 | -0.3739E-02 |
| 21 | 3 | 0.3222E+01 | 0.2477E+01 | 0.2807E+01 | 0.7222E-01 |
| 22 | 3 | 0.1386E+01 | 0.1055E+01 | 0.1247E+01 | 0.1392E-01 |
| 1 | 4 | 0.3641E+00 | 0.2979E+00 | 0.3277E+00 | 0.1210E+00 |
| 2 | 4 | 0.4230E+00 | 0.3461E+00 | 0.3807E+00 | 0.1247E+00 |
| 3 | 4 | 0.4492E+00 | 0.3675E+00 | 0.4042E+00 | 0.1351E+00 |
| 4 | 4 | 0.5436E+00 | 0.4448E+00 | 0.4893E+00 | 0.1705E+00 |
| 5 | 4 | 0.6729E+00 | 0.5506E+00 | 0.6056E+00 | 0.2126E+00 |
| 6 | 4 | 0.7247E+00 | 0.5929E+00 | 0.6522E+00 | 0.2175E+00 |
| 7 | 4 | 0.7602E+00 | 0.6219E+00 | 0.6841E+00 | 0.2239E+00 |
| 8 | 4 | 0.7858E+00 | 0.6430E+00 | 0.7073E+00 | 0.2449E+00 |
| 9 | 4 | 0.7898E+00 | 0.6462E+00 | 0.7108E+00 | 0.2547E+00 |
| 10 | 4 | 0.7975E+00 | 0.6525E+00 | 0.7178E+00 | 0.2639E+00 |
| 11 | 4 | 0.9901E+00 | 0.8101E+00 | 0.8911E+00 | 0.3204E+00 |
| 12 | 4 | 0.1072E+01 | 0.8774E+00 | 0.9651E+00 | 0.3203E+00 |
| 13 | 4 | 0.1708E+01 | 0.1398E+01 | 0.1537E+01 | 0.2436E+00 |
| 14 | 4 | 0.1280E+02 | 0.1047E+02 | 0.1152E+02 | 0.1319E+00 |
| 15 | 4 | 0.2513E+02 | 0.2056E+02 | 0.2262E+02 | 0.6232E-01 |
| 16 | 4 | 0.6255E+02 | 0.3900E+02 | 0.5203E+02 | 0.6731E-01 |
| 17 | 4 | 0.1065E+03 | 0.5159E+02 | 0.8520E+02 | 0.5236E-01 |
| 18 | 4 | 0.8837E+02 | 0.3927E+02 | 0.6718E+02 | 0.6912E-01 |
| 19 | 4 | 0.9453E+02 | 0.4091E+02 | 0.7263E+02 | 0.8024E-01 |
| 20 | 4 | 0.3892E+01 | 0.3185E+01 | 0.3503E+01 | -0.2597E-01 |
| 21 | 4 | 0.2442E+01 | 0.1998E+01 | 0.2198E+01 | -0.2280E-01 |
| 22 | 4 | 0.1315E+01 | 0.1076E+01 | 0.1183E+01 | -0.6465E-01 |

| | | | | | |
|---|---|---|---|---|---|
| 1 | 5 | 0.3174E+00 | 0.2597E+00 | 0.2856E+00 | 0.7923E-01 |
| 2 | 5 | 0.3678E+00 | 0.3009E+00 | 0.3310E+00 | 0.8124E-01 |
| 3 | 5 | 0.3915E+00 | 0.3203E+00 | 0.3523E+00 | 0.9807E-01 |
| 4 | 5 | 0.4758E+00 | 0.3893E+00 | 0.4282E+00 | 0.1486E+00 |
| 5 | 5 | 0.5926E+00 | 0.4849E+00 | 0.5334E+00 | 0.2045E+00 |
| 6 | 5 | 0.6362E+00 | 0.5205E+00 | 0.5726E+00 | 0.2130E+00 |
| 7 | 5 | 0.6702E+00 | 0.5483E+00 | 0.6032E+00 | 0.2225E+00 |
| 8 | 5 | 0.6937E+00 | 0.5676E+00 | 0.6243E+00 | 0.2477E+00 |
| 9 | 5 | 0.6944E+00 | 0.5681E+00 | 0.6250E+00 | 0.2582E+00 |
| 10 | 5 | 0.6952E+00 | 0.5688E+00 | 0.6257E+00 | 0.2671E+00 |
| 11 | 5 | 0.8629E+00 | 0.7060E+00 | 0.7766E+00 | 0.3355E+00 |
| 12 | 5 | 0.9284E+00 | 0.7596E+00 | 0.8356E+00 | 0.3407E+00 |
| 13 | 5 | 0.1471E+01 | 0.1204E+01 | 0.1324E+01 | 0.2597E+00 |
| 14 | 5 | 0.1244E+02 | 0.1018E+02 | 0.1120E+02 | 0.1702E+00 |
| 15 | 5 | 0.2848E+02 | 0.2330E+02 | 0.2563E+02 | 0.1152E+00 |
| 16 | 5 | 0.7320E+02 | 0.5989E+02 | 0.6588E+02 | 0.1169E+00 |
| 17 | 5 | 0.1129E+03 | 0.9238E+02 | 0.1016E+03 | 0.7909E-01 |
| 18 | 5 | 0.9718E+02 | 0.7951E+02 | 0.8746E+02 | 0.1004E+00 |
| 19 | 5 | 0.1030E+03 | 0.8423E+02 | 0.9266E+02 | 0.1107E+00 |
| 20 | 5 | 0.3792E+01 | 0.3102E+01 | 0.3413E+01 | -0.5352E-01 |
| 21 | 5 | 0.2117E+01 | 0.1732E+01 | 0.1906E+01 | -0.1003E+00 |
| 22 | 5 | 0.1127E+01 | 0.9225E+00 | 0.1015E+01 | -0.1445E+00 |
| 1 | 6 | 0.2708E+00 | 0.2215E+00 | 0.2437E+00 | -0.3899E-01 |
| 2 | 6 | 0.3126E+00 | 0.2557E+00 | 0.2813E+00 | -0.4116E-01 |

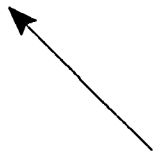
sample problem 1, radial neutron doses of dry depleted uranium cask thursday, september 7,1995
8 * array

| group | region | splitting wt | rr weight | surviving wt | stretch parameters |
|---|---|---|---|---|---|
| 3 | 6 | 0.3323E+00 | 0.2719E+00 | 0.2991E+00 | -0.2429E-02 |
| 4 | 6 | 0.3996E+00 | 0.3270E+00 | 0.3597E+00 | 0.9071E-01 |
| 5 | 6 | 0.4891E+00 | 0.4002E+00 | 0.4402E+00 | 0.1794E+00 |
| 6 | 6 | 0.5214E+00 | 0.4262E+00 | 0.4693E+00 | 0.1971E+00 |
| 7 | 6 | 0.5490E+00 | 0.4480E+00 | 0.4941E+00 | 0.2129E+00 |
| 8 | 6 | 0.5660E+00 | 0.4606E+00 | 0.5094E+00 | 0.2477E+00 |
| 9 | 6 | 0.5655E+00 | 0.4600E+00 | 0.5089E+00 | 0.2604E+00 |
| 10 | 6 | 0.5636E+00 | 0.4581E+00 | 0.5072E+00 | 0.2679E+00 |
| 11 | 6 | 0.6939E+00 | 0.5489E+00 | 0.6168E+00 | 0.3600E+00 |
| 12 | 6 | 0.7430E+00 | 0.5822E+00 | 0.6573E+00 | 0.3792E+00 |
| 13 | 6 | 0.1176E+01 | 0.9249E+00 | 0.1041E+01 | 0.2902E+00 |
| 14 | 6 | 0.1049E+02 | 0.8424E+01 | 0.9441E+01 | 0.2142E+00 |
| 15 | 6 | 0.2650E+02 | 0.2168E+02 | 0.2385E+02 | 0.1696E+00 |
| 16 | 6 | 0.6244E+02 | 0.4903E+02 | 0.5565E+02 | 0.1813E+00 |
| 17 | 6 | 0.9200E+02 | 0.7386E+02 | 0.8244E+02 | 0.1318E+00 |
| 18 | 6 | 0.7994E+02 | 0.6411E+02 | 0.7162E+02 | 0.1623E+00 |
| 19 | 6 | 0.8482E+02 | 0.6859E+02 | 0.7633E+02 | 0.1828E+00 |
| 20 | 6 | 0.3713E+01 | 0.3038E+01 | 0.3342E+01 | -0.1085E+00 |
| 21 | 6 | 0.1917E+01 | 0.1568E+01 | 0.1725E+01 | -0.2320E+00 |
| 22 | 6 | 0.9714E+00 | 0.7948E+00 | 0.8743E+00 | -0.3365E+00 |
| 1 | 7 | 0.2408E+00 | 0.1970E+00 | 0.2167E+00 | -0.3683E+00 |
| 2 | 7 | 0.2782E+00 | 0.2276E+00 | 0.2504E+00 | -0.3714E+00 |
| 3 | 7 | 0.2946E+00 | 0.2410E+00 | 0.2651E+00 | -0.2558E+00 |
| 4 | 7 | 0.3432E+00 | 0.2808E+00 | 0.3089E+00 | -0.4657E-01 |
| 5 | 7 | 0.3999E+00 | 0.3272E+00 | 0.3599E+00 | 0.1205E+00 |
| 6 | 7 | 0.4216E+00 | 0.3449E+00 | 0.3794E+00 | 0.1630E+00 |
| 7 | 7 | 0.4414E+00 | 0.3612E+00 | 0.3973E+00 | 0.1954E+00 |
| 8 | 7 | 0.4504E+00 | 0.3657E+00 | 0.4054E+00 | 0.2532E+00 |
| 9 | 7 | 0.4498E+00 | 0.3651E+00 | 0.4048E+00 | 0.2714E+00 |
| 10 | 7 | 0.4484E+00 | 0.3649E+00 | 0.4036E+00 | 0.2727E+00 |
| 11 | 7 | 0.5293E+00 | 0.4099E+00 | 0.4687E+00 | 0.4155E+00 |
| 12 | 7 | 0.5606E+00 | 0.4293E+00 | 0.4938E+00 | 0.4765E+00 |
| 13 | 7 | 0.8919E+00 | 0.6950E+00 | 0.7921E+00 | 0.3651E+00 |
| 14 | 7 | 0.8103E+01 | 0.6006E+01 | 0.7081E+01 | 0.2481E+00 |
| 15 | 7 | 0.2105E+02 | 0.1583E+02 | 0.1858E+02 | 0.2166E+00 |
| 16 | 7 | 0.4670E+02 | 0.2353E+02 | 0.3560E+02 | 0.3121E+00 |
| 17 | 7 | 0.7151E+02 | 0.2857E+02 | 0.5356E+02 | 0.3620E+00 |
| 18 | 7 | 0.6187E+02 | 0.2812E+02 | 0.4781E+02 | 0.4034E+00 |
| 19 | 7 | 0.6621E+02 | 0.2504E+02 | 0.4852E+02 | 0.4608E+00 |
| 20 | 7 | 0.3854E+01 | 0.3153E+01 | 0.3468E+01 | -0.1673E+00 |
| 21 | 7 | 0.2023E+01 | 0.1650E+01 | 0.1815E+01 | -0.3748E+00 |
| 22 | 7 | 0.1174E+01 | 0.8298E+00 | 0.9128E+00 | -0.6610E+00 |

sample problem 1, radial neutron doses of dry depleted uranium cask

9 * array

| group | region | relative importance |
|---|---|---|
| 1 | 1 | 0.1124E-05 |
| 2 | 1 | 0.9955E-06 |
| 3 | 1 | 0.9487E-06 |
| 4 | 1 | 0.7975E-06 |
| 5 | 1 | 0.6572E-06 |
| 6 | 1 | 0.6013E-06 |
| 7 | 1 | 0.5719E-06 |
| 8 | 1 | 0.5493E-06 |
| 9 | 1 | 0.5445E-06 |
| 10 | 1 | 0.5073E-06 |
| 11 | 1 | 0.4012E-06 |
| 12 | 1 | 0.3523E-06 |
| 13 | 1 | 0.2173E-06 |
| 14 | 1 | 0.4820E-07 |
| 15 | 1 | 0.3836E-07 |
| 16 | 1 | 0.2639E-07 |
| 17 | 1 | 0.2108E-07 |
| 18 | 1 | 0.3331E-07 |
| 19 | 1 | 0.1895E-07 |
| 20 | 1 | 0.1386E-06 |
| 21 | 1 | 0.1004E-06 |
| 22 | 1 | 0.6682E-06 |
| 1 | 2 | 0.1240E-05 |
| 2 | 2 | 0.1081E-05 |
| 3 | 2 | 0.1025E-05 |
| 4 | 2 | 0.8609E-06 |
| 5 | 2 | 0.7157E-06 |
| 6 | 2 | 0.6619E-06 |
| 7 | 2 | 0.6390E-06 |
| 8 | 2 | 0.6174E-06 |
| 9 | 2 | 0.6084E-06 |
| 10 | 2 | 0.5921E-06 |
| 11 | 2 | 0.4854E-06 |
| 12 | 2 | 0.4476E-06 |
| 13 | 2 | 0.2784E-06 |
| 14 | 2 | 0.4538E-07 |
| 15 | 2 | 0.3167E-07 |
| 16 | 2 | 0.2245E-07 |
| 17 | 2 | 0.1856E-07 |
| 18 | 2 | 0.2894E-07 |
| 19 | 2 | 0.2093E-07 |
| 20 | 2 | 0.1385E-06 |
| 21 | 2 | 0.1413E-06 |
| 22 | 2 | 0.5174E-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 | 0.1049E-05 |
| 4 | 3 | 0.8805E-06 |
| 5 | 3 | 0.7313E-06 |
| 6 | 3 | 0.6783E-06 |
| 7 | 3 | 0.6533E-06 |
| 8 | 3 | 0.6355E-06 |
| 9 | 3 | 0.6282E-06 |
| 10 | 3 | 0.6146E-06 |
| 11 | 3 | 0.5026E-06 |
| 12 | 3 | 0.4639E-06 |

sample problem 1, radial neutron doses of dry depleted uranium cask thursday, september 7,1995
9 * array

| group | region | relative importance |
|---|---|---|
| 13 | 3 | 0.2895E-06 |
| 14 | 3 | 0.4392E-07 |
| 15 | 3 | 0.2733E-07 |
| 16 | 3 | 0.1740E-07 |
| 17 | 3 | 0.1423E-07 |
| 18 | 3 | 0.2076E-07 |
| 19 | 3 | 0.1848E-07 |
| 20 | 3 | 0.1357E-06 |
| 21 | 3 | 0.1721E-06 |
| 22 | 3 | 0.3873E-06 |
| 1 | 4 | 0.1474E-05 |
| 2 | 4 | 0.1269E-05 |
| 3 | 4 | 0.1195E-05 |
| 4 | 4 | 0.9876E-06 |
| 5 | 4 | 0.7978E-06 |
| 6 | 4 | 0.7408E-06 |
| 7 | 4 | 0.7062E-06 |
| 8 | 4 | 0.6832E-06 |
| 9 | 4 | 0.6798E-06 |
| 10 | 4 | 0.6732E-06 |
| 11 | 4 | 0.5422E-06 |
| 12 | 4 | 0.5007E-06 |
| 13 | 4 | 0.3143E-06 |
| 14 | 4 | 0.4195E-07 |
| 15 | 4 | 0.2136E-07 |
| 16 | 4 | 0.9287E-08 |
| 17 | 4 | 0.5671E-08 |
| 18 | 4 | 0.7192E-08 |
| 19 | 4 | 0.6652E-08 |
| 20 | 4 | 0.1379E-06 |
| 21 | 4 | 0.2199E-06 |
| 22 | 4 | 0.4083E-06 |
| 1 | 5 | 0.1692E-05 |
| 2 | 5 | 0.1460E-05 |
| 3 | 5 | 0.1371E-05 |
| 4 | 5 | 0.1128E-05 |
| 5 | 5 | 0.9059E-06 |
| 6 | 5 | 0.8438E-06 |
| 7 | 5 | 0.8011E-06 |
| 8 | 5 | 0.7739E-06 |
| 9 | 5 | 0.7731E-06 |
| 10 | 5 | 0.7722E-06 |
| 11 | 5 | 0.6222E-06 |
| 12 | 5 | 0.5782E-06 |

sample problem 1, radial neutron doses of dry depleted uranium cask thursday, september 7,1995
9 * array

| group | region | relative importance |
|---|---|---|
| 13 | 5 | 0.3649E-06 |
| 14 | 5 | 0.4315E-07 |
| 15 | 5 | 0.1885E-07 |
| 16 | 5 | 0.7334E-08 |
| 17 | 5 | 0.4755E-08 |
| 18 | 5 | 0.5524E-08 |
| 19 | 5 | 0.5215E-08 |
| 20 | 5 | 0.1416E-06 |
| 21 | 5 | 0.2535E-06 |
| 22 | 5 | 0.4762E-06 |
| 1 | 6 | 0.1983E-05 |
| 2 | 6 | 0.1718E-05 |

| | | | |
|---|---|---|---|
| 3 | 6 | 0.1615E-05 | |
| 4 | 6 | 0.1343E-05 | |
| 5 | 6 | 0.1098E-05 | |
| 6 | 6 | 0.1030E-05 | |
| 7 | 6 | 0.9779E-06 | |
| 8 | 6 | 0.9485E-06 | |
| 9 | 6 | 0.9494E-06 | |
| 10 | 6 | 0.9526E-06 | |
| 11 | 6 | 0.7833E-06 | |
| 12 | 6 | 0.7351E-06 | |
| 13 | 6 | 0.4640E-06 | |
| 14 | 6 | 0.5118E-07 | |
| 15 | 6 | 0.2026E-07 | |
| 16 | 6 | 0.8602E-08 | |
| 17 | 6 | 0.5861E-08 | |
| 18 | 6 | 0.6746E-08 | |
| 19 | 6 | 0.6330E-08 | |
| 20 | 6 | 0.1446E-06 | |
| 21 | 6 | 0.2801E-06 | |
| 22 | 6 | 0.5527E-06 | |
| 1 | 7 | 0.2230E-05 | |
| 2 | 7 | 0.1930E-05 | |
| 3 | 7 | 0.1822E-05 | |
| 4 | 7 | 0.1564E-05 | |
| 5 | 7 | 0.1342E-05 | |
| 6 | 7 | 0.1273E-05 | |
| 7 | 7 | 0.1216E-05 | |
| 8 | 7 | 0.1192E-05 | |
| 9 | 7 | 0.1194E-05 | |
| 10 | 7 | 0.1197E-05 | |
| 11 | 7 | 0.1031E-05 | |
| 12 | 7 | 0.9785E-06 | |
| 13 | 7 | 0.6100E-06 | |
| 14 | 7 | 0.6824E-07 | |
| 15 | 7 | 0.2601E-07 | |
| 16 | 7 | 0.1357E-07 | |
| 17 | 7 | 0.9022E-08 | |
| 18 | 7 | 0.1011E-07 | |
| 19 | 7 | 0.9958E-08 | |
| 20 | 7 | 0.1393E-06 | |
| 21 | 7 | 0.2661E-06 | |
| 22 | 7 | 0.5293E-06 | |

10 * array, fission neutron weights

| region | neutron weight |
|---|---|
| 1 | 0.1353E+01 |
| 2 | 0.1150E+01 |
| 3 | 0.1121E+01 |
| 4 | 0.1054E+01 |
| 5 | 0.9341E+00 |
| 6 | 0.7529E+00 |
| 7 | 0.5790E+00 |
| 8 | 0.3541E+00 |

Weights given to fission neutrons as a function of importance region.

12$, 13$, and 14* arrays

| medium | element | density |
|---|---|---|
| 7 | 1092235 | 5.2672E-05 |
| 5 | 5092235 | 1.0700E-04 |
| 7 | 1092238 | 6.1692E-03 |
| 5 | 5092238 | 4.7700E-02 |
| 7 | 1094239 | 3.2759E-05 |
| 7 | 1094240 | 1.4960E-05 |
| 7 | 1008016 | 1.2550E-02 |
| 7 | 3008016 | 5.0430E-10 |
| 7 | 2040000 | 1.7799E-03 |
| 4 | 4024000 | 1.6620E-02 |
| 4 | 4025055 | 1.2000E-03 |
| 4 | 4026000 | 5.7750E-02 |
| 4 | 4028000 | 7.5200E-03 |
| 4 | 4042000 | 1.1000E-04 |
| 1 | 4042000 | 1.0000E-10 |
| 2 | 4042000 | 1.0000E-10 |
| 3 | 4042000 | 1.0000E-10 |
| 6 | 4042000 | 1.0000E-10 |
| 8 | 4042000 | 1.0000E-10 |

Cross-section mixing table

sample problem 1, radial neutron doses of dry depleted uranium cask  thursday, september 7,1995

17* and 18* arrays

| group | fs(ig) | bfs(ig) |
|---|---|---|
| 1 | 2.4740E-13 | 1.1239E-06 |
| 2 | 2.0960E-12 | 9.9549E-07 |
| 3 | 5.7660E-12 | 9.4869E-07 |
| 4 | 2.8990E-11 | 7.9747E-07 |
| 5 | 7.2280E-11 | 6.5718E-07 |
| 6 | 1.4570E-10 | 6.0130E-07 |
| 7 | 6.0990E-10 | 5.7194E-07 |
| 8 | 4.5420E-10 | 5.4933E-07 |
| 9 | 9.0700E-11 | 5.4455E-07 |
| 10 | 3.8240E-10 | 5.0733E-07 |
| 11 | 4.9900E-10 | 4.0123E-07 |
| 12 | 3.9820E-10 | 3.5235E-07 |
| 13 | 1.8360E-10 | 2.1728E-07 |
| 14 | 1.7610E-14 | 4.8203E-08 |
| 15 | 0.0000E+00 | 3.8356E-08 |
| 16 | 0.0000E+00 | 2.6394E-08 |
| 17 | 0.0000E+00 | 2.1085E-08 |
| 18 | 0.0000E+00 | 3.3307E-08 |
| 19 | 0.0000E+00 | 1.8953E-08 |
| 20 | 0.0000E+00 | 1.3860E-07 |
| 21 | 0.0000E+00 | 1.0041E-07 |
| 22 | 0.0000E+00 | 6.6821E-07 |

Source energy spectrum

Source energy biasing parameters

sample problem 1, radial neutron doses of dry depleted uranium cask  thursday, september 7,1995

19q array has 21 entries.

20q array has 22 entries.

21q array has 22 entries.

core available for mixing = 197394
core needed for mixing = 1154

total storage space = 200000
length of non cross section data = 16469
space for xsec data and supergroup data = 183531
minimum space needed for cross sections = 968
total storage needed for cross sections = 9614

number of supergroups = 1
space for cross sections = 183392

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 | 6.50128E-03 | 0.00000E+00 | 6.50128E-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 | 2.98588E-01 | 0.00000E+00 | 2.98588E-01 | 0.00000E+00 |
| 9 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 3.19252E-01 | 0.00000E+00 | 3.19252E-01 | 0.00000E+00 |
| 10 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 0.00000E+00 | 4.34712E-01 | 0.00000E+00 | 4.34712E-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 | 4.29921E-01 | 2.00291E-04 |
| 2 | 4.85363E-01 | 1.70334E-03 |
| 3 | 5.09305E-01 | 5.64380E-03 |
| 4 | 6.05880E-01 | 2.22975E-02 |
| 5 | 7.35218E-01 | 5.65153E-02 |
| 6 | 8.03546E-01 | 1.19625E-01 |
| 7 | 8.44794E-01 | 3.70905E-01 |
| 8 | 8.79573E-01 | 5.50637E-01 |
| 9 | 8.87298E-01 | 5.86215E-01 |
| 10 | 9.52385E-01 | 7.25967E-01 |
| 11 | 1.20422E+00 | 8.70193E-01 |
| 12 | 1.37130E+00 | 9.71262E-01 |
| 13 | 2.22371E+00 | 9.99999E-01 |
| 14 | 1.00238E+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 thursday, september 7,1995

| detector | | y | z | rad | t0 |
|---|---|---|---|---|---|
| 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          thursday, september 7,1995

                              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 less than one second.
****start batch    1                          random=    F2AE3EBFB1EB
source data
   wtave       iave    uave    vave    wave       xave       yave       zave       ageave
  9.968E+01     9.23  -0.0219 -0.1388  0.0625  -1.323E+00 -8.428E-01  9.576E+00   0.000E+00
 you are using the default version of gtmed which assumes  that the geometry and xsec media are the same
 uncol responses by resp. function & detector:
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 total responses by resp. function & detector:
   4.8215E-10  1.0974E-10  4.8524E-11  3.2272E-11  1.8373E-10  8.2896E-11  1.3861E-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      531     2645       61     3320        0     2838      158        0        0      534     1184        0
time required for the preceding batch was 2 seconds.
****start batch    2                          random=    1DF706314AAC
source data
   wtave       iave    uave    vave    wave       xave       yave       zave       ageave
  9.710E+01     9.01   0.0095 -0.0256 -0.0620  -6.476E-01  8.614E-01  1.261E+01   0.000E+00
 uncol responses by resp. function & detector:
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
 total responses by resp. function & detector:
   4.0994E-10  9.7217E-11  4.8508E-11  2.9282E-11  1.5097E-10  7.2747E-11  5.7533E-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       431     2122       43     2671        0     2470      134        0        0      440      947        0
time required for the preceding batch was 1 second.
****start batch    3                          random=    52F30D6D7819

source data
   wtave       iave    uave    vave    wave       xave       yave       zave       ageave
  1.035E+02     9.52   0.0438  0.0448 -0.0385  -9.189E-01 -3.406E+00 -1.423E+01   0.000E+00
 uncol responses by resp. function & detector:
   0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  5.0483E-13  1.9997E-13  1.0112E-18
 total responses by resp. function & detector:
   6.4353E-10  1.5511E-10  7.4484E-11  4.1041E-11  2.3439E-10  1.0389E-10  3.2819E-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       642     3189       60     4043        0     3416      211        0        0      591     1459        0

time required for the preceding batch was 2 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 directin cosinewith 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 + 531 + 61 = 158 + 0 + 0 + 534 = 692

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 | 9836 | 642 |
| | | 642 | 8 | 278 | 0 |
| 1 | -19 | | | | |
| | | 233 | 19 | 8426 | 0 |
| 2 | 2 | | | | |
| | | 239 | 3 | 17307 | 636 |
| | | 636 | 4 | 634 | 654 |
| | | 654 | 12 | 110 | 0 |
| 2 | -10 | | | | |
| | | 244 | 1 | 8513 | 675 |
| | | 675 | 8 | 13 | 0 |
| 3 | 3 | | | | |
| | | 250 | 4 | 17307 | 0 |
| 3 | -2 | | | | |
| | | 255 | 2 | 6212 | 0 |
| 4 | 4 | | | | |
| | | 261 | 5 | 17941 | 0 |
| 4 | -3 | | | | |
| | | 266 | 3 | 6212 | 0 |
| 5 | 5 | | | | |
| | | 272 | 6 | 25193 | 657 |
| | | 657 | 11 | 280 | 0 |
| 5 | -13 | | | | |
| | | 277 | 4 | 6212 | 663 |
| | | 663 | 12 | 26 | 672 |
| | | 672 | 10 | 17 | 0 |
| 6 | 6 | | | | |
| | | 283 | 7 | 25193 | 0 |
| 6 | -5 | | | | |
| | | 288 | 0 | 0 | 0 |
| 7 | 7 | | | | |
| | | 294 | 13 | 25193 | 0 |
| 7 | -6 | | | | |
| | | 299 | 0 | 0 | 0 |
| 7 | -5 | | | | |
| | | 304 | 0 | 0 | 0 |
| 8 | 8 | | | | |
| | | 310 | 9 | 173 | 660 |
| | | 660 | 2 | 76 | 0 |
| 8 | -1 | | | | |
| | | 315 | 1 | 92 | 0 |
| 9 | 9 | | | | |
| | | 321 | 10 | 171 | 669 |
| | | 669 | 2 | 2 | 0 |
| 9 | -8 | | | | |

combinatorial geometry zone transfer summary tables

| exit zone | exit body | loc. in ma array | entering zone | no. of entries | loc. for next zone |
|---|---|---|---|---|---|
| 9 | -8 | 326 | 8 | 17 | 0 |
| 10 | 10 | 332 | 5 | 171 | 0 |
| 10 | -9 | 337 | 9 | 17 | 0 |
| 11 | 11 | 343 | 13 | 280 | 0 |
| 11 | -5 | 348 | 0 | 0 | 0 |
| 11 | -12 | 353 | 0 | 0 | 0 |
| 12 | 13 | 359 | 5 | 110 | 0 |
| 12 | -4 | 364 | 2 | 26 | 0 |
| 12 | -10 | 369 | 0 | 0 | 0 |
| 13 | 14 | 375 | 15 | 9553 | 0 |
| 13 | -5 | 380 | 0 | 0 | 0 |
| 13 | -7 | 385 | 0 | 0 | 0 |
| 13 | -11 | 390 | 0 | 0 | 0 |
| 14 | 12 | 396 | 0 | 0 | 0 |
| 14 | -5 | 401 | 0 | 0 | 0 |
| 14 | -7 | 406 | 0 | 0 | 0 |
| 15 | 15 | 412 | 16 | 1593 | 0 |
| 15 | -14 | 417 | 0 | 0 | 0 |
| 16 | 16 | 423 | 17 | 1593 | 0 |
| 16 | -15 | 428 | 0 | 0 | 0 |
| 17 | 17 | 434 | 18 | 1593 | 0 |
| 17 | -16 | 439 | 0 | 0 | 0 |
| 18 | 18 | 445 | 0 | 0 | 0 |

combinatorial geometry zone transfer summary tables

| exit zone | exit body | loc. in ma array | entering zone | no. of entries | loc. for next zone |
|---|---|---|---|---|---|
| 18 | -17 | | | | |
| | | 450 | 0 | 0 | 0 |
| 19 | 19 | | | | |
| | | 456 | 1 | 9591 | 0 |
| 19 | -20 | | | | |
| | | 461 | 20 | 8426 | 0 |
| 20 | 20 | | | | |
| | | 467 | 19 | 9591 | 678 |
| | | 678 | 1 | 3 | 0 |
| 20 | -32 | | | | |
| | | 472 | 29 | 5926 | 639 |
| | | 639 | 31 | 137 | 645 |
| | | 645 | 22 | 41 | 666 |
| | | 666 | 30 | 19 | 0 |
| 21 | 31 | | | | |
| | | 478 | 29 | 2 | 0 |
| 21 | -30 | | | | |
| | | 483 | 0 | 0 | 0 |
| 21 | -25 | | | | |
| | | 488 | 0 | 0 | 0 |
| 22 | 29 | | | | |
| | | 494 | 20 | 117 | 648 |
| | | 648 | 28 | 11 | 0 |
| 22 | -28 | | | | |
| | | 499 | 0 | 0 | 0 |
| 22 | -23 | | | | |
| | | 504 | 25 | 41 | 0 |
| 23 | 27 | | | | |
| | | 510 | 27 | 1 | 0 |
| 23 | -21 | | | | |
| | | 515 | 0 | 0 | 0 |
| 24 | 25 | | | | |
| | | 521 | 29 | 6802 | 630 |
| | | 630 | 21 | 2 | 0 |
| 24 | -30 | | | | |
| | | 526 | 28 | 5926 | 0 |
| 25 | 23 | | | | |
| | | 532 | 28 | 3647 | 627 |
| | | 627 | 22 | 128 | 0 |
| 25 | -28 | | | | |
| | | 537 | 27 | 1975 | 0 |
| 26 | 21 | | | | |
| | | 543 | 23 | 1 | 0 |
| 27 | 22 | | | | |
| | | 549 | 25 | 2162 | 651 |
| | | 651 | 30 | 31 | 0 |

combinatorial geometry zone transfer summary tables

| exit zone | exit body | loc. in ma array | entering zone | no. of entries | loc. for next zone |
|---|---|---|---|---|---|
| 27 | -21 | 554 | 26 | 1 | 0 |
| 28 | 24 | 560 | 24 | 6804 | 633 |
| | | 633 | 31 | 339 | 0 |
| 28 | -23 | 565 | 25 | 3547 | 0 |
| 29 | 26 | 571 | 20 | 6804 | 0 |
| 29 | -25 | 576 | 24 | 5926 | 0 |
| 30 | 28 | 582 | 20 | 31 | 0 |
| 30 | -27 | 587 | 0 | 0 | 0 |
| 30 | -22 | 592 | 27 | 19 | 0 |
| 31 | 30 | 598 | 20 | 339 | 0 |
| 31 | -29 | 603 | 0 | 0 | 0 |
| 31 | -24 | 608 | 28 | 137 | 0 |
| 32 | 32 | 614 | 0 | 0 | 0 |
| 32 | -31 | 619 | 0 | 0 | 0 |
| 32 | -26 | 624 | 0 | 0 | 0 |

this case was run on thursday, september 7,1995

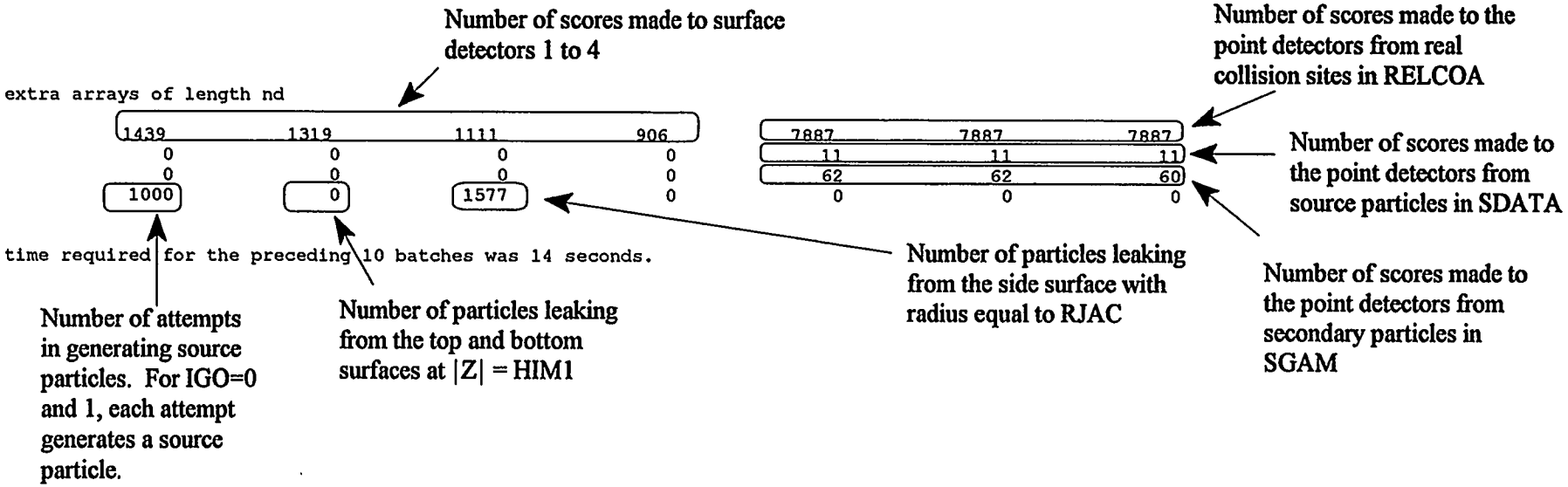
ansi standard neutron dose rate (rem per hour)

| | responses(detector) | | | |
|---|---|---|---|---|
| detector | uncoll response | fsd uncoll | total response | fsd total |
| 1 | 0.0000E+00 | 0.00000 | 4.8000E-10 | 0.05345 |
| 2 | 0.0000E+00 | 0.00000 | 1.1386E-10 | 0.06182 |
| 3 | 0.0000E+00 | 0.00000 | 5.5749E-11 | 0.07077 |
| 4 | 0.0000E+00 | 0.00000 | 3.1917E-11 | 0.06275 |
| 5 | 3.9557E-13 | 0.59908 | 1.5550E-10 | 0.09045 |
| 6 | 1.9712E-13 | 0.54340 | 7.6541E-11 | 0.06416 |
| 7 | 7.7966E-16 | 0.97327 | 1.9078E-11 | 0.25929 |

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 $2.614 \times 10^8$ neutrons per second, the total source strength is $1.8298 \times 10^9$ neutrons per second. Hence, the total responses must be multiplied by $1.8298 \times 10^9$ 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 | 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 |
| 1.000E+07 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 4.376E-16 | 2.690E-16 | 3.842E-19 |
| | 0.000 | 0.000 | 0.000 | 0.000 | 0.995 | 0.949 | 0.950 |
| 8.180E+06 | 8.885E-15 | 2.830E-15 | 1.405E-15 | 8.333E-16 | 2.650E-15 | 1.857E-15 | 9.590E-20 |
| | 0.596 | 0.573 | 0.527 | 0.569 | 0.630 | 0.407 | 0.485 |
| 6.360E+06 | 2.221E-14 | 7.577E-15 | 3.645E-15 | 1.579E-15 | 3.270E-15 | 4.262E-15 | 2.308E-16 |
| | 0.264 | 0.269 | 0.322 | 0.353 | 0.382 | 0.400 | 1.515 |
| 4.960E+06 | 3.156E-14 | 1.062E-14 | 5.054E-15 | 3.010E-15 | 6.849E-15 | 8.565E-16 | 4.501E-17 |
| | 0.392 | 0.389 | 0.383 | 0.387 | 0.546 | 1.238 | 0.990 |
| 4.060E+06 | 6.842E-14 | 1.894E-14 | 9.974E-15 | 6.207E-15 | 2.046E-14 | 8.905E-15 | 9.930E-15 |
| | 0.334 | 0.238 | 0.238 | 0.255 | 0.315 | 0.244 | 0.967 |
| 3.010E+06 | 9.194E-14 | 2.537E-14 | 1.365E-14 | 8.944E-15 | 3.628E-14 | 2.206E-14 | 7.244E-15 |
| | 0.141 | 0.135 | 0.174 | 0.192 | 0.256 | 0.225 | 0.734 |
| 2.460E+06 | 5.435E-13 | 3.032E-14 | 1.836E-14 | 9.495E-15 | 1.467E-13 | 4.552E-14 | 5.735E-15 |
| | 0.805 | 0.433 | 0.432 | 0.543 | 0.390 | 0.315 | 0.670 |
| 2.350E+06 | 2.038E-13 | 5.570E-14 | 2.270E-14 | 1.518E-14 | 6.040E-14 | 2.928E-14 | 3.234E-14 |
| | 0.193 | 0.168 | 0.256 | 0.285 | 0.380 | 0.326 | 0.673 |
| 1.830E+06 | 3.962E-13 | 8.158E-14 | 3.617E-14 | 1.835E-14 | 1.358E-13 | 6.936E-14 | 2.740E-14 |
| | 0.114 | 0.112 | 0.158 | 0.205 | 0.236 | 0.115 | 0.440 |
| 1.110E+06 | 2.207E-12 | 5.466E-13 | 2.820E-13 | 1.655E-13 | 7.119E-13 | 3.493E-13 | 6.125E-14 |
| | 0.087 | 0.106 | 0.105 | 0.102 | 0.096 | 0.097 | 0.201 |
| 5.500E+05 | 8.549E-12 | 1.986E-12 | 9.598E-13 | 5.433E-13 | 2.824E-12 | 1.380E-12 | 2.889E-13 |
| | 0.088 | 0.093 | 0.103 | 0.089 | 0.127 | 0.096 | 0.297 |
| 1.110E+05 | 4.352E-12 | 1.093E-12 | 3.846E-13 | 1.504E-13 | 1.334E-12 | 6.406E-13 | 2.690E-14 |
| | 0.378 | 0.374 | 0.371 | 0.392 | 0.322 | 0.349 | 0.689 |
| 3.350E+03 | 6.522E-11 | 6.370E-12 | 3.732E-12 | 2.656E-12 | 4.452E-12 | 3.699E-12 | 1.392E-14 |
| | 1.000 | 1.000 | 1.000 | 1.000 | 0.907 | 0.955 | 0.905 |
| 5.830E+02 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 4.362E-13 | 2.203E-13 | 4.797E-16 |
| | 0.000 | 0.000 | 0.000 | 0.000 | 0.990 | 0.991 | 0.298 |
| 1.010E+02 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 0.000E+00 | 1.901E-15 | 9.244E-16 | 2.080E-16 |
| | 0.000 | 0.000 | 0.000 | 0.000 | 0.113 | 0.096 | 0.222 |
| 2.900E+01 | | | | | | | |


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
1439 1319 1111 906
0 0 0 0
0 0 0 0
1000 0 1577 0
7887 7887 7887
11 11 11
62 62 60
0 0 0
Number of scores made to the point detectors from source particles in SDATA
time required for the preceding 10 batches was 14 seconds.
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
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

| neutron deaths | number | weight |
|---|---|---|
| killed by russian roulette | 4750 | 0.40620E+04 |
| escaped | 1593 | 0.55237E+03 |
| 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 | 6507 |
| 5 | 17416 |
| 6 | 0 |
| 7 | 7278 |
| 8 | 0 |

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 | 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 | 9 | 4.19E+00 | 0 | 0.00E+00 | 1 | 4.70E-01 | 2 | 9.80E-01 | 2 | 7.57E-01 | 0 | 0.00E+00 |
| 3 | 6 | 2.70E+00 | 0 | 0.00E+00 | 5 | 1.79E+00 | 1 | 4.87E-01 | 7 | 2.26E+00 | 10 | 2.94E+00 |
| 4 | 48 | 2.88E+01 | 1 | 4.75E-01 | 8 | 4.69E+00 | 4 | 2.90E+00 | 14 | 6.91E+00 | 17 | 7.18E+00 |
| 5 | 86 | 6.35E+01 | 1 | 7.28E-01 | 15 | 1.04E+01 | 9 | 6.12E+00 | 27 | 1.60E+01 | 31 | 1.42E+01 |
| 6 | 115 | 9.24E+01 | 0 | 0.00E+00 | 23 | 1.75E+01 | 28 | 1.83E+01 | 38 | 2.41E+01 | 42 | 2.13E+01 |
| 7 | 502 | 4.21E+02 | 14 | 1.11E+01 | 81 | 6.61E+01 | 68 | 5.10E+01 | 108 | 7.09E+01 | 110 | 5.89E+01 |
| 8 | 321 | 2.81E+02 | 1 | 3.98E-01 | 78 | 6.22E+01 | 73 | 5.51E+01 | 106 | 7.14E+01 | 64 | 3.72E+01 |
| 9 | 85 | 7.60E+01 | 0 | 0.00E+00 | 31 | 2.58E+01 | 27 | 2.09E+01 | 30 | 2.08E+01 | 46 | 2.70E+01 |
| 10 | 264 | 2.45E+02 | 3 | 2.59E+00 | 81 | 6.57E+01 | 63 | 4.98E+01 | 94 | 6.36E+01 | 95 | 5.43E+01 |
| 11 | 500 | 5.65E+02 | 10 | 9.89E+00 | 108 | 1.06E+02 | 134 | 1.24E+02 | 225 | 1.83E+02 | 268 | 1.65E+02 |
| 12 | 1617 | 2.08E+03 | 43 | 4.47E+01 | 394 | 4.08E+02 | 472 | 4.47E+02 | 895 | 7.23E+02 | 1028 | 6.67E+02 |
| 13 | 3749 | 7.74E+03 | 85 | 1.41E+02 | 1111 | 1.79E+03 | 1476 | 2.17E+03 | 2896 | 3.65E+03 | 3520 | 3.51E+03 |
| 14 | 347 | 3.38E+03 | 33 | 3.38E+02 | 171 | 1.83E+03 | 109 | 1.20E+03 | 168 | 1.81E+03 | 136 | 1.18E+03 |
| 15 | 5 | 6.74E+01 | 2 | 2.64E+01 | 23 | 3.86E+02 | 13 | 2.52E+02 | 3 | 6.10E+01 | 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 | region 7 weight | region 8 number | region 8 weight |
|---|---|---|---|---|
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 2 | 5.96E-01 | 0 | 0.00E+00 |
| 4 | 13 | 4.98E+00 | 14 | 3.76E+00 |
| 5 | 30 | 1.19E+01 | 16 | 4.80E+00 |
| 6 | 26 | 1.04E+01 | 21 | 6.65E+00 |
| 7 | 63 | 2.76E+01 | 62 | 1.87E+01 |
| 8 | 54 | 2.36E+01 | 66 | 1.93E+01 |
| 9 | 19 | 9.11E+00 | 10 | 3.30E+00 |
| 10 | 71 | 2.96E+01 | 100 | 2.90E+01 |
| 11 | 212 | 9.64E+01 | 242 | 7.63E+01 |
| 12 | 944 | 4.49E+02 | 903 | 3.12E+02 |
| 13 | 2945 | 2.19E+03 | 2596 | 1.36E+03 |
| 14 | 134 | 8.41E+02 | 210 | 7.85E+02 |
| 15 | 2 | 2.16E+01 | 10 | 9.34E+01 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

fission production 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 | 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 | 2 | 2.71E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 1.05E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 1 | 1.35E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 9.34E-01 | 3 | 2.26E+00 |
| 4 | 3 | 4.06E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 1.05E+00 | 5 | 4.67E+00 | 2 | 1.51E+00 |
| 5 | 11 | 1.49E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 2 | 2.11E+00 | 6 | 5.60E+00 | 4 | 3.01E+00 |
| 6 | 11 | 1.49E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 2 | 2.11E+00 | 2 | 1.87E+00 | 4 | 3.01E+00 |
| 7 | 32 | 4.33E+01 | 1 | 1.15E+00 | 0 | 0.00E+00 | 10 | 1.05E+01 | 13 | 1.21E+01 | 12 | 9.03E+00 |
| 8 | 25 | 3.38E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 9 | 9.49E+00 | 15 | 1.40E+01 | 10 | 7.53E+00 |
| 9 | 11 | 1.49E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 4 | 4.22E+00 | 2 | 1.87E+00 | 7 | 5.27E+00 |
| 10 | 18 | 2.44E+01 | 2 | 2.30E+00 | 0 | 0.00E+00 | 8 | 8.43E+00 | 14 | 1.31E+01 | 12 | 9.03E+00 |
| 11 | 14 | 1.89E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 7 | 7.38E+00 | 21 | 1.96E+01 | 27 | 2.03E+01 |
| 12 | 11 | 1.49E+01 | 1 | 1.15E+00 | 0 | 0.00E+00 | 2 | 2.11E+00 | 6 | 5.60E+00 | 1 | 7.53E-01 |
| 13 | 17 | 2.30E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 9.34E-01 | 3 | 2.26E+00 |
| 14 | 8 | 1.08E+01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 1.05E+00 | 2 | 1.87E+00 | 2 | 1.51E+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 | region 7 weight | region 8 number | region 8 weight |
|---|---|---|---|---|
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 4 | 3 | 1.74E+00 | 0 | 0.00E+00 |
| 5 | 7 | 4.05E+00 | 0 | 0.00E+00 |
| 6 | 8 | 4.63E+00 | 0 | 0.00E+00 |
| 7 | 7 | 4.05E+00 | 0 | 0.00E+00 |
| 8 | 11 | 6.37E+00 | 0 | 0.00E+00 |
| 9 | 6 | 3.47E+00 | 0 | 0.00E+00 |
| 10 | 14 | 8.11E+00 | 0 | 0.00E+00 |
| 11 | 12 | 6.95E+00 | 0 | 0.00E+00 |
| 12 | 3 | 1.74E+00 | 0 | 0.00E+00 |
| 13 | 2 | 1.16E+00 | 0 | 0.00E+00 |
| 14 | 1 | 5.79E-01 | 0 | 0.00E+00 |
| 15 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

number of splittings

| 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 | 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 | 3 | 1.35E+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 | 3 | 9.34E-01 | 3 | 7.53E-01 |
| 4 | 9 | 4.06E+00 | 1 | 5.75E-01 | 0 | 0.00E+00 | 1 | 3.64E-01 | 2 | 7.54E-01 | 0 | 0.00E+00 |
| 5 | 15 | 9.94E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 6 | 2.68E+00 | 3 | 1.13E+00 |
| 6 | 5 | 3.38E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 3 | 1.58E+00 | 7 | 3.12E+00 | 10 | 3.50E+00 |
| 7 | 23 | 1.48E+01 | 1 | 5.75E-01 | 9 | 4.01E+00 | 5 | 2.64E+00 | 7 | 3.30E+00 | 19 | 6.63E+00 |
| 8 | 11 | 7.26E+00 | 1 | 4.46E-01 | 14 | 6.29E+00 | 8 | 4.11E+00 | 15 | 6.71E+00 | 11 | 3.65E+00 |
| 9 | 4 | 2.71E+00 | 0 | 0.00E+00 | 3 | 1.40E+00 | 5 | 2.51E+00 | 5 | 2.35E+00 | 6 | 2.36E+00 |
| 10 | 20 | 1.35E+01 | 0 | 0.00E+00 | 19 | 9.05E+00 | 9 | 4.74E+00 | 16 | 7.03E+00 | 23 | 7.84E+00 |
| 11 | 45 | 3.12E+01 | 1 | 5.75E-01 | 36 | 2.15E+01 | 24 | 1.32E+01 | 48 | 2.32E+01 | 50 | 1.93E+01 |
| 12 | 71 | 6.15E+01 | 8 | 5.42E+00 | 94 | 6.25E+01 | 77 | 4.87E+01 | 189 | 1.01E+02 | 227 | 9.80E+01 |
| 13 | 128 | 1.80E+02 | 13 | 1.33E+01 | 202 | 2.19E+02 | 267 | 2.57E+02 | 499 | 4.07E+02 | 620 | 4.14E+02 |
| 14 | 10 | 6.10E+01 | 1 | 5.98E+00 | 8 | 5.25E+01 | 2 | 1.48E+01 | 3 | 2.08E+01 | 10 | 5.55E+01 |
| 15 | 3 | 2.36E+01 | 0 | 0.00E+00 | 3 | 3.37E+01 | 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 | region 7 weight | region 8 number | region 8 weight |
|---|---|---|---|---|
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 2 | 5.79E-01 | 0 | 0.00E+00 |
| 4 | 4 | 9.45E-01 | 1 | 1.60E-01 |
| 5 | 5 | 1.29E+00 | 6 | 1.08E+00 |
| 6 | 3 | 8.68E-01 | 3 | 6.19E-01 |
| 7 | 13 | 3.49E+00 | 14 | 2.70E+00 |
| 8 | 13 | 3.84E+00 | 21 | 4.46E+00 |
| 9 | 3 | 7.61E-01 | 1 | 2.08E-01 |
| 10 | 16 | 4.13E+00 | 21 | 4.40E+00 |
| 11 | 46 | 1.37E+01 | 56 | 1.30E+01 |
| 12 | 212 | 6.99E+01 | 267 | 6.73E+01 |
| 13 | 617 | 3.16E+02 | 575 | 2.28E+02 |
| 14 | 12 | 5.39E+01 | 23 | 7.43E+01 |
| 15 | 0 | 0.00E+00 | 1 | 9.05E+00 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

number of splittings prevented by lack of room

| energy | region 1 | | region 2 | | region 3 | | region 4 | | region 5 | | region 6 | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| group | 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 | region 7 | | region 8 | |
|---|---|---|---|---|
| group | number | weight | number | weight |
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 4 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 5 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 6 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 7 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 8 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 9 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 10 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 11 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 12 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 13 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 14 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 15 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

number of russian roulette kills

| 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 | 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 | 2 | 7.55E-01 | 0 | 0.00E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 2.73E-01 | 0 | 0.00E+00 |
| 3 | 1 | 3.10E-01 | 0 | 0.00E+00 | 1 | 2.30E-01 | 0 | 0.00E+00 | 4 | 8.94E-01 | 3 | 5.46E-01 |
| 4 | 9 | 3.91E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 3.64E-01 | 1 | 3.09E-01 | 2 | 5.12E-01 |
| 5 | 14 | 7.92E+00 | 0 | 0.00E+00 | 2 | 1.03E+00 | 1 | 3.55E-01 | 1 | 4.21E-01 | 3 | 9.99E-01 |
| 6 | 9 | 6.04E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 4 | 1.88E+00 | 2 | 8.56E-01 | 5 | 1.79E+00 |
| 7 | 57 | 3.88E+01 | 0 | 0.00E+00 | 4 | 2.10E+00 | 8 | 3.92E+00 | 15 | 6.68E+00 | 17 | 5.67E+00 |
| 8 | 47 | 3.27E+01 | 2 | 8.17E-01 | 13 | 5.98E+00 | 10 | 4.89E+00 | 16 | 6.43E+00 | 11 | 3.67E+00 |
| 9 | 12 | 8.24E+00 | 0 | 0.00E+00 | 2 | 8.86E-01 | 3 | 1.55E+00 | 5 | 2.37E+00 | 6 | 1.99E+00 |
| 10 | 47 | 3.31E+01 | 0 | 0.00E+00 | 15 | 7.58E+00 | 9 | 4.19E+00 | 20 | 8.35E+00 | 21 | 7.13E+00 |
| 11 | 98 | 7.59E+01 | 0 | 0.00E+00 | 22 | 1.28E+01 | 19 | 1.04E+01 | 49 | 2.44E+01 | 53 | 2.07E+01 |
| 12 | 165 | 1.46E+02 | 8 | 5.38E+00 | 75 | 5.24E+01 | 93 | 6.09E+01 | 211 | 1.11E+02 | 239 | 1.01E+02 |
| 13 | 348 | 5.14E+02 | 13 | 1.40E+01 | 157 | 1.79E+02 | 271 | 2.77E+02 | 517 | 4.40E+02 | 648 | 4.36E+02 |
| 14 | 20 | 1.40E+02 | 3 | 2.00E+01 | 13 | 9.96E+01 | 9 | 7.22E+01 | 18 | 1.65E+02 | 25 | 1.48E+02 |
| 15 | 3 | 2.35E+01 | 0 | 0.00E+00 | 1 | 1.14E+01 | 2 | 2.38E+01 | 3 | 5.37E+01 | 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 | region 7 weight | region 8 number | region 8 weight |
|---|---|---|---|---|
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 1 | 2.31E-01 | 0 | 0.00E+00 |
| 4 | 3 | 6.87E-01 | 1 | 1.60E-01 |
| 5 | 1 | 2.85E-01 | 0 | 0.00E+00 |
| 6 | 4 | 1.21E+00 | 0 | 0.00E+00 |
| 7 | 13 | 3.23E+00 | 0 | 0.00E+00 |
| 8 | 14 | 3.06E+00 | 4 | 6.87E-01 |
| 9 | 2 | 5.43E-01 | 0 | 0.00E+00 |
| 10 | 13 | 3.24E+00 | 5 | 8.44E-01 |
| 11 | 53 | 1.46E+01 | 19 | 3.14E+00 |
| 12 | 207 | 6.08E+01 | 53 | 9.45E+00 |
| 13 | 661 | 3.21E+02 | 167 | 5.22E+01 |
| 14 | 32 | 1.09E+02 | 7 | 1.63E+01 |
| 15 | 1 | 7.10E+00 | 0 | 0.00E+00 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

number of russian roulette survivals

| 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 | 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 | 7 | 2.45E+00 | 0 | 0.00E+00 | 0 | 0.00E+00 | 1 | 3.31E-01 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 2 | 6.46E-01 | 0 | 0.00E+00 | 3 | 7.64E-01 | 0 | 0.00E+00 | 4 | 8.39E-01 | 7 | 1.47E+00 |
| 4 | 32 | 1.39E+01 | 1 | 3.45E-01 | 6 | 2.74E+00 | 1 | 4.22E-01 | 10 | 3.15E+00 | 7 | 2.07E+00 |
| 5 | 43 | 2.57E+01 | 0 | 0.00E+00 | 2 | 1.04E+00 | 2 | 1.05E+00 | 18 | 7.29E+00 | 18 | 6.29E+00 |
| 6 | 66 | 4.43E+01 | 0 | 0.00E+00 | 8 | 4.66E+00 | 15 | 7.35E+00 | 23 | 1.02E+01 | 22 | 7.73E+00 |
| 7 | 259 | 1.82E+02 | 7 | 4.23E+00 | 17 | 9.02E+00 | 21 | 1.13E+01 | 36 | 1.68E+01 | 48 | 1.77E+01 |
| 8 | 171 | 1.22E+02 | 0 | 0.00E+00 | 16 | 8.68E+00 | 32 | 1.78E+01 | 39 | 1.83E+01 | 23 | 8.36E+00 |
| 9 | 58 | 4.08E+01 | 0 | 0.00E+00 | 9 | 5.33E+00 | 13 | 6.90E+00 | 16 | 7.64E+00 | 17 | 6.66E+00 |
| 10 | 134 | 9.84E+01 | 1 | 6.58E-01 | 31 | 1.72E+01 | 32 | 1.77E+01 | 45 | 2.12E+01 | 42 | 1.55E+01 |
| 11 | 183 | 1.61E+02 | 6 | 4.78E+00 | 56 | 3.81E+01 | 62 | 3.74E+01 | 101 | 5.57E+01 | 128 | 5.46E+01 |
| 12 | 365 | 3.57E+02 | 24 | 1.96E+01 | 199 | 1.53E+02 | 240 | 1.68E+02 | 444 | 2.66E+02 | 486 | 2.25E+02 |
| 13 | 678 | 1.06E+03 | 34 | 4.23E+01 | 522 | 6.52E+02 | 693 | 7.77E+02 | 1285 | 1.23E+03 | 1420 | 1.05E+03 |
| 14 | 81 | 6.73E+02 | 8 | 7.63E+01 | 30 | 2.56E+02 | 29 | 2.70E+02 | 50 | 4.65E+02 | 42 | 2.92E+02 |
| 15 | 2 | 1.45E+01 | 1 | 1.09E+01 | 8 | 9.42E+01 | 11 | 1.98E+02 | 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 | region 7 weight | region 8 number | region 8 weight |
|---|---|---|---|---|
| 1 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 2 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 3 | 1 | 2.29E-01 | 0 | 0.00E+00 |
| 4 | 6 | 1.27E+00 | 0 | 0.00E+00 |
| 5 | 13 | 3.47E+00 | 0 | 0.00E+00 |
| 6 | 9 | 2.50E+00 | 0 | 0.00E+00 |
| 7 | 22 | 6.59E+00 | 3 | 4.81E-01 |
| 8 | 16 | 4.70E+00 | 4 | 6.82E-01 |
| 9 | 5 | 1.51E+00 | 0 | 0.00E+00 |
| 10 | 38 | 1.03E+01 | 8 | 1.41E+00 |
| 11 | 96 | 2.97E+01 | 18 | 3.07E+00 |
| 12 | 458 | 1.54E+02 | 84 | 1.52E+01 |
| 13 | 1269 | 6.84E+02 | 258 | 8.24E+01 |
| 14 | 33 | 1.47E+02 | 8 | 1.82E+01 |
| 15 | 1 | 1.19E+01 | 0 | 0.00E+00 |
| 16 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 17 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 18 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 19 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 20 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 21 | 0 | 0.00E+00 | 0 | 0.00E+00 |
| 22 | 0 | 0.00E+00 | 0 | 0.00E+00 |

**next random number is 200503995F32

total cpu time for this problem was 0.23 minutes.

```
 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
 roth      1.0000 theoretical density
 nel            1 no. elements
 icp            1 0/1 mixture/compound
           92235      1.00 atom/molecule
 end

 sc  u-238        standard composition
 mx             1 mixture no.
 den   1.9602E-02 atomic density
 roth      1.0000 theoretical density
 nel            1 no. elements
 icp            1 0/1 mixture/compound
           92238      1.00 atom/molecule
 end

 sc  pu-239       standard composition
 mx             1 mixture no.
 den   1.0409E-04 atomic density
 roth      1.0000 theoretical density
 nel            1 no. elements
```

```
icp            1 0/1 mixture/compound
           94239      1.00 atom/molecule
end

sc  pu-240       standard composition
mx             1 mixture no.
den   4.7534E-05 atomic density
roth      1.0000 theoretical density
nel            1 no. elements
icp            1 0/1 mixture/compound
           94240      1.00 atom/molecule
end

sc  o            standard composition
mx             1 mixture no.
den   3.9877E-02 atomic density
roth      1.0000 theoretical density
nel            1 no. elements
icp            1 0/1 mixture/compound
            8016      1.00 atom/molecule
end

sc  zr           standard composition
mx             2 mixture no.
den   1.9350E-02 atomic density
roth      6.4900 theoretical density
nel            1 no. elements
icp            1 0/1 mixture/compound
           40000      1.00 atom/molecule
end

sc  o            standard composition
mx             3 mixture no.
den   1.0000E-09 atomic density
roth      1.0000 theoretical density
nel            1 no. elements
icp            1 0/1 mixture/compound
```

```
            8016      1.00 atom/molecule
end

sc  cr            standard composition
mx              4 mixture no.
den   1.6620E-02 atomic density
roth      7.2000 theoretical density
nel             1 no. elements
icp             1 0/1 mixture/compound
           24000      1.00 atom/molecule
end

sc  mn            standard composition
mx              4 mixture no.
den   1.2000E-03 atomic density
roth      7.2000 theoretical density
nel             1 no. elements
icp             1 0/1 mixture/compound
           25055      1.00 atom/molecule
end

sc  fe            standard composition
mx              4 mixture no.
den   5.7750E-02 atomic density
roth      7.8600 theoretical density
nel             1 no. elements
icp           . 1 0/1 mixture/compound
           26000      1.00 atom/molecule
end

sc  ni            standard composition
mx              4 mixture no.
den   7.5200E-03 atomic density
roth      8.9000 theoretical density
nel             1 no. elements

icp             1 0/1 mixture/compound
```

```
           28000      1.00 atom/molecule
end

sc  mo             standard composition
mx              4 mixture no.
den    1.1000E-04 atomic density
roth      10.2000 theoretical density
nel             1 no. elements
icp             1 0/1 mixture/compound
           42000      1.00 atom/molecule
end

sc  u-235          standard composition
mx              5 mixture no.
den    1.0700E-04 atomic density
roth       1.0000 theoretical density
nel             1 no. elements
icp             1 0/1 mixture/compound
           92235      1.00 atom/molecule
end

sc  u-238          standard composition
mx              5 mixture no.
den    4.7700E-02 atomic density
roth       1.0000 theoretical density
nel             1 no. elements
icp             1 0/1 mixture/compound
           92238      1.00 atom/molecule
end
```

**Output from cell-weighting calculation**

```
**** problem geometry ****

 ctp squarepitch  cell type
 pitch     1.2600 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


**** 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 ****

    7 mesh intervals in zone  1
    4 mesh intervals in zone  2
    4 mesh intervals in zone  3
   41 mesh intervals in zone  4
```

```
     5 mesh intervals in zone  5


  **** source energy 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
```

**** morse importance region informations ****

| region | # of xsdrn int. | region boundry | estimation prob |
|---|---|---|---|
| 1 | 7 | 3.6420E+01 | 1.8781E-02 |
| 2 | 4 | 4.4550E+01 | 3.1959E-02 |
| 3 | 4 | 4.5820E+01 | 3.9234E-02 |
| 4 | 17 | 4.6899E+01 | 5.4257E-02 |
| 5 | 8 | 4.8928E+01 | 9.3833E-02 |
| 6 | 8 | 5.1334E+01 | 1.8504E-01 |
| 7 | 8 | 5.3440E+01 | 4.0710E-01 |
| 8 | 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 location 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  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
          0.3642000E+02
rcc   25  0.0000000E+00  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
          0.3642100E+02
rcc   26  0.0000000E+00  0.0000000E+00 -0.1828800E+03  0.0000000E+00  0.0000000E+00  0.3657600E+03
          0.3642200E+02
rcc   27  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.1000000E-02
rcc   28  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.1210000E+02
rcc   29  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.2116000E+02
rcc   30  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.3642000E+02
rcc   31  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.3642100E+02
rcc   32  0.0000000E+00  0.0000000E+00 -0.1828900E+03  0.0000000E+00  0.0000000E+00  0.3657800E+03
          0.3642200E+02
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 |

| i | kr1(i) | kr2(i) |
|---|---|---|
| 1 | 1 | 1 |
| 2 | 2 | 2 |
| 3 | 3 | 3 |
| 4 | 4 | 4 |
| 5 | 5 | 5 |
| 6 | 6 | 6 |
| 7 | 7 | 7 |
| 8 | 8 | 8 |
| 9 | 9 | 9 |
| 10 | 10 | 10 |
| 11 | 11 | 11 |
| 12 | 12 | 12 |
| 13 | 13 | 14 |
| 14 | 15 | 15 |
| 15 | 16 | 16 |
| 16 | 17 | 17 |
| 17 | 18 | 18 |
| 18 | 19 | 19 |
| 19 | 20 | 26 |
| 20 | 27 | 27 |
| 21 | 28 | 28 |
| 22 | 29 | 29 |
| 23 | 30 | 30 |
| 24 | 31 | 31 |
| 25 | 32 | 32 |

```
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    197999 locations

control module sas4     is complete.
```

```
module sas4     will be called

   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 1.000-9  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 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=10 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
secondary module o0o008   has been called.

module o0o008   is finished. completion code     0. cpu time used     0.00 (seconds).

secondary module o0o002   has been called.

module o0o002   is finished. completion code     0. cpu time used     1.00 (seconds).

secondary module o0o001   has been called.

module o0o001   is finished. completion code     0. cpu time used     1.00 (seconds).

secondary module o0o001   has been called.

module o0o001   is finished. completion code     0. cpu time used     4.00 (seconds).

secondary module o0o106   has been called.

module o0o106   is finished. completion code     0. cpu time used    15.00 (seconds).

module sas4     is finished. completion code     0. cpu time used    22.00 (seconds).
```

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# QADS: A MULTIDIMENSIONAL POINT-KERNEL ANALYSIS MODULE

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## ABSTRACT

QADS is a multidimensional point-kernel computer code that utilizes the simplified free-form input of the SCALE system as well as compatibility with ORIGEN-S produced sources, SCALE cross-section libraries, and standard composition data sets. QADS consists of a preprocessor that takes the free-form input and prepares input for the widely available QAD-CGGP code, which is then automatically executed by a driver module. This report describes the point-kernel theory briefly, followed by numerous tips on successfully applying the theory to various types of shielding problems. The remainder of the document is devoted to input and output descriptions of the QADS code with several illustrative sample problems.

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## S5.1 INTRODUCTION

QADS is a module that performs multidimensional point kernel estimation of gamma transport through practically any type of shielding materials using a simplified input scheme that follows the general input philosophy of the SCALE shielding sequences, SAS1, SAS2, etc. Conceptually, QADS was designed to capture the flexibility and power of the QAD technique for problems amenable to point-kernel solution while allowing for an efficient and user-friendly input interface. Functionally, the QADS module is called via the SCALE driver and first reads the free-form input values and then preprocesses the actual input for the QAD-CGGP code.[1] The driver then calls and executes QAD-CGGP automatically. For this version of QADS, QAD-CGGP was unchanged from the RSIC-distributed version to allow future updates of the QAD-CGGP code to be easily implemented into QADS. The QADS module has a number of similarities with other SCALE modules that facilitate rapid transfer of input data from other setups. The SCALE standard composition library is used to allow simplified input of materials. The problem geometry is coded using the well-known MORSE combinatorial geometry package. Finally, the dose portion of the input follows similarly the XSDOSE input data in module SAS1. The combined use of the SCALE standard compositions and free-form input with the multidimensional geometry capabilities and generally short running time of point kernel techniques produces a very powerful procedure for shielding analysis of a wide variety of problems.

## S5.2 POINT-KERNEL DOSE ESTIMATION THEORY

### S5.2.1 POINT-KERNEL THEORY

Point- kernel techniques have been widely used in gamma-ray radiation shielding analyses through the years and the methods are well known. However, for completeness the discussion of the method in Ref. 1 is repeated herein. For gamma-ray calculations, the QADS module uses the point-kernel ray-tracing technique. In this method, the point kernel representing the transfer of energy by the uncollided flux along a line-of-sight path is combined with an appropriate buildup factor to account for the contribution from the scattered photons. With a distributed source, the point kernel is integrated over the source volume for each source energy considered. Expressed as an equation, the gamma-ray dose rate, $D(\bar{r})$, at any point due to an isotropic source emitting $s$ photons of energy $E$ per second per unit volume is

$$D(\bar{r}) = \int_v \frac{Ks(\bar{r}')B(\mu|\bar{r}-\bar{r}'|,E)\exp(-\mu|\bar{r}-\bar{r}'|)dv}{4\pi|\bar{r}-\bar{r}'|^2}, \qquad \text{(S5.1)}$$

where

$\bar{r}$ = point at which gamma dose rate is to be calculated,
$\bar{r}'$ = location of source in volume $v$,
$v$ = volume of source region,
$\mu$ = total attenuation coefficient at energy $E$,
$|\bar{r}-\bar{r}'|$ = distance between source point and point at which gamma intensity is to be calculated,
K = flux-to-dose conversion factor,
B = dose buildup factor.

### S5.2.2 BUILDUP FACTOR OPTIONS

#### S5.2.2.1 Governing Equations

Two buildup factor options are available in the QADS module. The first option is the use of the original QAD-P5A code[1] values based on the Goldstein and Wilkins moments method calculations for gamma-ray transport in infinite homogeneous media. This method uses Capo's fit to the Goldstein-Wilkins data with bivariant polynomial expressions to calculate the appropriate buildup factors as a function of the gamma-ray energy and the number of mean free paths (mfp) from the source to the detector. For high atomic number materials, the polynomial fit has the form

$$B(\mu|\bar{r}-\bar{r}'|,E) = \sum_{j=0}^{4}\sum_{i=0}^{3} C^{ij}(\mu|\bar{r}-\bar{r}'|)^i(E)^j, \qquad \text{(S5.2a)}$$

and for low atomic number materials it has the form

$$B(\mu|\bar{r}-\bar{r}'|,E) = \sum_{j=0}^{4}\sum_{i=0}^{3} C_{ij}(\mu|\bar{r}-\bar{r}'|)^i\left(\frac{1}{E}\right)^j, \qquad \text{(S5.2b)}$$

where the $C_{ij}$'s are the coefficients of the expansion.

The second buildup factor method that can be selected is the geometrical progression approximation (GP method).[2] This method has recently received a lot of attention and appears to more closely reproduce actual calculations than other methods. The buildup factors are approximated by the equations

$$B(X,E) = 1 + (b-1)\frac{k^x - 1}{k-1} \qquad (k \neq 1);$$

$$= 1 + (b-1)X \qquad (k = 1); \qquad \text{(S5.3a)}$$

$$k(X) = cX^a + d\cdot\frac{\tanh(X/X_k - 2) - \tanh(-2)}{1 - \tanh(-2)}; \qquad \text{(S5.3b)}$$

where X is the source-detector distance in mean-free-paths of the medium, b is the value of the buildup factor at 1 mfp, and k represents the photon dose multiplication per mfp penetration. The parameters a, c, d, and $X_k$ are the fitting parameters and are allowed to vary with energy. A differing form of Eq. (S5.3b) is used for penetrations greater than 40 mfp.

### S5.2.2.2 Buildup Factor Usage Guidelines

Using these infinite-medium buildup factors should result in an overestimate of the dose rate at a surface external to the source region since it implies that reflecting material is located beyond the surface. However, because of the strong preferential forward scattering of photons, the error will usually not be more than a few percent and only in rather unusual cases will it reach 20 or 30%.

Using single-material buildup factors for multilayered shields or for shields made up of mixtures of materials can be another source of error. For multilayered structures having an outer layer that is thicker than 2 or 3 mfp, the buildup factor used should be the one representing the outer layer, but the total number of mean free paths should be the number along the line-of-sight through all materials in the structure. This is a reasonable procedure since the gamma-ray spectrum would readjust to the new medium and tend to approach the spectrum that would exist if the whole structure consisted of the outer layer, particularly when a low atomic number material is followed by a high atomic number material. For homogeneous mixtures or compounds, the so-called equivalent Z (atomic number) method can be used.

For multilayered structures in which each layer is less than 2 mfp thick, no clear-cut procedure is available. If one assumes that the structure is made entirely of the material having the largest buildup factor, then the dose is overestimated. Conversely, if one assumes that the material having the lowest buildup factor is representative of the structure, then the dose is underestimated.

## S5.2.3 DOSE ESTIMATION

The QADS module calculates the dose at a detector for each source energy group j with the following equation, which is a finite difference form of Eq. (S5.1):

$$D_j = \sum_i K_j \frac{S_{ij}}{4\pi R_i^2} \exp\left[-\sum_k (\mu_j t)_k\right] B_{jk}, \qquad \text{(S5.4)}$$

where

j = energy group index,
i = source point index,
k = region index,
K = flux-to-dose conversion factor,
S = volume-weighted gamma-ray point source strength (photons/s),
R = distance from source point to detector (cm),
B = dose buildup factor,
$\mu$ = total attenuation coefficient ($cm^{-1}$),
t = zone penetration distance (cm).

The i index is used to completely describe the source. The source is broken into i mesh cells with each mesh treated as a point source. The energy index j is treated in a similar manner. The source energy is assumed to be at the midpoint of the *jth* energy or group interval. All relevant constants are then evaluated at j points in energy. The total dose is obtained by summing the contribution from each of the source energies.

The QADS module also will perform a neutron calculation, although the range of applicability of the solutions is fairly limited. The methods used for the neutron calculations are discussed in Ref. 1. The neutron calculations are performed in a fixed 10-group structure and a fission spectrum source.

## S5.2.4. LIMITATIONS

The point-kernel procedure as implemented in QADS is quite general and is useful for a large number of applications. However, a number of limitations exist as discussed previously in Sect. S5.2.2.2 for buildup factors. Other limitations arise from (1) the use of a finite source mesh which can in some cases produce erroneous results, (2) the inaccuracies due to particle streaming which are not adequately modeled by the ray-tracing techniques, (3) the lack of capability for QAD-CGGP to treat off-centered cylindrical sources, and (4) the so-called oblique angle breakdown of the point-kernel method.

The default mesh generator in the QADS code should produce a source mesh that is accurate for most applications. However, if the mesh becomes large relative to the source-to-detector distance in either direction perpendicular to the primary axis connecting the source and detector, large inaccuracies can result. For example, the default source mesh, particularly in the axial direction, is inadequate for a tall, thin pipe with appreciable shielding. In these situations, the maximum number of mesh intervals (100) can be specified and advantage taken of the problem symmetry or only a portion of the problem modeled in order to obtain accurate results.

Particle streaming is an area that point kernel has much difficulty due to the ray-tracing technique utilized. For a small streaming path, the ray-tracing lines from each source mesh to the detector can completely miss an

explicitly modeled penetration. Larger void or low-density regions can be detected by the ray-tracing procedure; however, multiple scatters or grazing along the streaming paths cannot be accurately represented.

The QAD-CGGP code, which QADS prepares input for and executes, cannot treat off-centered cylindrical sources. Approximate procedures are available where the cylindrical sources are modeled as rectangular-parallelepiped which can be located off the coordinate axis. Similar procedures can also be used to overcome the QAD-CGGP limitation of a single source by surrounding multiple sources by a single body and selective zeroing the source from nonsource regions via the judicial use of weight factors (see Sect. S5.3.1.2).

The vulnerability of point-kernel techniques to the so-called oblique angle has been widely recognized for a number of years. A point-kernel inaccuracy can arise when nearly all the ray traces from the source to the detector pass through the shield at very sharp (oblique) angles. Under these circumstances, the preferred penetration path is directly through the shield with a few scattering events on the opposite side of the shield before reaching the detector, rather than the many scattering events required before the particle reaches the detector along the oblique ray traces. The point-kernel solution for such problems can be severely underestimated, depending on the specifics of the configuration.

## S5.3 INPUT SPECIFICATIONS

### S5.3.1 INPUT OVERVIEW

The QADS module input can be broken into the following areas: (1) material component specification, (2) source specification, (3) problem geometry, and (4) selection of built-in data and detector options. A brief description of each input group follows.

#### S5.3.1.1 Material Component Specification

The selection of the constituent material compositions is straightforward since the SCALE standard composition library and material input processor are utilized by QADS. Therefore the input specifications for QADS materials should be unchanged from those of the SCALE sequences. Unlike the SCALE shielding sequences, the QADS module does not call the BONAMI and NITAWL modules (see Sects. F2 and F3 of the SCALE manual) since the data in QADS are fixed and do not require any resonance processing.

#### S5.3.1.2 Source Specification

The specification of a source in QADS allows for a great deal of flexibility to handle a large number of source situations ranging from a flat source to one that has arbitrary shape and limitations in any of the three directions. The input is such that the description of most source situations is straightforward; however, as the source complexity increases so does the detail necessary to describe the given situation. This section is designed to give the user sufficient understanding to describe practically any given source configuration. The source description internal to the code includes an overall normalization, a spatial mesh and corresponding spatial distribution by mesh point, an energy structure and corresponding energy spectral shape, and a specified coordinate system. The source description can use a Cartesian, cylindrical, or a spherical coordinate system; however, the Cartesian system is recommended if the source is off-centered, or if there are multiple sources. The technique utilized for off-centered or multiple sources is to describe a source geometry that encloses the origin and all sources, then selectively zero-out nonsource regions by use of zero weights. [See Eq. (S5.6).]

The use of keywords in the source geometry and shape, and defaults in the source mesh points, energy group structure, and in some cases the source spectrum, greatly simplifies the typical source description and will suffice for many practical applications. The source shape description for a flat (keyword FLATS) or a cosine (keyword COSIN) shape are handled internally by the following equation for the point variation in the source:

$$P(a,b,c) = \cos\{xiso(1,1)[a - xiso(2,1)]\} * \cos\{xiso(1,2)[b - xiso(2,2)]\}; * \cos\{xiso(1,3)[c - xiso(2,3)]\}; \quad \text{(S5.5)}$$

where a, b, and c are the coordinates of the point in the appropriate coordinate systems, and the xiso values are either calculated internally by the code or input by the user. For the FLATS and COSIN options the values of xiso are computed internally (e.g., all xiso values are zero for the flat option). For the COSIN options the values of xiso are computed such that the power or source strength peak occurs at the midplane and is equal to zero at the external boundary. Only for the Cartesian coordinates are COSIN specifications allowed in all three directions. As an option, the QADS module allows the user to input a unique set of xiso values.

The final option for specifying the source shape is to input the relative shape by mesh point along each axis. This option assumes separability in each of the three directions and the user inputs the power or source shape independently along each axis. The source shape is entered via the WEIGHTS option and then specifying relative shape values (for cylindrical geometry) P(r), P(z), P(θ) at each **mesh boundary** using the *WAT*= keyword. The

relative magnitudes of the shape function for each different axis are not important since the code normalizes to the input value ASO. The overall normalization is performed (for cylindrical geometry) by using the input shapes P(r), P(z), and P(θ), to calculate the weights $F_l$, $F_m$, and $F_n'$:

$$F_l = \int_{r_l}^{r_l+1} rP(r)dr;$$

$$F_m = \int_{z_m}^{z_m+1} P(z)dz; \qquad \text{(S5.6)}$$

$$F_n' = \int_{\theta_n}^{\theta_n+1} P(\theta)d\theta.$$

The $F_n$ value is primed to allow overall normalization to be performed as follows:

$$A = \frac{ASO}{\left(\sum_{l=1}^{L} F_l\right)\left(\sum_{m=1}^{M} F_m\right)\left(\sum_{n=1}^{N} F_n\right)}; \qquad \text{(S5.7)}$$

$$F_n = A F_n'.$$

Thus the total power and the input value ASO can be equated,

$$P = ASO = \left(\sum_{l=1}^{L} F_l\right)\left(\sum_{m=1}^{M} F_m\right)\left(\sum_{n=1}^{N} F_n\right), \qquad \text{(S5.8)}$$

and the power at any point is given by

$$P_{lmn} = F_l F_m F_n. \qquad \text{(S5.9)}$$

In this manner the correct normalization is given regardless of the relative magnitudes of the individual coordinates.

### S5.3.1.3 Problem Geometry Specification

The problem geometry input uses the MORSE combinatorial geometry description. The input includes first a description of each body type, where the nine different body types are defined in the next section. The user then defines the corresponding body types for each zone and, finally, the mixtures numbers for each zone. The input geometry description should be obvious to MORSE combinatorial geometry users; for those unfamiliar with MORSE geometry input the user is referred to Sect. M9 for more details.

#### S5.3.1.4 Built-In Database Description

QADS contains a large database of built-in quantities, which simplifies the user input for most problems of interest. These built-in data consist of (1) buildup factors for both the standard and GP techniques, (2) dose factors that can be user input, read from a SCALE library or internally computed using the ANSI-standard description, and (3) mass attenuation coefficients for any element.

### S5.3.2 INPUT DESCRIPTION

The user input to QADS is designed to be very similar to other SCALE sequences. Thus with minimal effort a problem set up for another sequence can be rerun using the QADS sequence. Also, a user who is familiar with SCALE input and execution should have little problem becoming proficient in the operation of QADS.

#### S5.3.2.1 Sequence Specifier

Under the SCALE driver, QADS is invoked by the use of the sequence specifier "=QADS" and corresponding data shown in Table S5.3.1. The input sections following the sequence specifier consist of a title, cross-section library name, calculation-type standard composition data, QADS source specification, QADS problem geometry specification, QADS dose and detector specifications, and, finally, a QADS input terminator.

#### S5.3.2.2 Title Card

The sequence specifier card is followed by an 80-character title card. Any descriptive title containing 80 or fewer characters is allowed.

#### S5.3.2.3 Cross-Section Library Name

The input value for the cross-section library name has four options: 27N-18COUPLE, 22N-18COUPLE, ORIGENGP-SRC, and READINGP-SRC. The first two options specify that the problem group structure will be read from the corresponding SCALE library, while the input source spectrum will be read in the job input stream. Note that the cross sections on the SCALE library are not used since QADS has built-in attenuation coefficients. The third option, ORIGENGP-SRC, signals the code to read both the problem group structure and the source spectrum and magnitude from the ORIGEN-S output saved on disk. This is a useful option for coupling ORIGEN-S source calculations and QADS shielding calculations. The final option, READINGP-SRC, directs the code to read both the problem group structure and source spectrum from the job input stream. While more cumbersome in preparing the input, this option provides flexibility in that any group structure can be used and it gives QADS the option of easily specifying gamma line sources. This is accomplished by specifying narrow energy bins with the midpoint energy equal to the gamma line source energy.

#### S5.3.2.4 Calculation Type

The next input value, the calculational type, is included simply to minimize changes to existing decks that have been used in other SCALE sequences. The only value that is acceptable for this input is INFHOMMEDIUM. QADS does not perform any resonance processing on the cross sections since it uses built-in attenuation coefficients.

Table S5.3.1 Outline of material information processor data for QADS

| Data position | Type of data | Data entry | Comments |
|---|---|---|---|
| 1 | Sequence specifier | =QADS | Begin in column 1. PARM=CHK beginning in column 11 checks the input for errors |
| 2 | Title | Enter a title | 80 characters |
| 3 | Cross-section library name | 27N-18COUPLE<br>22N-18COUPLE<br>ORIGENGP-SRC<br>READINGP-SRC | These keywords are used to select the problem group structure only. QADS has built-in cross sections |
| 4 | Calculation type | INFHOMMEDIUM | This is only valid option for QADS calculation |
| 5 | Standard composition data | Enter the appropriate data | Terminate this data block with END COMP. See Table S5.3.2 |
| 6 | QADS source specification | Enter the appropriate data | End this data block with END SOURCE. See Table S5.3.3 |
| 7 | QADS problem geometry specification | Enter the combinatorial geometry data | End this data block with END GEOM. See Table S5.3.4 |
| 8 | QADS dose and detector specification | Enter the appropriate data | Terminate this block with END DOSE. See Table S5.3.6 |
| 9 | Terminate QADS sequence | END | Must begin in column 1 |

### S5.3.2.5 Standard Composition Data

The QADS standard composition data input is exactly like that of the standard SCALE input; thus problem input descriptions should be easily transported from other applications to QADS. A brief input description is given in Table S5.2; for more detailed explanations of each input value see the description given in Sect. M7.4.

### S5.3.2.6 QADS Source Specification

The QADS source specification input follows and is summarized in Table S5.3. Following selection of the appropriate source geometry, the user enters the source strength, normally in units of photons/s. This is the value ASO discussed in the previous section. For the ORIGENGP-SRC option this value should be entered as zero, since the overall normalization is read directly from the ORIGEN-S output (see Sect. F7). If a number other than zero is entered, the value from ORIGEN-S is discarded and the new value is used as the normalization. The use of eight different keyword inputs describes the spatial shape of the source within the defined source body. The first six options give a simple definition of the spatial variation of the source and no further information is needed to describe this variation. If either XISOS or WEIGHTS are specified, then a more detailed description of the spatial shape of the source is given in the More Data array parameters, XIS or WAT, respectively. Specifying XISOS directs the code to read the six values of XIS [xiso values of Eq. (S5.5)] in the following order:

$$XIS=XIS(1,1),XIS(2,1),XIS(1,2),XIS(2,2),XIS(1,3),XIS(2,3).$$

If the user specifies WEIGHTS, then the relative shapes for each mesh point for each coordinate axis should follow the WAT=keyword in the More Data array. The order of weights by axis is R, Z, $\theta$ for cylindrical; X, Z, Y for Cartesian; and $\rho$, $\theta$, $\psi$ for spherical. The optional fields of group structure and particle spectrum are read in next; the option is determined by the value of the cross-section library name specified previously. The group structure array is read in only if the cross-section library input value READINGPSRC is specified. Similarly, the particle spectrum array is read in only if the cross-section library input value is specified as either READINGP-SRC or one of the SCALE libraries (27N-18COUPLE or 22N-18COUPLE).

The More Data array contains seven different keywords that in many instances will not have to be changed from their default values; however, using the keyword options increases the module's flexibility. This is easily illustrated by the first keyword, NZS. The value of NZS defaults to 1 and describes the body number corresponding to the source body. In many instances, the source will be the central body in the problem description and a common convention is to number the innermost body as 1. However, in some instances the source may incorporate several boundaries and simply specifying the body number for the outermost body will effectively spread the source out over all intermediate boundaries. An example of this is given in the sample problems. This is an important parameter since the source mesh is generated from the body data corresponding to the body number specified. The procedure used internally is to determine, based on the data for the specified body number, the innermost and outermost dimensions of the source body and then construct the mesh based on the specified number of equally spaced meshes (determined by the MSH= parameter). If MSH=0, then the number of mesh intervals is set to 30 for the R, X, Y, Z, and $\rho$ axes and 20 for the $\theta$ and $\psi$ axes. These values can be changed by specifying MSH= and entering the new number of mesh intervals for each of the three coordinate axes in the same order as previously given for the weights. Should changes from the defaults be attempted, care should be exercised in the selection of an appropriate number of mesh cells (the maximum number of mesh cells is 100 for each direction). Since the source representation is completely described by the source mesh, the mesh should be fine enough to adequately model the source body. This is particularly important

Table S5.3.2 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 Sect. M8.2. 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 | No longer used but must still be entered | ARBM | Enter once for each standard composition compo-nent that is an arbitrary material. Enter 0 or 1 |
| A4 | ICP | Compound indicator | ARBM | Enter once for each standard composition component that is an arbitrary material.<br>Enter 1 for a compound, 0 for alloys, mixtures, etc. |
| A5 | IRS | No longer used but must still be entered | ARBM | Enter once for each standard composition component that is an arbitrary material.<br>Enter 0 or 1 |
| A6 | NCZA | ID number (from far right column of Table M8.2.1 or M8.2.2) | ARBM | Repeat the sequences A6 and A7 for each element or isotope in the arbitrary material before entering entry number 2. Enter the number from the far right column of Table M8.2.1 or M8.2.2. (Premixed standard compositions cannot be used in an arbitrary material definition) |
| A7 | ATPM | Number of atoms of this element per molecule of arbitrary material<br>or<br>Weight percent of this element in this arbitrary material | ARBM & ICP=1<br>or<br>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=1<br>or<br>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 S5.3.2 (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<br>or<br>ROTH | Specific gravity of the solution<br>or<br>Density of the basic standard composition | Optional | If the specific gravity (SPGR) of the solution is known, it should be entered as SPG=SPGR<br>or<br>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* | 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.

Table S5.3.3 Input data description for QADS source specification

| Data position | Type of data | Data entry | Comments |
|---|---|---|---|
| 1 | Source geometry | CYLINDRICAL<br>CARTESIAN<br>SPHERICAL | Select the appropriate source geometry |
| 2 | Source strength | Enter the appropriate data | Enter the number of source particles/s. Enter 0 for source read from ORIGEN-S |
| 3 | Source shape | FLATS<br>COSINX<br>COSINY<br>COSINZ<br>COSINR<br>COSINRHO<br>XISOS<br>WEIGHTS | Terminate with an END card |
| 4 | Group structure (optional) | Enter number of groups, then group bounds (high-to-low in eV) | Input only if READING-SRC is specified |
| 5 | Particle spectrum (optional) | Enter value for each group | Input only if READINGP-SRC or SCALE library is specified |
| 6 | More Data array (optional) | NZS=<br>INU=<br>NSO=<br>NPS=<br>XIS=<br>MSH=<br><br>WAT= | [1] - body # for source<br>[0] - neutron calculation if > 0<br>[71] - ORIGEN-S unit number<br>[0] - source position number, 0=last<br>[0] - xiso values (6 values)<br>[0] - number of mesh intervals (values for each coordinate direction)[a,b]<br>[0] - weights read in[a] |
| 7 | End Source array | END SOURCE | Terminate source input |

[a]The mesh intervals and weights for each axis are input in the following order: Cartesian (X,Z,Y), cylindrical (R,Z,θ), and spherical (ρ, θ, ψ).

[b]The default number of mesh intervals is 30 for R, X, Y, Z, and ρ axes and 20 for θ and ψ axes. The user can input the actual mesh by specifying a **negative** number of mesh intervals for a given axis, followed by the mesh boundaries along that axis.

for surface or near-surface doses where errors can occur if the mesh size is larger than the surface-to-detector distance. Alternately, if the value of MSH is entered as a negative number, the actual mesh can then be entered immediately after each MSH value has been input (e.g., if MSH= -15 then enter 16 r mesh values; if -10, enter 11 Z mesh values; if -5, enter 6 θ mesh values). This will allow for special situations when the intermediate boundaries, not just the endpoints, need to be specified.

The NSO and NPS parameters give the ORIGEN-S unit number and source position for the ORIGEN-S data saved to disk in an earlier run. Only in a few instances should values other than the defaults have to be entered. The XIS and WAT parameters allow the user to enter their own set of source shapes. The last optional parameter is INU. Specifying INU greater than 0 allows the user to perform a neutron calculation. This document assumes that a gamma only calculation is the intent of most users and further information on the neutron capabilities is given in the original QAD document.[1]

### S5.3.2.7 QADS Problem Geometry Specification

Tables S5.4 and S5.5 outline the user input for the QADS problem geometry input. This input is very similar to that of the MORSE-SGC. See Sect. M9.2 for more detailed information.

### S5.3.2.8 QADS Dose and Detector Specification

The description of the final input section, QADS detector and buildup factor specification, is given in Table S5.6. This section consists of buildup factor selection followed by two optional inputs: the number and type of flux-to-dose conversion factors and the number and position of detectors for the problem. The first 8 options for the buildup factors given in Table S5.6 correspond to the standard buildup factors [Eq. (S5.2)], while the 43 options given in Table S5.7 correspond to the GP buildup factor data [Eq. (S5.3)]. For the standard buildup factor data, the DOSE keyword indicates that the buildup factors are for an air exposure response with penetration through the given material and the ENG keyword indicates a response of the energy absorbed in the material itself. Similarly for the GP buildup factor data, the ABS keyword indicates a response of the energy absorbed in the material, while the keyword EXP indicates the air exposure response with penetration through the given material.

The next input parameter is NFACTR, which specifies the number and/or type of flux-to-dose conversion factors. For all but a very few cases, the default value is sufficient. If the default value is used, ANSI-standard dose factors are either read from the SCALE library or calculated internally. The user can optionally specify other dose IDs from the SCALE library if that option is being utilized in the problem. Lastly, the user can input dose response values by specifying a number between 0 and 9000. This allows NFACTR sets of conversion factor sets to be read from the job input stream. The default for the number of detectors is four, NDETEC=0 and the detectors are located at 0, 1, 2, and 4 m from the outermost edge of the outermost nonvoid cylinder along the midplane of the cylinder. This default option. is valid only for cylindrical source geometries. For other geometries and/or other detector locations the user enters the number of detectors desired, NDETEC=number of detectors, followed by the location of each detector. The default detector geometry is cylindrical and need not be entered unless the user desires another geometry for the detector.

### S5.3.2.9 Terminate QADS Sequence

An END card should be included to terminate the user input to QADS. No built-in mechanisms for stacking several cases within a QADS sequence exist. The use of the SCALE driver provides such an option since additional cases can be stacked by simply respecifying the entire QADS sequence input following the END card (i.e., including an =QADS as the card following the END card).

Table S5.3.4 Input data description for QADS geometry specification

| Data position | Type of data | Data entry | Comments |
|---|---|---|---|
| 0 | Title card | Geometry title | Enter geometry title (80 characters) |
| 1A | Body type | BOX<br>RPP<br>SPH<br>RCC<br>REC<br>ELL<br>TRC<br>WED<br>ARB | See Table S5.3.5 for body definitions. Refer to Sect. M9.2 for complete information |
| 1B | Body number | Enter appropriate body number | Enter body number corresponding to above body type |
| 1C | Body data | Enter appropriate data for given body | See Table S5.3.5 for required data for each body type |
| 1D | Terminate body data | END BODY | After all body descriptions have been entered, terminate with END BODY |
| 2A | Zone name | Three letter zone title (e.g, ZN1, ZN3) | The first zone name corresponds to zone 1, second to zone 2, etc., regardless of its title |
| 2B | Number of adjacent zones | Integer # | Enter number of zones that can be entered from this zone |
| 2C | Body numbers for this zone | +integer<br>-integer<br>OR +integer<br>OR -integer | Enter the body numbers that comprise this zone. See Appendix A for more information |
| 2D | Terminate zone data | END ZONE | After all zones have been described, terminate with END ZONE |
| 3 | Mixtures by zone | Integer for each zone | Enter the mixture number for each zone. Enter 1000 for internal voids, 0 for external voids |
| 4 | End geometry input | END GEOM | |

Table S5.3.5 Input required for each body type

| Body description | Body type | Body No. | Real data defining particular body[a] | | | | | |
|---|---|---|---|---|---|---|---|---|
| Box | BOX | Assigned by the user | Vx<br>H2x | Vy<br>H2y | Vz<br>H2z | H1x<br>H3x | H1y<br>H3y | H1z<br>H3z |
| Rectangular parallelepiped | RPP | Assigned by the user | Xmin | Xmax | Ymin | Ymax | Zmin | Zmax |
| Sphere | SPH | Assigned by the user | Vx | Vy | Vz | R | | |
| Right circular cylinder | RCC | Assigned by the user | Vx<br>R | Vy | Vz | Hx | Hy | Hz |
| Right elliptic cylinder | REC | Assigned by the user | Vx<br>R1x | Vy<br>R1y | Vz<br>R1z | Hx<br>R2x | Hy<br>R2y | Hz<br>R2z |
| Ellipsoid | ELL | Assigned by the user | V1x<br>R | V1y | V1z | Hx | Hy | Hz |
| Truncated right cone | TRC | Assigned by the user | Vx<br>R1 | Vy<br>R2 | Vz | Hx | Hy | Hz |
| Right angle wedge | WED | Assigned by the user | Vx<br>H2x | Vy<br>H2y | Vz<br>H2z | H1x<br>H3x | H1y<br>H3y | H1z<br>H3z |
| Arbitrary convex polyhedron | ARB | Assigned by the user | V1x<br>V3x<br>V5x<br>V7x<br>Face descriptions[b] | V1y<br>V3y<br>V5y<br>V7y | V1z<br>V3z<br>V5z<br>V7z | V2x<br>V4x<br>V6x<br>V8x | V2y<br>V4y<br>V6y<br>V8y | V2z<br>V4z<br>V6z<br>V8z |

[a]For definitions of these values, see Sect. M9.2 on MARS geometry.
[b]Line 5 of the arbitrary polyhedron input contains a four-digit integer for each of the six faces of an ARB body.

Table S5.3.6 Input data description for QADS detector specification

| Data position | Type of data | Data entry | Comments |
|---|---|---|---|
| 1 | Buildup factors | WATE DOSE or ENG<br>ALUM ENG<br>IRON DOSE or ENG<br>LEAD DOSE or ENG<br>CONC DOSE | These buildup factors correspond to the standard exponential buildup factor data. For GP values, see Table S5.7 |
| 2 | Number/type flux-to-dose conversion factor (optional) | NFACTR=[0]<br>NFACTR > 9000<br>0 < NFACTR < 9000<br>END | Use ANSI-Standard dose factors<br>SCALE dose factor IDs[a]<br>Read NFACTR responses from input[b]<br>Terminate dose factor input |
| 3 | Number of detectors (optional) | NDETEC= [0] | Defaults of 0, 1, 2, 4 m from mid-plane (valid only for CYLINDRICAL source) |
| 4 | Detector data (NDETEC ≠ 0) | RRC<br>ZRC<br>PHIRC<br>NRCOP<br>for each detector | R, X, or ρ value<br>Z, Z, or θ value<br>θ, Y, or ψ value<br>CYLINDRICAL (default if source geometry is cylindrical)<br>CARTESIAN<br>SPHERICAL |
| 5 | Terminate input | END DOSE | Terminate dose input |

[a] Refer to Table S1.4.8 in Sect. S1.4 for available SCALE dose factor IDs.

[b] NFACTR for values between 0 and 9000 is the number of response sets, not the total number of values entered. After the value of NFACTR is entered, response values are entered by group for each of the NFACTOR responses.

Table S5.3.7 Index of materials and responses used in QADS

| MATGP | Material | ICGP[a] | Response | ICGP | Response |
|---|---|---|---|---|---|
| BERY | Beryllium | _ABS | Beryllium | _EXP | Air |
| BORO | Boron | _ABS | Boron | _EXP | Air |
| CARB | Carbon | _ABS | Carbon | _EXP | Air |
| NITR | Nitrogen | _ABS | Nitrogen | _EXP | Air |
| OXYG | Oxygen | _ABS | Oxygen | _EXP | Air |
| SODI | Sodium | _ABS | Sodium | _EXP | Air |
| MAGN | Magnesium | _ABS | Magnesium | _EXP | Air |
| ALUM | Aluminum | _ABS | Aluminum | _EXP | Air |
| SILI | Silicon | _ABS | Silicon | _EXP | Air |
| PHOS | Phosphorus | _ABS | Phosphorus | _EXP | Air |
| SULP | Sulphur | _ABS | Sulphur | _EXP | Air |
| ARGO | Argon | _ABS | Argon | _EXP | Air |
| POTA | Potassium | _ABS | Potassium | _EXP | Air |
| CALC | Calcium | _ABS | Calcium | _EXP | Air |
| IRON | Iron | _ABS | Iron | _EXP | Air |
| COPP | Copper | _ABS | Copper | _EXP | Air |
| MOLY | Molybdenum | _ABS | Molybdenum | _EXP | Air |
| LEAD | Lead | _ABS | Lead | _EXP | Air |
| URAN | Uranium | _ABS | Uranium | _EXP | Air |
| WATE | Water | _ABS | Water | _EXP | Air |
| AIR_ | Air | _ABS | Air | _EXP | Air |
| CONC | Concrete | _ABS | Concrete | _EXP | Air |

[a] _ means blank.

## S5.4 SAMPLE PROBLEMS AND OUTPUT DESCRIPTION

QADS was developed largely to provide a simplified input scheme to expedite shielding analyses of spent fuel shipping casks. Of course, many other applications are well suited for analysis using the QADS module. However, the two sample problems and their corresponding outputs given here are examples of how QADS could be used in shipping cask analysis. The examples were designed to use as many options as possible, in some cases more than are actually necessary, to give the user insight into how the particular options can be best utilized. Note that these problems are not the standard QADS sample problems distributed with SCALE. They may be downloaded from the SCALE home page on the World-Wide Web (WWW). A pointer for the SCALE home page may be found at http://www.cad.ornl.gov

The first sample problem involves a 38-cm-thick cylindrical cast-iron shipping cask with a dry 40-cm radius inner cavity[3] shown in Fig. S5.4.1. The input listing is provided in Fig. S5.4.2. The source has a total source strength of $5.078 \times 10^{16}$ photons/s and is distributed into an 18-group structure as shown in the input. This spectrum was derived from individual line sources by binning into the specified energy ranges while conserving energy. The weights option was specified to show its use; however, the actual weights are all set to 1, thus specifying a flat source. The problem geometry described is a cylindrical shield 38 cm thick with a 40-cm-radius cavity. The bottom of the cask is also 38 cm thick with the top cover 42 cm in thickness. These body descriptions are followed by surrounding bodies of first internal void and lastly external void in order that dose estimations external to the cask can be performed in QADS. In this case, these regions were made arbitrarily large.

Figure S5.4.3 contains the complete QADS output of the first sample problem with appropriate notations made to aid the user in understanding the printed results. The results for receiver 1 (i.e., a detector at the outer cask surface on the axial midplane) appear near the end of the output. The calculated dose rates are shown in the sixth column, both as a total dose rate and by group. The value of $3.53 \times 10^{-2}$ rem/h agrees well with both one-dimensional (1-D) and two-dimensional (2-D) transport results.[3]

The second sample problem illustrates one of many shielding situations that QADS can handle quite easily. The physical situation is a storage container consisting of 52 cans of enriched uranium. The cans are stacked 4 high in 13 compartments as shown in Fig. S5.4.4. QADS cannot handle the source geometry exactly for this case. The cylinders themselves can be modeled but only one distinct source body can be input. There are several ways to approximate this shielding situation. The first is to make the geometry 1-D by modeling the middle cylinder exactly, then smearing the remaining 12 cylinders into an outer cylindrical ring. This method was chosen as an approximation since one aim of the code checkout was to compare QADS results with 1-D transport calculations. Another possibility is to model all 13 cylinders in Cartesian geometry with checkerboard patterns approximating the cylinders and the use of zero and nonzero weights to selectively "punchout" the "cylindrical" regions of the source. This approach more closely reproduces the actual configuration but at the expense of simplicity in the problem setup. The input for this sample problem (Fig. S5.4.5) also demonstrates the use of the optional parameter NZS. The default value for NZS is 1, which describes the body number of the source description. In many applications the innermost body is both the source body and body 1; thus the default should be appropriate for many situations. In this and other similar situations, however, there are multiple source bodies. The procedure used here specifies the outermost source body number as NZS. This designation incorporates all the remaining internal bodies. It also places a portion of the source in the structural regions which, if desired, can be assigned zero weights. The error in this problem was deemed small enough to ignore. Excerpts of the resulting QADS output for the second sample problem are shown in Fig. S5.4.6.

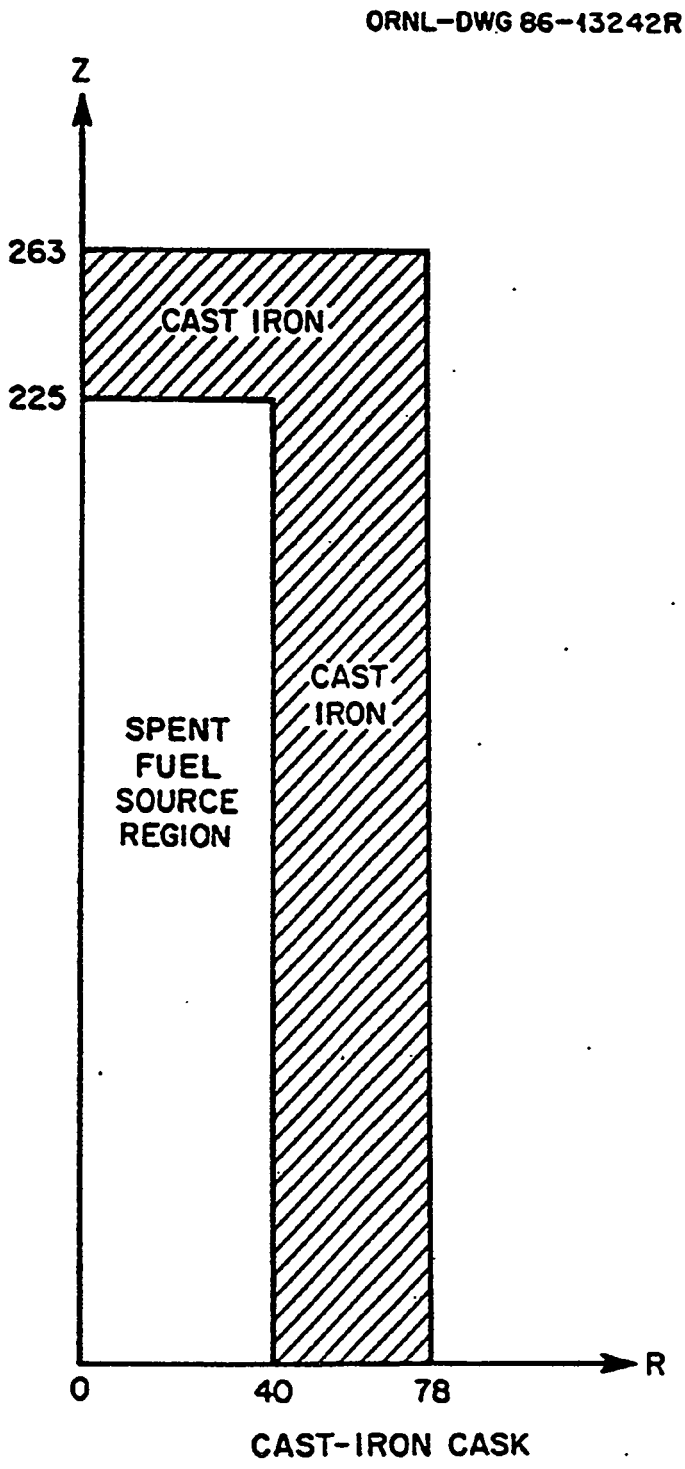



Figure S5.4.1 Geometry of cast-iron cask

```
=QADS
QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK
READINGP-SRC INFHOMMEDIUM
ARBM-CASTFE 7.0 4 0 0 1 6012 3.25 14000 1.4 28000 1.1 26000 94.25 2 END
ARBM-POLY .91 2 0 1 0 6012 2 1001 4 3 END
ARBM-1.4541 2.81 4 0 0 1 25055 2. 24000 18. 28000 10. 26000 70. 1 .186 END
ARBM-ZIRC4 2.81 3 0 0 1 40000 97.9 50000 1.6 26000 0.5 1 .116 END
ARBM-U235 2.81 1 0 0 1 92235 100. 1 .011 END
ARBM-U238 2.81 1 0 0 1 92238 100. 1 .344 END
ARBM-OXYGEN 2.81 1 0 0 0 8016 100. 1 .043 END
END COMP
CYLINDRICAL 5.078E16 WEIGHTS END
18 10+6 8+6 6.5+6 5+6 4+6 3+6 2.5+6 2+6 1.66+6 1.33+6 1+6 8+5
6+5 4+5 3+5 2+5 1+5 5+4 1+4
5Z 2.64-5 5.02-3 1.13-4 0 1.80-2 7.60-3 6.70-1 2.99-1 5Z
MSH=15 15 10 WAT=43*1
END SOURCE
CYLINDRICAL SHELL CASK
RCC 1 0 0 38 0 0 450 40
RCC 2 0 0 0  0 0 488 78
RCC 3 0 0 488 0 0 42 78
RCC 4 0 0 -10000 0 0 20000 20000
RCC 5 0 0 -10001 0 0 20002 20002
END BODY
ZN1 2 1
ZN2 2 2 -1
ZN3 2 3
ZN4 2 4 -3 -2
ZN5 2 5 -4
END ZONE
1 2 2 1000 0
END GEOM
IRON EXP
NDETEC=2
78. 265. 0. 178. 265. 0.
END DOSE
END
```

Figure S5.4.2 Input listing for first sample problem

```
      PRIMARY MODULE ACCESS AND INPUT RECORD ( SCALE DRIVER - 95/03/29 - 09:06:37 )
MODULE QADS     WILL BE CALLED
  QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK
  READINGP-SRC INFHOMMEDIUM
  ARBM-CASTFE 7.0 4 0 0 1 6012 3.25 14000 1.4 28000 1.1 26000 94.25 2 END
  ARBM-POLY .91 2 0 1 0 6012 2 1001 4 3 END
  ARBM-1.4541 2.81 4 0 0 1 25055 2. 24000 18. 28000 10. 26000 70. 1 .186 END
  ARBM-ZIRC4 2.81 3 0 0 1 40000 97.9 50000 1.6 26000 0.5 1 .116 END
  ARBM-U235 2.81 1 0 0 1 92235 100. 1 .011 END
  ARBM-U238 2.81 1 0 0 1 92238 100. 1 .344 END
  ARBM-OXYGEN 2.81 1 0 0 0 8016 100. 1 .043 END
  END COMP
  CYLINDRICAL 5.078E16 WEIGHTS END
  18 10+6 8+6 6.5+6 5+6 4+6 3+6 2.5+6 2+6 1.66+6 1.33+6 1+6 8+5
  6+5 4+5 3+5 2+5 1+5 5+4 1+4
  5Z 2.64-5 5.02-3 1.13-4 0 1.80-2 7.60-3 6.70-1 2.99-1 5Z
  MSH=15 15 10 WAT=43*1
  END SOURCE
  CYLINDRICAL SHELL CASK
  RCC 1 0 0 38 0 0 450 40

  RCC 2 0 0 0  0 0 488 78

  RCC 3 0 0 488 0 0 42 78

  RCC 4 0 0 -10000 0 0 20000 20000

  RCC 5 0 0 -10001 0 0 20002 20002
  END BODY
  ZN1 2 1
  ZN2 2 2 -1
  ZN3 2 3
  ZN4 2 4 -3 -2
  ZN5 2 5 -4
  END ZONE
  1 2 2 1000 0
  END GEOM
  IRON EXP
  NDETEC=2
  78. 265. 0. 178. 265. 0.
  END DOSE

SECONDARY MODULE QADCGGP  HAS BEEN CALLED.

MODULE QADCGGP  IS FINISHED. COMPLETION CODE     0. CPU TIME USED     2.36 (SECONDS).

MODULE QADS     IS FINISHED. COMPLETION CODE     0. CPU TIME USED     4.18 (SECONDS).
```

QADS sample problem input list

Figure S5.4.3 Complete output listing of first sample problem

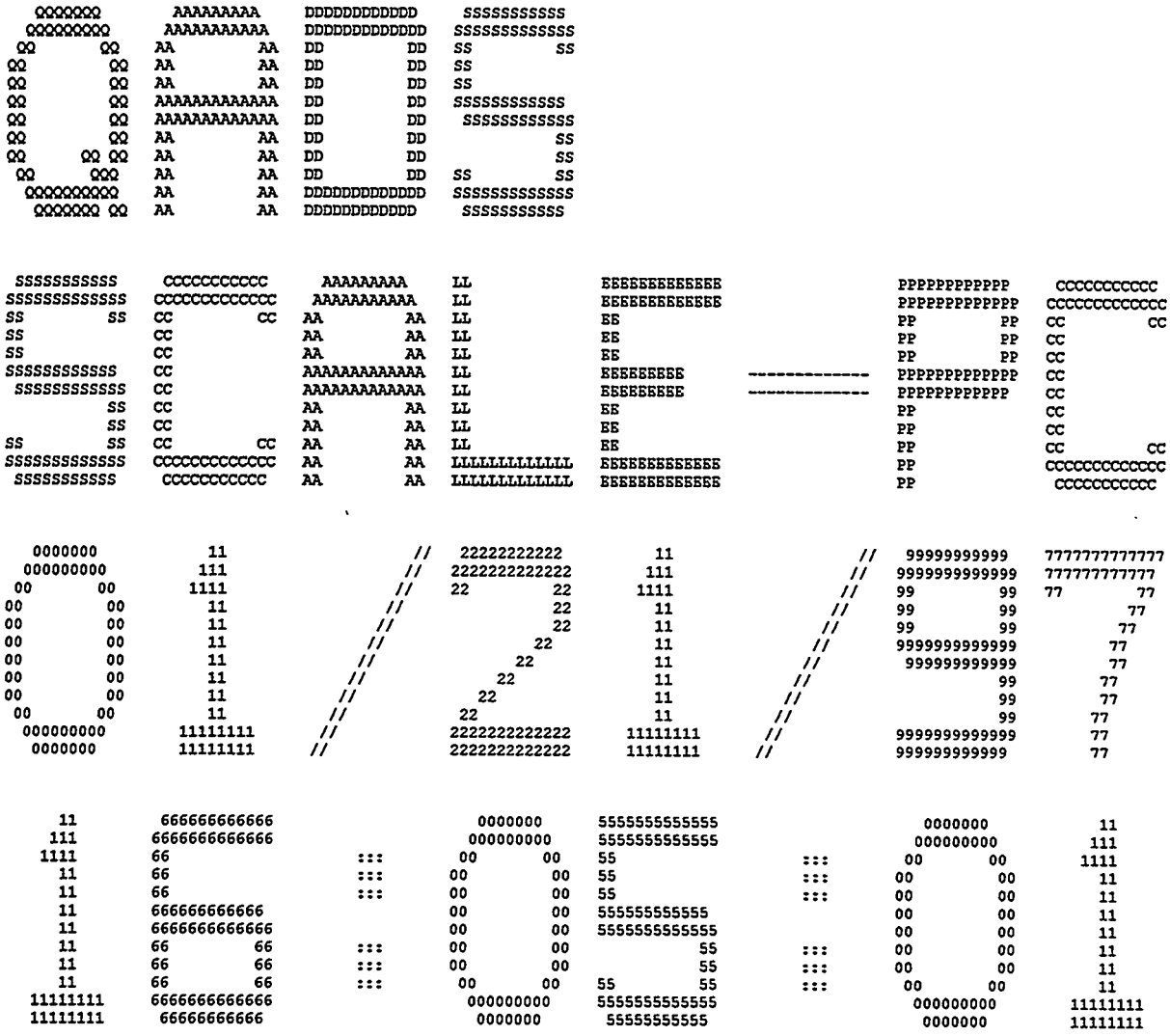



Figure S5.4.3 (continued)

```
 SSSSSSSSSS     CCCCCCCCCC      AAAAAAAA     LL             EEEEEEEEEEEE                 PPPPPPPPPPP     CCCCCCCCCC
SSSSSSSSSSS    CCCCCCCCCCCC    AAAAAAAAAA    LL             EEEEEEEEEEEE                 PPPPPPPPPPPP   CCCCCCCCCCCC
SS        SS   CC          CC  AA        AA  LL             EE                           PP          PP  CC          CC
SS             CC              AA        AA  LL             EE                           PP          PP  CC
SS             CC              AA        AA  LL             EE                           PP          PP  CC
SSSSSSSSSSS    CC              AAAAAAAAAAAA  LL             EEEEEEEEE      ----------    PPPPPPPPPPPP    CC
 SSSSSSSSSSS   CC              AAAAAAAAAAAA  LL             EEEEEEEEE      ----------    PPPPPPPPPPP     CC
          SS   CC              AA        AA  LL             EE                           PP              CC
          SS   CC              AA        AA  LL             EE                           PP              CC
SS        SS   CC          CC  AA        AA  LL             EE                           PP              CC          CC
SSSSSSSSSSSS   CCCCCCCCCCCC    AA        AA  LLLLLLLLLLLL   EEEEEEEEEEEE                 PP              CCCCCCCCCCCC
 SSSSSSSSSS     CCCCCCCCCC     AA        AA  LLLLLLLLLLLL   EEEEEEEEEEEE                 PP               CCCCCCCCCC
```

```
**********************************************************************************
**********************************************************************************
**********************************************************************************
*****                                                                        *****
*****                  PROGRAM VERIFICATION INFORMATION                      *****
*****                                                                        *****
*****                CODE SYSTEM:  SCALE-PC VERSION:  4.3                    *****
*****                                                                        *****
**********************************************************************************
**********************************************************************************
*****                                                                        *****
*****                                                                        *****
*****              PROGRAM:  QADS                                            *****
*****                                                                        *****
*****         CREATION DATE:  09-15-95                                       *****
*****                                                                        *****
*****              VOLUME:   SCSIDRIVED                                      *****
*****                                                                        *****
*****              LIBRARY:  D:\scale43\EXE                                  *****
*****                                                                        *****
*****                                                                        *****
*****       PRODUCTION CODE:  QADS                                           *****
*****                                                                        *****
*****              VERSION:  3.0                                             *****
*****                                                                        *****
*****              JOBNAME:  SCALE-PC                                        *****
*****                                                                        *****
*****     DATE OF EXECUTION:  01/21/97                                       *****
*****                                                                        *****
*****     TIME OF EXECUTION:  16:05:01                                       *****
*****                                                                        *****
*****                                                                        *****
**********************************************************************************
**********************************************************************************
**********************************************************************************
```

Figure S5.4.3 (continued)

```
QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

**** PROBLEM PARAMETERS ****

LIB NO_LIB_USED  LIBRARY
MXX            3 MIXTURES
MSC            7 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  ARBM-CASTFE  STANDARD COMPOSITION
MX             2 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH      7.0000 SPECIFIED DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
            6012     3.250 WT%
           14000     1.400 WT%
           28000     1.100 WT%
           26000    94.250 WT%
END

SC  ARBM-POLY    STANDARD COMPOSITION
MX             3 MIXTURE NO.
VF        1.0000 VOLUME FRACTION
ROTH      0.9100 SPECIFIED DENSITY
NEL            2 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
            6012      2.00 ATOMS/MOLECULE
            1001      4.00 ATOMS/MOLECULE
END

SC  ARBM-1.4541  STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.1860 VOLUME FRACTION
ROTH      2.8100 SPECIFIED DENSITY
NEL            4 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           25055     2.000 WT%
           24000    18.000 WT%
           28000    10.000 WT%
           26000    70.000 WT%
END

SC  ARBM-ZIRC4   STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.1160 VOLUME FRACTION
ROTH      2.8100 SPECIFIED DENSITY
NEL            3 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           40000    97.900 WT%
           50000     1.600 WT%
           26000     0.500 WT%
END

SC  ARBM-U235    STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0110 VOLUME FRACTION
ROTH      2.8100 SPECIFIED DENSITY
NEL            1 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           92235   100.000 WT%
END

SC  ARBM-U238    STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.3440 VOLUME FRACTION
ROTH      2.8100 SPECIFIED DENSITY
NEL            1 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
           92238   100.000 WT%
END

SC  ARBM-OXYGEN  STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0430 VOLUME FRACTION
ROTH      2.8100 SPECIFIED DENSITY
NEL            1 NO. ELEMENTS
ICP            0 0/1 MIXTURE/COMPOUND
            8016   100.000 WT%
END
```

SCALE material processor input

Figure S5.4.3 (continued)

```
**** PROBLEM GEOMETRY ****

**** INFINITE HOMOGENEOUS MEDIUM ****
MFUEL          1 MIXTURE NO. OF THE INFINITE HOMOGENEOUS MEDIUM

**** SOURCE PARAMETERS ****

QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

SRC    CYLINDRICAL   SOURCE COORDINATE SYSTEM
ASO     5.07800E+16 . SOURCE STRENGTH
SHAPE      WEIGHTS   SOURCE SHAPE

GROUP STRUCTURE READ FROM CARDS
SOURCE SPECTRUM READ FROM CARDS

OPTIONAL PARAMETERS

MSH VALUES READ FROM CARDS

OPTIONAL PARAMETERS

    43 WAT VALUES READ FROM CARDS

**** DOSE DATA ****

BFMAT      IRON  BUILDUP FACTOR MATERIAL
BFRSP       EXP  BUILDUP FACTOR RESPONSE

NFACTR         0  DOSE FACTOR ID (READ FROM CARDS IF      < 9000)
NDETEC         2  NUMBER OF DETECTORS

DETECTOR NO.  1
RRC= 7.8000E+01 ZRC= 2.6500E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
DETECTOR NO.  2
RRC= 1.7800E+02 ZRC= 2.6500E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
```

source description

detector and dose data

Figure S5.4.3 (continued)

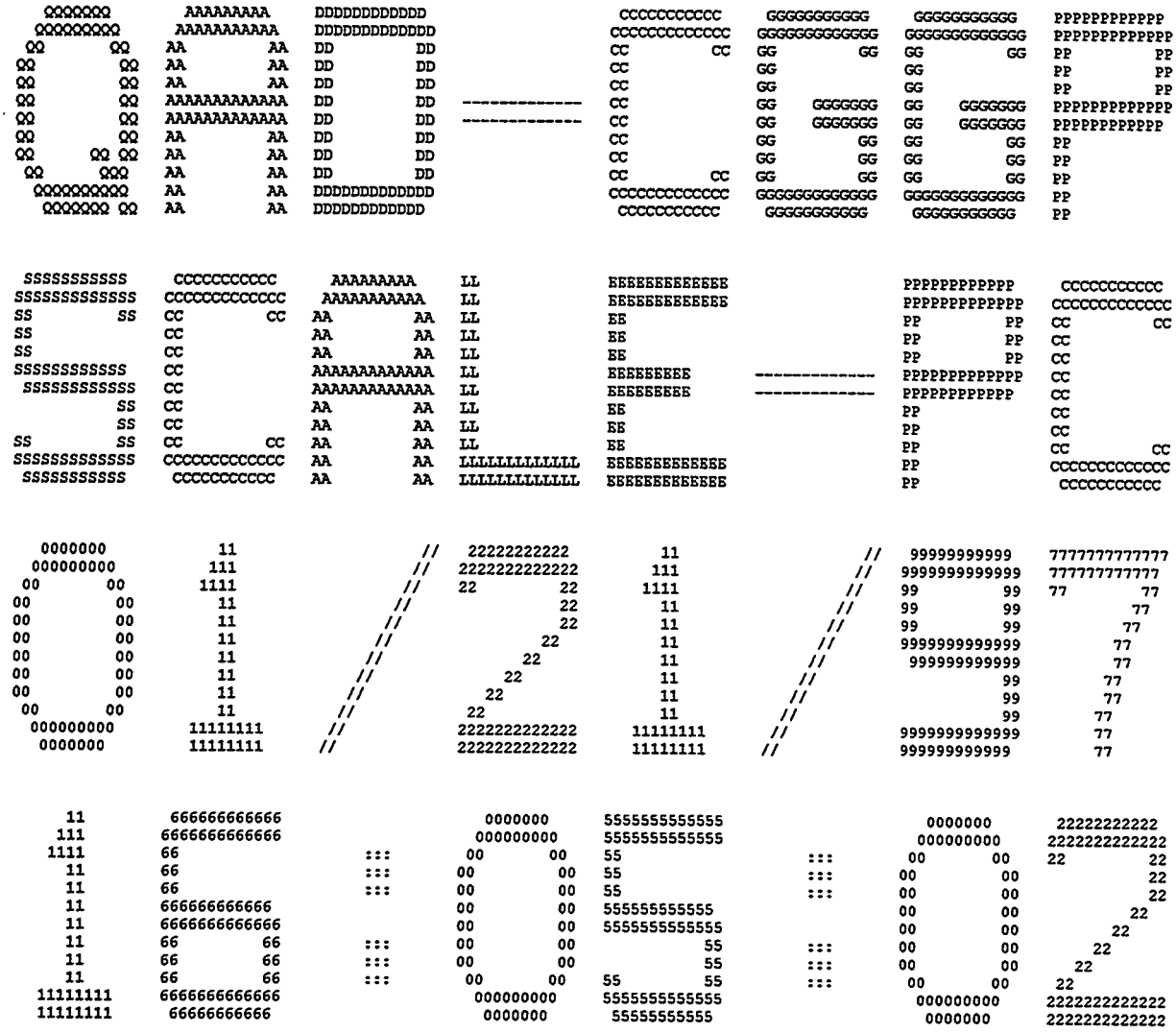


Figure S5.4.3 (continued)

```
 SSSSSSSSSS     CCCCCCCCCC      AAAAAAAAA     LL             EEEEEEEEEEEE                 PPPPPPPPPPP     CCCCCCCCCC
SSSSSSSSSSSS   CCCCCCCCCCCC    AAAAAAAAAAA    LL             EEEEEEEEEEEE                 PPPPPPPPPPPP   CCCCCCCCCCCC
SS         SS  CC          CC  AA         AA  LL             EE                           PP         PP  CC          CC
SS             CC              AA         AA  LL             EE                           PP         PP  CC
SS             CC              AA         AA  LL             EE                           PP         PP  CC
SSSSSSSSSSS    CC              AAAAAAAAAAAAA  LL             EEEEEEEEE       ----------   PPPPPPPPPPPP   CC
 SSSSSSSSSSS   CC              AAAAAAAAAAAAA  LL             EEEEEEEEE       ----------   PPPPPPPPPPP    CC
          SS   CC              AA         AA  LL             EE                           PP             CC
          SS   CC              AA         AA  LL             EE                           PP             CC
SS        SS   CC          CC  AA         AA  LL             EE                           PP             CC          CC
SSSSSSSSSSSS   CCCCCCCCCCCC    AA         AA  LLLLLLLLLLLL   EEEEEEEEEEEE                 PP             CCCCCCCCCCCC
 SSSSSSSSSS     CCCCCCCCCC     AA         AA  LLLLLLLLLLLL   EEEEEEEEEEEE                 PP              CCCCCCCCCC
```

```
*********************************************************************************
*********************************************************************************
*********************************************************************************
*****                                                                       *****
*****                  PROGRAM VERIFICATION INFORMATION                     *****
*****                                                                       *****
*****                CODE SYSTEM:  SCALE-PC VERSION:  4.3                   *****
*****                                                                       *****
*********************************************************************************
*********************************************************************************
*****                                                                       *****
*****                                                                       *****
*****              PROGRAM:  QADCGGP                                        *****
*****                                                                       *****
*****         CREATION DATE:  09-15-95                                      *****
*****                                                                       *****
*****              VOLUME:   SCSIDRIVED                                     *****
*****                                                                       *****
*****              LIBRARY:  D:\scale43\EXE                                 *****
*****                                                                       *****
*****                                                                       *****
*****       PRODUCTION CODE:  QAD-CGGP                                      *****
*****                                                                       *****
*****              VERSION:  3.0                                            *****
*****                                                                       *****
*****              JOBNAME:  SCALE-PC                                       *****
*****                                                                       *****
*****     DATE OF EXECUTION:  01/21/97                                      *****
*****                                                                       *****
*****     TIME OF EXECUTION:  16:05:02                                      *****
*****                                                                       *****
*****                                                                       *****
*********************************************************************************
*********************************************************************************
*********************************************************************************
```

Figure S5.4.3 (continued)

```
INPUT DATA LIST

  1          QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK
  2             15  15   10  11    3   1   18   0    0   1    2   0    0   0    0   0
  3             0.507800E+17   0.000000       0.000000       0.000000       0.000000
  4             0.000000       0.000000
  5             0.000000        2.66667        5.33333        8.00000        10.6667
  6              13.3333        16.0000        18.6667        21.3333        24.0000
  7              26.6667        29.3333        32.0000        34.6667        37.3333
  8              40.0000
  9              38.0000        68.0000        98.0000        128.000        158.000
 10              188.000        218.000        248.000        278.000        308.000
 11              338.000        368.000        398.000        428.000        458.000
 12              488.000
 13             0.000000       0.628318        1.25664        1.88495        2.51327
 14              3.14159        3.76991        4.39823        5.02654        5.65486
 15              6.28318
 16              1.00000        1.00000        1.00000        1.00000        1.00000
 17              1.00000        1.00000        1.00000        1.00000        1.00000
 18              1.00000        1.00000        1.00000        1.00000        1.00000
 19              1.00000
 20              1.00000        1.00000        1.00000        1.00000        1.00000
 21              1.00000        1.00000        1.00000        1.00000        1.00000
 22              1.00000        1.00000        1.00000        1.00000        1.00000
 23              1.00000
 24              1.00000        1.00000        1.00000        1.00000        1.00000
 25              1.00000        1.00000        1.00000        1.00000        1.00000
 26              1.00000
 27              0    0           CYLINDRICAL SHELL CASK
 28            RCC    1      0.+0      0.+0 380000.-4      0.+0      0.+0 450000.-3
 29                       400000.-4
 30            RCC    2      0.+0      0.+0      0.+0      0.+0      0.+0 488000.-3
 31                       780000.-4
 32            RCC    3      0.+0      0.+0 488000.-3      0.+0      0.+0 420000.-4
 33                       780000.-4
 34            RCC    4      0.+0      0.+0-100000.-1      0.+0      0.+0 200000.-1
 35                       200000.-1
 36            RCC    5      0.+0      0.+0-100010.-1      0.+0      0.+0 200020.-1
 37                       200020.-1
 38            END
 39            ZN1    2      1
 40            ZN2    2      2     -1
 41            ZN3    2      3
 42            ZN4    2      4     -3     -2
 43            ZN5    2      5     -4
 44            END
 45              1    1    1    1    1
 46              1    2    2 1000    0
 47             11   6   14  28   26   1   25  24   40  50   92   8
 48          IRON EXP
 49             0.000000       0.000000       0.522660E-01   0.367492       0.000000
 50             0.104532E-01   0.940788E-01   0.319115       0.521536E-02   0.997550
 51             0.120830
 52             0.227500       0.980000E-01   0.770000E-01    6.59750       0.000000
 53             0.000000       0.000000       0.000000       0.000000       0.000000
 54             0.000000
 55             0.779132       0.000000       0.000000       0.000000       0.130868
 56             0.000000       0.000000       0.000000       0.000000       0.000000
 57             0.000000
 58              9.00000        7.25000        5.75000        4.50000        3.50000
 59              2.75000        2.25000        1.83000        1.49500        1.16500
 60             0.900000       0.700000       0.500000       0.350000       0.250000
 61             0.150000       0.750000E-01   0.300000E-01
 62             0.000000       0.000000       0.000000       0.000000       0.000000
 63             0.264000E-04   0.502000E-02   0.113000E-03   0.000000       0.180000E-01
 64             0.760000E-02   0.670000       0.299000       0.000000       0.000000
 65             0.000000       0.000000       0.000000
 66             0.877162E-05   0.747850E-05   0.637482E-05   0.541365E-05   0.462207E-05
 67             0.395963E-05   0.346860E-05   0.301918E-05   0.262760E-05   0.220512E-05
 68             0.183257E-05   0.152276E-05   0.117245E-05   0.875938E-06   0.630604E-06
 69             0.383374E-06   0.266928E-06   0.934763E-06
 70             0.000000       0.000000       0.000000       0.000000       0.000000
 71             0.000000       0.000000       0.000000       0.000000       0.000000
 72             0.000000       0.000000       0.000000       0.000000       0.000000
 73             0.000000       0.000000       0.000000
 74           0.01 -10.00
 75          10.00 - 8.00 8.00 - 6.50 6.50 - 5.00 5.00 - 4.00 4.00 - 3.00 3.00 - 2.50
 76           2.50 - 2.00 2.00 - 1.66 1.66 - 1.33 1.33 - 1.00 1.00 - 0.80 0.80 - 0.60
 77           0.60 - 0.40 0.40 - 0.30 0.30 - 0.20 0.20 - 0.10 0.10 - 0.05 0.05 - 0.01
 78
 79              78.0000        265.000       0.000000              0           0
 80                    0              0
 81              178.000        265.000       0.000000              0           0
 82                    0              0
 83             0.000000       0.000000       0.000000             -1           0
 84                    0              0
```

Listing of actual QAD-CGGP input

Figure S5.4.3 (continued)

```
QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

CONTROL    15    15    10    11     3     1    18     0     0     1     2     0     0     0     0     0
                       0    -9     1    10     0     0     0     0     0     0     0     0     0     0

SOURCE  5.0780E+16  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00

     R  0.0000E+00  2.6667E+00  5.3333E+00  8.0000E+00  1.0667E+01  1.3333E+01  1.6000E+01  1.8667E+01
        2.1333E+01  2.4000E+01  2.6667E+01  2.9333E+01  3.2000E+01  3.4667E+01  3.7333E+01  4.0000E+01

     Z  3.8000E+01  6.8000E+01  9.8000E+01  1.2800E+02  1.5800E+02  1.8800E+02  2.1800E+02  2.4800E+02
        2.7800E+02  3.0800E+02  3.3800E+02  3.6800E+02  3.9800E+02  4.2800E+02  4.5800E+02  4.8800E+02

   PHI  0.0000E+00  6.2832E-01  1.2566E+00  1.8850E+00  2.5133E+00  3.1416E+00  3.7699E+00  4.3982E+00
        5.0265E+00  5.6549E+00  6.2832E+00

  F(L)  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
        1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00

  F(M)  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
        1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00

  F(N)  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00  1.0000E+00
        1.0000E+00  1.0000E+00  1.0000E+00
```

Control parameters

3-D mesh description

Weight factors

Figure S5.4.3 (continued)

```
        CYLINDRICAL SHELL CASK

                IVOPT = 0          IDBG = 0
```

Geometry description

```
                                                BODY DATA
 RCC    1  0.0000000E+00  0.0000000E+00  0.3800000E+02  0.0000000E+00  0.0000000E+00  0.4500000E+03    3
           0.4000000E+02
 RCC    2  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.4880000E+03   12
           0.7800000E+02
 RCC    3  0.0000000E+00  0.0000000E+00  0.4880000E+03  0.0000000E+00  0.0000000E+00  0.4200000E+02   21
           0.7800000E+02
 RCC    4  0.0000000E+00  0.0000000E+00 -0.1000000E+05  0.0000000E+00  0.0000000E+00  0.2000000E+05   30
           0.2000000E+05
 RCC    5  0.0000000E+00  0.0000000E+00 -0.1000100E+05  0.0000000E+00  0.0000000E+00  0.2000200E+05   39
           0.2000200E+05
 END    6  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00  0.0000000E+00   48
NUMBER OF BODIES       5
LENGTH OF FPD-ARRAY   53


                                          INPUT ZONE DATA
 ZN1    2     1     0     0     0     0     0     0     0     0 Z 1
 ZN2    2     2    -1     0     0     0     0     0     0     0 Z 2
 ZN3    2     3     0     0     0     0     0     0     0     0 Z 3
 ZN4    2     4    -3    -2     0     0     0     0     0     0 Z 4
 ZN5    2     5    -4     0     0     0     0     0     0     0 Z 5
 END    0     0     0     0     0     0     0     0     0     0 Z 6
NUMBER OF INPUT ZONES      5
NUMBER OF  CODE ZONES      5
LENGTH OF INTEGER ARRAY   97


CODE ZONE    INPUT ZONE    ZONE DATA LOC.    NO. OF BODIES    REGION NO.    MEDIA NO.
    1            1              36               1              1             1
    2            2              41               2              1             2
    3            3              50               1              1             2
    4            4              55               3              1          1000
    5            5              68               2              1             0

  I    KR1(I)    KR2(I)
  1       1         1
  2       2         2
  3       3         3
  4       4         4
  5       5         5

        MORSE REGION IN INPUT ZONE(I) ARRAY   MRIZ(I),I=1, 5)

           1   1   1   1   1

        MORSE MEDIA IN INPUT ZONE(I) ARRAY  MMIZ(I),I=1, 5)

           1   2   21000   0
```

mixture numbers by zone

```
 OPTION 0 WAS USED IN CALCULATING VOLUMES, FOR  1 REGIONS
0-SET VOLUMES = 1, 1-CONCENTRIC SPHERES, 2-SLABS, 3-INPUTVOLUMES.

        VOLUMES (CM**) USED IN COLLISIONS DENSITY AND TRACK LENGTH ESTIMATORS.
   REG       1
VOLUME  1.000E+00
```

Figure S5.4.3 (continued)

| COMP/MAT | C | SI | NI | FE | H | MN | CR | ZR | SN |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 0.0000E+00 | 0.0000E+00 | 5.2266E-02 | 3.6749E-01 | 0.0000E+00 | 1.0453E-02 | 9.4079E-02 | 3.1912E-01 | 5.2154E-03 |
| 2 | 2.2750E-01 | 9.8000E-02 | 7.7000E-02 | 6.5975E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3 | 7.7913E-01 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 1.3087E-01 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

partial densities by material

| COMP/MAT | U | O |
|---|---|---|
| 1 | 9.9755E-01 | 1.2083E-01 |
| 2 | 0.0000E+00 | 0.0000E+00 |
| 3 | 0.0000E+00 | 0.0000E+00 |

DATA FOUND: IRON MEDIUM, AIR RESPONSE

| GRP/MAT | C | SI | NI | FE | H | MN | CR | ZR | SN | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | NEUTRON REMOVAL CROSS-SECTION | | | | | | | |
| | 4.0630E-02 | 2.8980E-02 | 1.9400E-02 | 2.1360E-02 | 6.0200E-01 | 2.0500E-02 | 2.1090E-02 | 1.5590E-02 | 1.3780E-02 | |
| | | | MATERIAL HYDROGEN DENSITY | | | | | | | |
| | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 1.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | |
| | | | GAMMA ATTENUATION COEFFICIENT | | | | | | | |
| 1 | 2.0433E-02 | 2.5088E-02 | 3.1696E-02 | 2.9871E-02 | 3.4672E-02 | 2.8679E-02 | 2.8566E-02 | 3.4947E-02 | 3.8079E-02 | 9.00 |
| 2 | 2.2510E-02 | 2.6390E-02 | 3.1730E-02 | 3.0071E-02 | 3.9767E-02 | 2.8954E-02 | 2.8931E-02 | 3.4116E-02 | 3.6681E-02 | 7.25 |
| 3 | 2.5166E-02 | 2.8218E-02 | 3.2203E-02 | 3.0705E-02 | 4.6088E-02 | 2.9665E-02 | 2.9730E-02 | 3.3691E-02 | 3.5673E-02 | 5.75 |
| 4 | 2.8561E-02 | 3.0859E-02 | 3.3528E-02 | 3.2154E-02 | 5.3802E-02 | 3.1153E-02 | 3.1323E-02 | 3.4065E-02 | 3.5442E-02 | 4.50 |
| 5 | 3.2690E-02 | 3.4290E-02 | 3.5707E-02 | 3.4426E-02 | 6.2870E-02 | 3.3443E-02 | 3.3727E-02 | 3.5275E-02 | 3.6052E-02 | 3.50 |
| 6 | 3.7278E-02 | 3.8285E-02 | 3.8622E-02 | 3.7395E-02 | 7.2705E-02 | 3.6413E-02 | 3.6796E-02 | 3.7306E-02 | 3.7546E-02 | 2.75 |
| 7 | 4.1590E-02 | 4.2205E-02 | 4.1748E-02 | 4.0535E-02 | 8.1753E-02 | 3.9529E-02 | 3.9995E-02 | 3.9733E-02 | 3.9571E-02 | 2.25 |
| 8 | 4.6492E-02 | 4.6749E-02 | 4.5530E-02 | 4.4303E-02 | 9.1967E-02 | 4.3250E-02 | 4.3807E-02 | 4.2827E-02 | 4.2313E-02 | 1.83 |
| 9 | 5.1758E-02 | 5.1797E-02 | 4.9994E-02 | 4.8701E-02 | 1.0278E-01 | 4.7569E-02 | 4.8221E-02 | 4.6710E-02 | 4.5962E-02 | 1.50 |
| 10 | 5.8767E-02 | 5.8738E-02 | 5.6652E-02 | 5.5183E-02 | 1.1673E-01 | 5.3891E-02 | 5.4631E-02 | 5.3056E-02 | 5.2503E-02 | 1.16 |
| 11 | 6.6814E-02 | 6.6716E-02 | 6.4420E-02 | 6.2720E-02 | 1.3272E-01 | 6.1243E-02 | 6.2066E-02 | 6.0667E-02 | 6.0637E-02 | 0.90 |
| 12 | 7.5078E-02 | 7.4984E-02 | 7.2776E-02 | 7.0765E-02 | 1.4909E-01 | 6.9062E-02 | 6.9953E-02 | 6.9485E-02 | 7.0888E-02 | 0.70 |
| 13 | 8.7000E-02 | 8.6980E-02 | 8.5450E-02 | 8.2820E-02 | 1.7280E-01 | 8.0730E-02 | 8.1680E-02 | 8.4200E-02 | 8.9760E-02 | 0.50 |
| 14 | 1.0024E-01 | 1.0059E-01 | 1.0241E-01 | 9.8424E-02 | 1.9911E-01 | 9.5531E-02 | 9.6347E-02 | 1.0926E-01 | 1.2797E-01 | 0.35 |
| 15 | 1.1322E-01 | 1.1457E-01 | 1.2690E-01 | 1.1972E-01 | 2.2491E-01 | 1.1519E-01 | 1.1527E-01 | 1.5658E-01 | 2.0806E-01 | 0.25 |
| 16 | 1.3380E-01 | 1.3990E-01 | 2.0490E-01 | 1.8290E-01 | 2.6500E-01 | 1.7150E-01 | 1.6740E-01 | 3.5090E-01 | 5.6900E-01 | 0.15 |
| 17 | 1.6042E-01 | 2.2331E-01 | 8.0149E-01 | 6.4746E-01 | 3.1281E-01 | 5.7430E-01 | 5.2777E-01 | 1.9470E+00 | 3.4590E+00 | 0.08 |
| 18 | 2.3680E-01 | 1.3400E+00 | 1.0050E+01 | 7.9300E+00 | 3.5700E-01 | 6.9170E+00 | 6.2210E+00 | 2.4380E+01 | 4.0580E+01 | 0.03 |

| GRP/MAT | U | O | |
|---|---|---|---|
| | | NEUTRON REMOVAL CROSS-SECTION | |
| | 9.1100E-03 | 3.7280E-02 | |
| | | MATERIAL HYDROGEN DENSITY | |
| | 0.0000E+00 | 0.0000E+00 | |
| | | GAMMA ATTENUATION COEFFICIENT | |
| 1 | 5.0343E-02 | 2.1644E-02 | 9.0000E+00 |
| 2 | 4.7642E-02 | 2.3527E-02 | 7.2500E+00 |
| 3 | 4.5397E-02 | 2.5966E-02 | 5.7500E+00 |
| 4 | 4.4070E-02 | 2.9181E-02 | 4.5000E+00 |
| 5 | 4.3826E-02 | 3.3141E-02 | 3.5000E+00 |
| 6 | 4.4831E-02 | 3.7585E-02 | 2.7500E+00 |
| 7 | 4.6735E-02 | 4.1805E-02 | 2.2500E+00 |
| 8 | 4.9801E-02 | 4.6631E-02 | 1.8300E+00 |
| 9 | 5.4508E-02 | 5.1868E-02 | 1.4950E+00 |
| 10 | 6.6818E-02 | 5.8872E-02 | 1.1650E+00 |
| 11 | 8.4938E-02 | 6.6901E-02 | 9.0000E-01 |
| 12 | 1.1488E-01 | 7.5157E-02 | 7.0000E-01 |
| 13 | 1.8540E-01 | 8.7080E-02 | 5.0000E-01 |
| 14 | 3.5759E-01 | 1.0043E-01 | 3.5000E-01 |
| 15 | 7.3894E-01 | 1.1356E-01 | 2.5000E-01 |
| 16 | 2.4770E+00 | 1.3440E-01 | 1.5000E-01 |
| 17 | 3.6193E+00 | 1.6626E-01 | 7.5000E-02 |
| 18 | 3.9760E+01 | 3.4400E-01 | 3.0000E-02 |

attenuation coefficients by group for each material

Figure S5.4.3 (continued)

***** CONVERSION FACTORS AND BUILD FACTORS

***** BUILDUP FACTORS OF GEOMETRIC-PROGRESSION METHOD ARE USED
***** IRON MEDIUM, AIR RESPONSE

GP method build-up factors

| GRP | ENERGY | CONV. | B | C | A | XK | D | |
|---|---|---|---|---|---|---|---|---|
| 1 | 0.0000E+00 | 8.7716E-06 | 1.3232 | 0.9606 | 0.0358 | 13.818 | -0.04970 | 9.00 |
| 2 | 0.0000E+00 | 7.4785E-06 | 1.3848 | 0.9750 | 0.0270 | 13.554 | -0.03994 | 7.25 |
| 3 | 0.0000E+00 | 6.3748E-06 | 1.4514 | 0.9865 | 0.0205 | 13.310 | -0.03325 | 5.75 |
| 4 | 0.0000E+00 | 5.4136E-06 | 1.5154 | 1.0178 | 0.0083 | 13.052 | -0.02217 | 4.50 |
| 5 | 0.0000E+00 | 4.6221E-06 | 1.5895 | 1.0392 | 0.0008 | 12.185 | -0.01660 | 3.50 |
| 6 | 2.6400E-05 | 3.9596E-06 | 1.6452 | 1.0756 | -0.0098 | 14.048 | -0.00873 | 2.75 |
| 7 | 5.0200E-03 | 3.4686E-06 | 1.6832 | 1.1168 | -0.0211 | 18.275 | 0.00129 | 2.25 |
| 8 | 1.1300E-04 | 3.0192E-06 | 1.7170 | 1.1606 | -0.0322 | 19.176 | 0.00878 | 1.83 |
| 9 | 0.0000E+00 | 2.6276E-06 | 1.7507 | 1.1975 | -0.0401 | 15.911 | 0.01105 | 1.50 |
| 10 | 1.8000E-02 | 2.2051E-06 | 1.8060 | 1.2329 | -0.0459 | 17.614 | 0.01355 | 1.16 |
| 11 | 7.6000E-03 | 1.8326E-06 | 1.8619 | 1.2608 | -0.0492 | 19.862 | 0.01321 | 0.90 |
| 12 | 6.7000E-01 | 1.5228E-06 | 1.9075 | 1.2752 | -0.0501 | 21.324 | 0.01089 | 0.70 |
| 13 | 2.9900E-01 | 1.1724E-06 | 1.9570 | 1.2610 | -0.0460 | 24.770 | 0.00840 | 0.50 |
| 14 | 0.0000E+00 | 8.7594E-07 | 1.9916 | 1.1460 | -0.0188 | 9.909 | -0.01739 | 0.35 |
| 15 | 0.0000E+00 | 6.3060E-07 | 1.9291 | 1.0200 | 0.0076 | 12.502 | -0.02408 | 0.25 |
| 16 | 0.0000E+00 | 3.8337E-07 | 1.6600 | 0.7430 | 0.0790 | 14.120 | -0.04760 | 0.15 |
| 17 | 0.0000E+00 | 2.6693E-07 | 1.2362 | 0.4529 | 0.1867 | 14.446 | -0.10061 | 0.08 |
| 18 | 0.0000E+00 | 9.3476E-07 | 1.0280 | 0.3740 | 0.1900 | 29.340 | -0.31700 | 0.03 |

| GRP | EG | 0.5MFP | 1.0MFP | 2.0MFP | 4.0MFP | 8.0MFP | 10.0MFP | 20.0MFP | 40.0MFP | 60.0MFP |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | 9.00 | 1.164E+00 | 1.323E+00 | 1.641E+00 | 2.310E+00 | 3.904E+00 | 4.888E+00 | 1.260E+01 | 4.388E+01 | 1.265E+02 |
| 2 | 7.25 | 1.195E+00 | 1.385E+00 | 1.767E+00 | 2.566E+00 | 4.420E+00 | 5.521E+00 | 1.339E+01 | 3.990E+01 | 9.647E+01 |
| 3 | 5.75 | 1.227E+00 | 1.451E+00 | 1.903E+00 | 2.845E+00 | 4.987E+00 | 6.227E+00 | 1.449E+01 | 3.884E+01 | 8.287E+01 |
| 4 | 4.50 | 1.257E+00 | 1.515E+00 | 2.043E+00 | 3.154E+00 | 5.659E+00 | 7.077E+00 | 1.595E+01 | 3.958E+01 | 7.539E+01 |
| 5 | 3.50 | 1.292E+00 | 1.590E+00 | 2.202E+00 | 3.503E+00 | 6.432E+00 | 8.072E+00 | 1.789E+01 | 4.223E+01 | 7.629E+01 |
| 6 | 2.75 | 1.316E+00 | 1.645E+00 | 2.334E+00 | 3.826E+00 | 7.240E+00 | 9.157E+00 | 2.072E+01 | 4.969E+01 | 8.457E+01 |
| 7 | 2.25 | 1.331E+00 | 1.683E+00 | 2.435E+00 | 4.099E+00 | 7.979E+00 | 1.017E+01 | 2.322E+01 | 5.713E+01 | 9.890E+01 |
| 8 | 1.83 | 1.343E+00 | 1.717E+00 | 2.531E+00 | 4.378E+00 | 8.787E+00 | 1.129E+01 | 2.600E+01 | 6.224E+01 | 1.053E+02 |
| 9 | 1.50 | 1.356E+00 | 1.751E+00 | 2.625E+00 | 4.656E+00 | 9.650E+00 | 1.254E+01 | 2.979E+01 | 7.397E+01 | 1.263E+02 |
| 10 | 1.16 | 1.379E+00 | 1.806E+00 | 2.769E+00 | 5.066E+00 | 1.095E+01 | 1.446E+01 | 3.638E+01 | 9.652E+01 | 1.751E+02 |
| 11 | 0.90 | 1.402E+00 | 1.862E+00 | 2.912E+00 | 5.481E+00 | 1.234E+01 | 1.658E+01 | 4.478E+01 | 1.281E+02 | 2.437E+02 |
| 12 | 0.70 | 1.422E+00 | 1.907E+00 | 3.025E+00 | 5.800E+00 | 1.343E+01 | 1.827E+01 | 5.216E+01 | 1.597E+02 | 3.147E+02 |
| 13 | 0.50 | 1.447E+00 | 1.957E+00 | 3.126E+00 | 6.014E+00 | 1.395E+01 | 1.901E+01 | 5.534E+01 | 1.767E+02 | 3.578E+02 |
| 14 | 0.35 | 1.477E+00 | 1.992E+00 | 3.113E+00 | 5.712E+00 | 1.238E+01 | 1.647E+01 | 4.369E+01 | 1.269E+02 | 2.687E+02 |
| 15 | 0.25 | 1.463E+00 | 1.929E+00 | 2.882E+00 | 4.889E+00 | 9.414E+00 | 1.197E+01 | 2.762E+01 | 6.634E+01 | 1.227E+02 |
| 16 | 0.15 | 1.359E+00 | 1.660E+00 | 2.178E+00 | 3.035E+00 | 4.454E+00 | 5.108E+00 | 8.262E+00 | 1.325E+01 | 1.815E+01 |
| 17 | 0.08 | 1.145E+00 | 1.236E+00 | 1.358E+00 | 1.503E+00 | 1.677E+00 | 1.745E+00 | 2.026E+00 | 2.306E+00 | 2.534E+00 |
| 18 | 0.03 | 1.018E+00 | 1.028E+00 | 1.040E+00 | 1.051E+00 | 1.062E+00 | 1.065E+00 | 1.079E+00 | 1.090E+00 | 1.092E+00 |

ALBERT-WELTON COEFFICIENTS

7.7200E-09 3.4900E-01 4.2200E-01 6.9800E-01

Figure S5.4.3 (continued)

```
EG-
  9.0000E+00  7.2500E+00  5.7500E+00  4.5000E+00  3.5000E+00  2.7500E+00  2.2500E+00  1.8300E+00  1.4950E+00
  1.1650E+00  9.0000E-01  7.0000E-01  5.0000E-01  3.5000E-01  2.5000E-01  1.5000E-01  7.5000E-02  3.0000E-02
FE ABS G-
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
EN-
  1.0000E+01  8.0000E+00  6.0000E+00  5.0000E+00  4.0000E+00  3.0000E+00  2.0000E+00  1.0000E+00  6.7000E-01
  3.3000E-01
FE ABS N-
  2.2500E-15  9.2700E-16  5.4700E-16  4.6800E-16  3.8000E-16  3.0700E-16  2.1600E-16  1.0400E-16  8.3500E-17
  4.6700E-17
WIDTH T-
                0.01 -10.00 12.0-0.10
WIDTH G-
               10.00 - 8.00 8.00 - 6.50 6.50 - 5.00 5.00 - 4.00 4.00 - 3.00 3.00 - 2.50
                2.50 - 2.00 2.00 - 1.66 1.66 - 1.33 1.33 - 1.00 1.00 - 0.80 0.80 - 0.60
                0.60 - 0.40 0.40 - 0.30 0.30 - 0.20 0.20 - 0.10 0.10 - 0.05 0.05 - 0.01
WIDTH N-
                12.0-9.00   9.00-7.00   7.00-5.50   5.50-4.50   4.50-3.50   3.50-2.50
                2.50-1.50   1.50-0.835  0.835-0.50  0.50-0.10
UNIT G-


UNIT N-
                  RAD       WATTS PER    PER HOUR     GRAM      RAD PER  HR


                                COORDINATE TYPE 0          SOURCE INTENSITY OPTION 2

          R COORDINATE
      COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY

    1  1.3333E+00   2.1333E+01   4.0000E+00   6.4000E+01   6.6667E+00   1.0667E+02   9.3334E+00   1.4934E+02
    5  1.2000E+01   1.9200E+02   1.4667E+01   2.3467E+02   1.7333E+01   2.7734E+02   2.0000E+01   3.1999E+02
    9  2.2667E+01   3.6267E+02   2.5333E+01   4.0534E+02   2.8000E+01   4.4799E+02   3.0667E+01   4.9067E+02
   13  3.3333E+01   5.3334E+02   3.6000E+01   5.7599E+02   3.8667E+01   6.1867E+02

          PHI COORDINATE
      COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY

    1  3.1416E-01   1.2566E+00   9.4248E-01   1.2566E+00   1.5708E+00   1.2566E+00   2.1991E+00   1.2566E+00
    5  2.8274E+00   1.2566E+00   3.4557E+00   1.2566E+00   4.0841E+00   1.2566E+00   4.7124E+00   1.2566E+00
    9  5.3407E+00   1.2566E+00   5.9690E+00   1.2566E+00

          Z COORDINATE
      COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY    COORDINATE    INTENSITY

    1  5.3000E+01   5.6124E+10   8.3000E+01   5.6124E+10   1.1300E+02   5.6124E+10   1.4300E+02   5.6124E+10
    5  1.7300E+02   5.6124E+10   2.0300E+02   5.6124E+10   2.3300E+02   5.6124E+10   2.6300E+02   5.6124E+10
    9  2.9300E+02   5.6124E+10   3.2300E+02   5.6124E+10   3.5300E+02   5.6124E+10   3.8300E+02   5.6124E+10
   13  4.1300E+02   5.6124E+10   4.4300E+02   5.6124E+10   4.7300E+02   5.6124E+10
```

Source intensity by mesh intervals

Figure S5.4.3 (continued)

QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

RECEIVER NUMBER 1 COORDINATES - R 7.8000E+01 PHI 0.0000E+00 Z 2.6500E+02

detector coordinates

GEOMETRY PRINT FOR PSEUDO SOURCE POINT AT THE COORDINATE ORIGIN

| ZONE | DISTANCE | X | Y | Z |
|---|---|---|---|---|
| | SOURCE PNT | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2 | 3.9612E+01 | 1.1185E+01 | 0.0000E+00 | 3.8000E+01 |
| 1 | 1.0205E+02 | 4.0000E+01 | 0.0000E+00 | 1.3590E+02 |
| 2 | 1.3458E+02 | 7.8000E+01 | 0.0000E+00 | 2.6500E+02 |
| 1000 | 9.7512E-05 | 7.8000E+01 | 0.0000E+00 | 2.6500E+02 |

QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

RECEIVER NUMBER 1 COORDINATES - R 7.8000E+01 PHI 0.0000E+00 Z 2.6500E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL | 2.1136 | 0.01 -10.00 | 7.4125E+02 | 1.3958E+01 | 2.5265E-03 | 3.5266E-02 | 0.0000E+00 | 0.0000E+00 |
| W/BU | 2.2004 | | | | | | | |
| 1 | 9.0000 | 10.00 - 8.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 9.7213E+00 | 1.1078E+01 | 3.8493E-05 | 4.2643E-04 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 6.9338E+02 | 1.3427E+01 | 2.4051E-03 | 3.2293E-02 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 4.8228E+00 | 1.6520E+01 | 1.4561E-05 | 2.4055E-04 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 2.5448E+01 | 2.8885E+01 | 5.6117E-05 | 1.6209E-03 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 1.0052E+00 | 4.1665E+01 | 1.8421E-06 | 7.6749E-05 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 6.8098E+00 | 5.8108E+01 | 1.0370E-05 | 6.0256E-04 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 6.1046E-02 | 8.0132E+01 | 7.1573E-08 | 5.7353E-06 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

total dose rate

dose rate by group

Figure S5.4.3 (continued)

QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

RECEIVER NUMBER 2 COORDINATES -

R 1.7800E+02 PHI 0.0000E+00 Z 2.6500E+02

GEOMETRY PRINT FOR PSEUDO SOURCE POINT AT THE COORDINATE ORIGIN

| ZONE | DISTANCE | X | Y | Z |
|---|---|---|---|---|
| | SOURCE PNT | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2 | 4.5777E+01 | 2.5525E+01 | 0.0000E+00 | 3.8000E+01 |
| 1 | 2.5961E+01 | 4.0000E+01 | 0.0000E+00 | 5.9551E+01 |
| 2 | 6.8151E+01 | 7.8000E+01 | 0.0000E+00 | 1.1612E+02 |
| 1000 | 1.7934E+02 | 1.7800E+02 | 0.0000E+00 | 2.6500E+02 |

QADS SAMPLE PROBLEM #1 - OECD BENCHMARK SHIPPING CASK

RECEIVER NUMBER 2 COORDINATES -

R 1.7800E+02 PHI 0.0000E+00 Z 2.6500E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL | 2.1038 | 0.01 -10.00 | 3.3516E+02 | 1.3862E+01 | 1.1408E-03 | 1.5813E-02 | 0.0000E+00 | 0.0000E+00 |
| W/BU | 2.1964 | | | | | | | |
| 1 | 9.0000 | 10.00 - 8.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 4.3510E+00 | 1.0983E+01 | 1.7228E-05 | 1.8921E-04 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 3.1255E+02 | 1.3300E+01 | 1.0841E-03 | 1.4419E-02 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 2.1944E+00 | 1.6347E+01 | 6.6254E-06 | 1.0831E-04 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 1.2016E+01 | 2.8438E+01 | 2.6497E-05 | 7.5353E-04 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 4.9239E-01 | 4.0798E+01 | 9.0234E-07 | 3.6814E-05 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 3.5275E+00 | 5.6472E+01 | 5.3715E-06 | 3.0334E-04 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 3.5670E-02 | 7.6963E+01 | 4.1821E-08 | 3.2187E-06 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 | 0.0000E+00 |

Subroutine EXIT has been called. Probably from INPUT.

Figure S5.4.3 (continued)

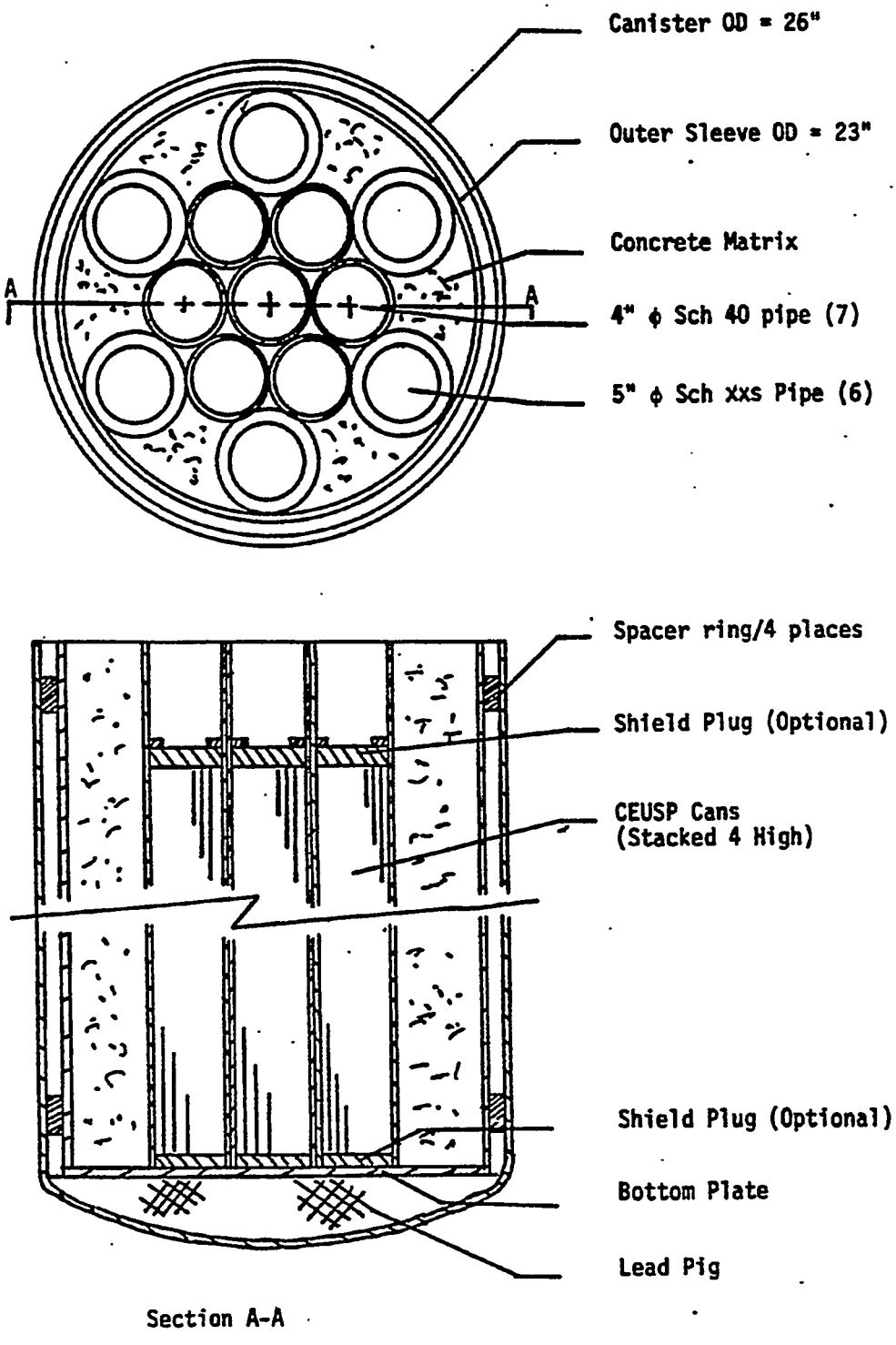



Figure S5.4.4 Enriched uranium storage containers

```
=QADS
CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL
ORIGENGP-SRC      INFHOMMEDIUM
URANIUM 1 .03045 293 92233 9.700 92234 1.400 92235 76.5
          92236 5.600 92238 6.800 END
O   1   .13591   END
CD  1   .02141   END
GD  1   .02788   END
URANIUM 5 .01473 293 92233 9.700 92234 1.400 92235 76.5
          92236 5.600 92238 6.800 END
O   5   .06575   END
CD  5   .01035   END
GD  5   .01349   END
SS304 2  END
CARBONSTEEL   3   END
MGCONCRETE   4   END
END COMP
CYLINDRICAL   0.   FLATS   END
NZS=4
END SOURCE
CYLINDRICAL SHELL CASK
RCC 1 0 0 .940 0 0 246.28  4.808
RCC 2 0 0 .635 0 0 247.58  5.113
RCC 3 0 0 .635 0 0 271.78  5.715
RCC 4 0 0 .940 0 0 246.28  24.620
RCC 5 0 0 .635 0 0 247.58  24.925
RCC 6 0 0 .635 0 0 271.75  26.797
RCC 7 0 0 .635 0 0 271.78  32.385
RCC 8 0 0 .635 0 0 271.78  33.020
RCC 9 0 0 -10000 0 0  20000  20000
RCC 10 0 0 -10001 0 0 20002 20002
END BODY
ZNL 2 1
ZN2 2 2 -1
ZN3 2 3 -2
ZN4 2 4 -3
ZN5 2 5 -4
ZN6 2 6 -5
ZN7 2 7 -6
ZN8 2 8 -7
ZN9 2 9 -8
ZN10 2 10 -9
END ZONE
1 2 3 5 2  3  1000  2  1000  0
END GEOM
IRON EXP
END DOSE
END
```

Figure S5.4.5 Input listing of second sample problem

```
CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

**** PROBLEM PARAMETERS ****

LIB NO_LIB_USED  LIBRARY
MXX            5 MIXTURES
MSC           11 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        0.0304 VOLUME FRACTION
ROTH     19.0500 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       293.0 DEG KELVIN
           92000      1.00 ATOM/MOLECULE
                         92233     9.700 WT%
                         92234     1.400 WT%
                         92235    76.500 WT%
                         92236     5.600 WT%
                         92238     6.800 WT%
END

SC  O            STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.1359 VOLUME FRACTION
ROTH      1.0000 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
            8016      1.00 ATOM/MOLECULE
END

SC  CD           STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0214 VOLUME FRACTION
ROTH      8.6420 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
           48000      1.00 ATOM/MOLECULE
END

SC  GD           STANDARD COMPOSITION
MX             1 MIXTURE NO.
VF        0.0279 VOLUME FRACTION
ROTH      7.9000 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
           64000      1.00 ATOM/MOLECULE
END

SC  URANIUM      STANDARD COMPOSITION
MX             5 MIXTURE NO.
VF        0.0147 VOLUME FRACTION
ROTH     19.0500 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
TEMP       293.0 DEG KELVIN
           92000      1.00 ATOM/MOLECULE
                         92233     9.700 WT%
                         92234     1.400 WT%
                         92235    76.500 WT%
                         92236     5.600 WT%
                         92238     6.800 WT%
END

SC  O            STANDARD COMPOSITION
MX             5 MIXTURE NO.
VF        0.0658 VOLUME FRACTION
ROTH      1.0000 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
            8016      1.00 ATOM/MOLECULE
END

SC  CD           STANDARD COMPOSITION
MX             5 MIXTURE NO.
VF        0.0104 VOLUME FRACTION
ROTH      8.6420 THEORETICAL DENSITY
NEL            1 NO. ELEMENTS
ICP            1 0/1 MIXTURE/COMPOUND
           48000      1.00 ATOM/MOLECULE
END
```

Figure S5.4.6 Abbreviated output listing of second sample problem

```
SC  GD            STANDARD COMPOSITION
MX                5 MIXTURE NO.
VF           0.0135 VOLUME FRACTION
ROTH         7.9000 THEORETICAL DENSITY
NEL               1 NO. ELEMENTS
ICP               1 0/1 MIXTURE/COMPOUND
            64000       1.00 ATOM/MOLECULE
END

SC  SS304         STANDARD COMPOSITION
MX                2 MIXTURE NO.
VF           1.0000 VOLUME FRACTION
ROTH         7.9200 THEORETICAL DENSITY
NEL               4 NO. ELEMENTS
ICP               0 0/1 MIXTURE/COMPOUND
            24304     19.000 WT%
            25055      2.000 WT%
            26304     69.500 WT%
            28304      9.500 WT%
END

SC  CARBONSTEEL   STANDARD COMPOSITION
MX                3 MIXTURE NO.
VF           1.0000 VOLUME FRACTION
ROTH         7.8212 THEORETICAL DENSITY
NEL               2 NO. ELEMENTS
ICP               0 0/1 MIXTURE/COMPOUND
            26000     99.000 WT%
             6012      1.000 WT%
END

SC  MGCONCRETE    STANDARD COMPOSITION
MX                4 MIXTURE NO.
VF           1.0000 VOLUME FRACTION
ROTH         2.1470 THEORETICAL DENSITY
NEL              14 NO. ELEMENTS
ICP               0 0/1 MIXTURE/COMPOUND
            26000      0.559 WT%
             1001      0.332 WT%
             6012     10.532 WT%
             8016     49.943 WT%
            11023      0.141 WT%
            12000      9.420 WT%
            13027      0.786 WT%
            14000      4.210 WT%
            16000      0.248 WT%
            17000      0.052 WT%
            19000      0.945 WT%
            20000     22.632 WT%
            22000      0.149 WT%
            25055      0.051 WT%
END

**** PROBLEM GEOMETRY ****

**** INFINITE HOMOGENEOUS MEDIUM ****
MFUEL             1 MIXTURE NO. OF THE INFINITE HOMOGENEOUS MEDIUM

**** SOURCE PARAMETERS ****

CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

SRC     CYLINDRICAL   SOURCE COORDINATE SYSTEM
ASO      0.00000E+00  SOURCE STRENGTH
SHAPE        FLATS    SOURCE SHAPE



OPTIONAL PARAMETERS

NZS           4  SOURCE BODY NUMBER

GROUP STRUCTURE AND SOURCE SPECTRUM READ FROM UNIT 71 POSITION     0
```

Figure S5.4.6 (continued)

```
**** DOSE DATA ****

BFMAT       IRON  BUILDUP FACTOR MATERIAL
BFRSP        EXP  BUILDUP FACTOR RESPONSE


NFACTR          0  DOSE FACTOR ID (READ FROM CARDS IF      < 9000)
NDETEC          4  NUMBER OF DETECTORS

DETECTOR NO.  1
RRC= 3.3020E+01 ZRC= 1.2361E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
DETECTOR NO.  2
RRC= 1.3302E+02 ZRC= 1.2361E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
DETECTOR NO.  3
RRC= 2.3302E+02 ZRC= 1.2361E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
DETECTOR NO.  4
RRC= 4.3302E+02 ZRC= 1.2361E+02 PHIRC= 0.0000E+00 NRCOP= CYLINDRICAL
```

Figure S5.4.6 (continued)

CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

RECEIVER NUMBER 1 COORDINATES - R 3.3020E+01 PHI 0.0000E+00 Z 1.2361E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL W/BU | 1.8406 2.1758 | 0.01 -10.00 | 5.0261E+05 | 2.3528E+00 | 1.6445E+00 | 3.8692E+00 | 0.0000E+00 | 0.0000E+00 |
| 1 | 9.0000 | 10.00 - 8.00 | 1.8490E-06 | 1.4734E+00 | 1.6219E-11 | 2.3896E-11 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 1.3960E-05 | 1.5627E+00 | 1.0440E-10 | 1.6314E-10 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 1.0864E-04 | 1.6656E+00 | 6.9253E-10 | 1.1535E-09 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 3.6020E-04 | 1.7855E+00 | 1.9500E-09 | 3.4818E-09 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 1.3163E-03 | 1.9448E+00 | 6.0839E-09 | 1.1832E-08 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 3.5529E+05 | 2.1099E+00 | 1.4068E+00 | 2.9682E+00 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 3.1142E-01 | 2.2684E+00 | 1.0802E-06 | 2.4502E-06 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 2.5770E+03 | 2.4552E+00 | 7.7803E-03 | 1.9102E-02 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 2.3376E+04 | 2.6803E+00 | 6.1422E-02 | 1.6463E-01 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 5.4825E+03 | 3.0726E+00 | 1.2090E-02 | 3.7147E-02 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 1.8406E+04 | 3.5677E+00 | 3.3731E-02 | 1.2034E-01 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 3.5715E+04 | 4.1192E+00 | 5.4385E-02 | 2.2402E-01 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 5.3543E+04 | 4.8879E+00 | 6.2777E-02 | 3.0684E-01 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 1.2006E+03 | 5.3945E+00 | 1.0516E-03 | 5.6731E-03 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 6.9870E+03 | 5.2466E+00 | 4.4060E-03 | 2.3117E-02 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 3.8218E+01 | 3.7872E+00 | 1.4652E-05 | 5.5490E-05 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 5.3293E-04 | 1.9954E+00 | 1.4225E-10 | 2.8385E-10 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 1.2612E-24 | 1.0917E+00 | 1.1790E-30 | 1.2871E-30 | 0.0000E+00 | 0.0000E+00 |

CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

RECEIVER NUMBER 2 COORDINATES - R 1.3302E+02 PHI 0.0000E+00 Z 1.2361E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL W/BU | 1.7659 2.1235 | 0.01 -10.00 | 9.7647E+04 | 2.2409E+00 | 3.1320E-01 | 7.0185E-01 | 0.0000E+00 | 0.0000E+00 |
| 1 | 9.0000 | 10.00 - 8.00 | 3.3688E-07 | 1.4166E+00 | 2.9550E-12 | 4.1861E-12 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 2.5412E-06 | 1.4945E+00 | 1.9005E-11 | 2.8402E-11 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 1.9806E-05 | 1.5848E+00 | 1.2626E-10 | 2.0009E-10 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 6.6056E-05 | 1.6904E+00 | 3.5760E-10 | 6.0449E-10 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 2.4380E-04 | 1.8334E+00 | 1.1269E-09 | 2.0660E-09 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 6.6669E+04 | 1.9830E+00 | 2.6399E-01 | 5.2348E-01 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 5.9218E-02 | 2.1278E+00 | 2.0540E-07 | 4.3707E-07 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 4.9746E+02 | 2.3004E+00 | 1.5019E-03 | 3.4550E-03 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 4.5872E+03 | 2.5111E+00 | 1.2053E-02 | 3.0267E-02 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 1.1010E+03 | 2.8829E+00 | 2.4279E-03 | 6.9993E-03 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 3.7845E+03 | 3.3573E+00 | 6.9353E-03 | 2.3284E-02 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 7.5121E+03 | 3.8949E+00 | 1.1439E-02 | 4.4555E-02 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 1.1596E+04 | 4.6618E+00 | 1.3596E-02 | 6.3382E-02 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 2.6842E+02 | 5.2001E+00 | 2.3512E-04 | 1.2226E-03 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 1.6208E+03 | 5.0856E+00 | 1.0221E-03 | 5.1980E-03 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 1.0085E+01 | 3.6614E+00 | 3.8663E-06 | 1.4156E-05 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 5.4683E-04 | 1.9309E+00 | 1.4596E-10 | 2.8184E-10 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 1.6269E-25 | 1.0917E+00 | 1.5208E-31 | 1.6603E-31 | 0.0000E+00 | 0.0000E+00 |

Figure S5.4.6 (continued)

CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

RECEIVER NUMBER 3 COORDINATES - R 2.3302E+02 PHI 0.0000E+00 Z 1.2361E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL | 1.7324 | 0.01 -10.00 | 3.9888E+04 | 2.1949E+00 | 1.2643E-01 | 2.7751E-01 | 0.0000E+00 | 0.0000E+00 |
| W/BU | 2.0930 | | | | | | | |
| 1 | 9.0000 | 10.00 - 8.00 | 1.3336E-07 | 1.3974E+00 | 1.1698E-12 | 1.6346E-12 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 1.0057E-06 | 1.4714E+00 | 7.5213E-12 | 1.1067E-11 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 7.8427E-06 | 1.5572E+00 | 4.9996E-11 | 7.7856E-11 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 2.6211E-05 | 1.6573E+00 | 1.4190E-10 | 2.3517E-10 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 9.7095E-05 | 1.7931E+00 | 4.4878E-10 | 8.0470E-10 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 2.6685E+04 | 1.9347E+00 | 1.0566E-01 | 2.0442E-01 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 2.3830E-02 | 2.0715E+00 | 8.2657E-08 | 1.7123E-07 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 2.0149E+02 | 2.2345E+00 | 6.0832E-04 | 1.3593E-03 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 1.8722E+03 | 2.4337E+00 | 4.9194E-03 | 1.1972E-02 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 4.5469E+02 | 2.7861E+00 | 1.0026E-03 | 2.7935E-03 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 1.5841E+03 | 3.2367E+00 | 2.9030E-03 | 9.3961E-03 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 3.1909E+03 | 3.7497E+00 | 4.8590E-03 | 1.8220E-02 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 5.0331E+03 | 4.4895E+00 | 5.9011E-03 | 2.6493E-02 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 1.1954E+02 | 5.0309E+00 | 1.0471E-04 | 5.2677E-04 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 7.4229E+02 | 4.9507E+00 | 4.6809E-04 | 2.3174E-03 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 4.9036E+00 | 3.6121E+00 | 1.8799E-06 | 6.7905E-06 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 3.0559E-04 | 1.9295E+00 | 8.1571E-11 | 1.5739E-10 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 6.0101E-26 | 1.0917E+00 | 5.6180E-32 | 6.1334E-32 | 0.0000E+00 | 0.0000E+00 |

CEUSP CANISTER, NO. 4 SCH. 40, .5" BARREL

RECEIVER NUMBER 4 COORDINATES - R 4.3302E+02 PHI 0.0000E+00 Z 1.2361E+02

| GRP NO | MEAN ENERGY MEV | ENERGY GROUP LIMITS MEV | DIRECT BEAM FLUX | MEAN BUILDUP FACTORS | DOSE RATE DIRECT BEAM | DOSE RATE WITH BUILDUP | HEATING RATES IN IRON DIRECT BEAM | HEATING RATES IN IRON WITH BUILDUP |
|---|---|---|---|---|---|---|---|---|
| TOTAL | 1.7187 | 0.01 -10.00 | 1.2711E+04 | 2.1749E+00 | 4.0070E-02 | 8.7149E-02 | 0.0000E+00 | 0.0000E+00 |
| W/BU | 2.0792 | | | | | | | |
| 1 | 9.0000 | 10.00 - 8.00 | 4.1894E-08 | 1.3896E+00 | 3.6748E-13 | 5.1064E-13 | 0.0000E+00 | 0.0000E+00 |
| 2 | 7.2500 | 8.00 - 6.50 | 3.1594E-07 | 1.4620E+00 | 2.3627E-12 | 3.4543E-12 | 0.0000E+00 | 0.0000E+00 |
| 3 | 5.7500 | 6.50 - 5.00 | 2.4644E-06 | 1.5460E+00 | 1.5710E-11 | 2.4288E-11 | 0.0000E+00 | 0.0000E+00 |
| 4 | 4.5000 | 5.00 - 4.00 | 8.2443E-06 | 1.6437E+00 | 4.4632E-11 | 7.3362E-11 | 0.0000E+00 | 0.0000E+00 |
| 5 | 3.5000 | 4.00 - 3.00 | 3.0588E-05 | 1.7764E+00 | 1.4138E-10 | 2.5115E-10 | 0.0000E+00 | 0.0000E+00 |
| 6 | 2.7500 | 3.00 - 2.50 | 8.4247E+03 | 1.9145E+00 | 3.3359E-02 | 6.3866E-02 | 0.0000E+00 | 0.0000E+00 |
| 7 | 2.2500 | 2.50 - 2.00 | 7.5409E-03 | 2.0478E+00 | 2.6156E-08 | 5.3564E-08 | 0.0000E+00 | 0.0000E+00 |
| 8 | 1.8300 | 2.00 - 1.66 | 6.3939E+01 | 2.2065E+00 | 1.9304E-04 | 4.2594E-04 | 0.0000E+00 | 0.0000E+00 |
| 9 | 1.4950 | 1.66 - 1.33 | 5.9608E+02 | 2.4004E+00 | 1.5663E-03 | 3.7597E-03 | 0.0000E+00 | 0.0000E+00 |
| 10 | 1.1650 | 1.33 - 1.00 | 1.4551E+02 | 2.7438E+00 | 3.2086E-04 | 8.8038E-04 | 0.0000E+00 | 0.0000E+00 |
| 11 | 0.9000 | 1.00 - 0.80 | 5.0995E+02 | 3.1827E+00 | 9.3452E-04 | 2.9743E-03 | 0.0000E+00 | 0.0000E+00 |
| 12 | 0.7000 | 0.80 - 0.60 | 1.0339E+03 | 3.6830E+00 | 1.5744E-03 | 5.7984E-03 | 0.0000E+00 | 0.0000E+00 |
| 13 | 0.5000 | 0.60 - 0.40 | 1.6463E+03 | 4.4069E+00 | 1.9303E-03 | 8.5064E-03 | 0.0000E+00 | 0.0000E+00 |
| 14 | 0.3500 | 0.40 - 0.30 | 3.9549E+01 | 4.9429E+00 | 3.4642E-05 | 1.7123E-04 | 0.0000E+00 | 0.0000E+00 |
| 15 | 0.2500 | 0.30 - 0.20 | 2.4901E+02 | 4.8706E+00 | 1.5703E-04 | 7.6482E-04 | 0.0000E+00 | 0.0000E+00 |
| 16 | 0.1500 | 0.20 - 0.10 | 1.7114E+00 | 3.5724E+00 | 6.5611E-07 | 2.3439E-06 | 0.0000E+00 | 0.0000E+00 |
| 17 | 0.0750 | 0.10 - 0.05 | 1.3069E-04 | 1.9241E+00 | 3.4885E-11 | 6.7121E-11 | 0.0000E+00 | 0.0000E+00 |
| 18 | 0.0300 | 0.05 - 0.01 | 1.8377E-26 | 1.0917E+00 | 1.7178E-32 | 1.8754E-32 | 0.0000E+00 | 0.0000E+00 |

Figure S5.4.6 (continued)

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Computational Physics and Engineering 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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## ACKNOWLEDGMENTS

HTAS1 was originally developed by W. D. Turner, with extensive modifications by C. K. Cobb, M. W. Wendel, and the present author.

## 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.

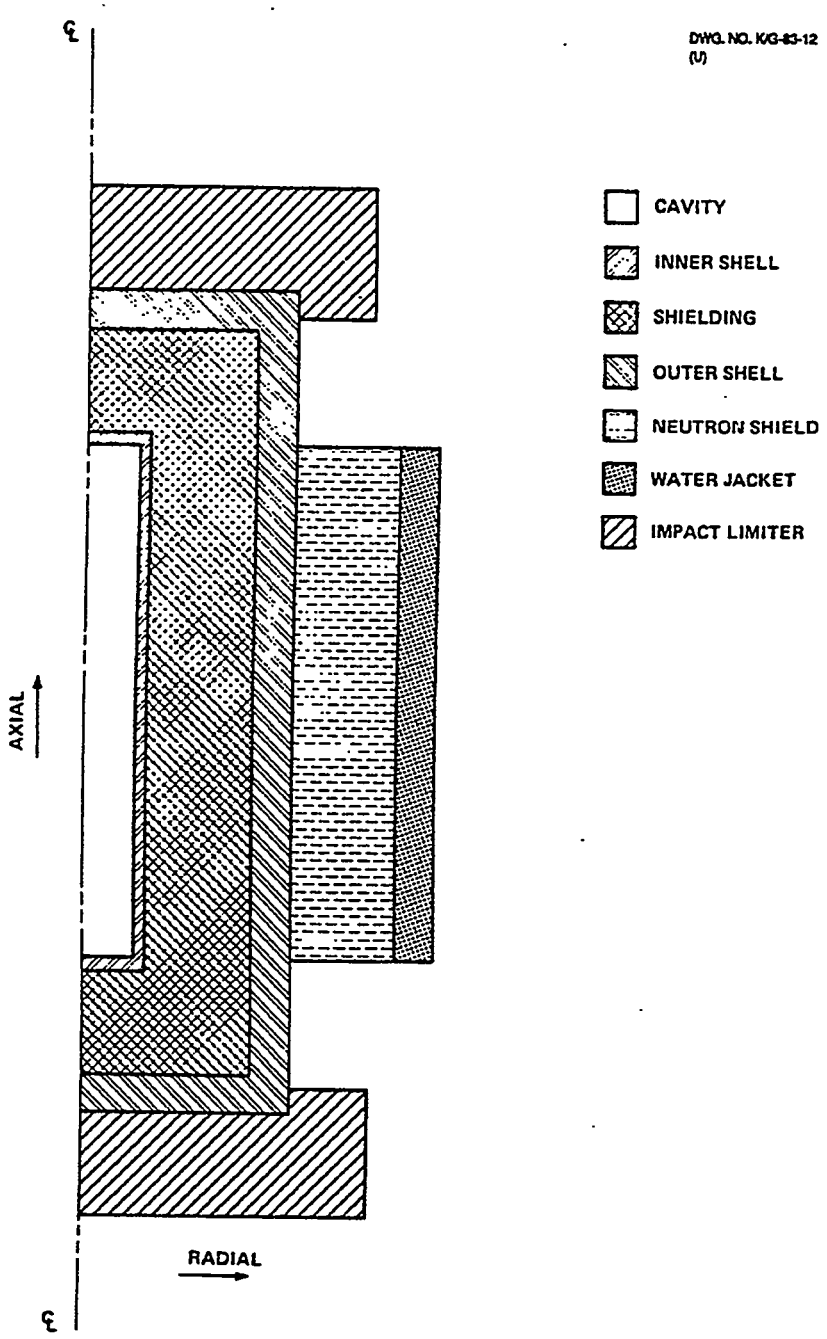



Figure H1.1.1 Zone configuration in HTAS1 general model

## 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.

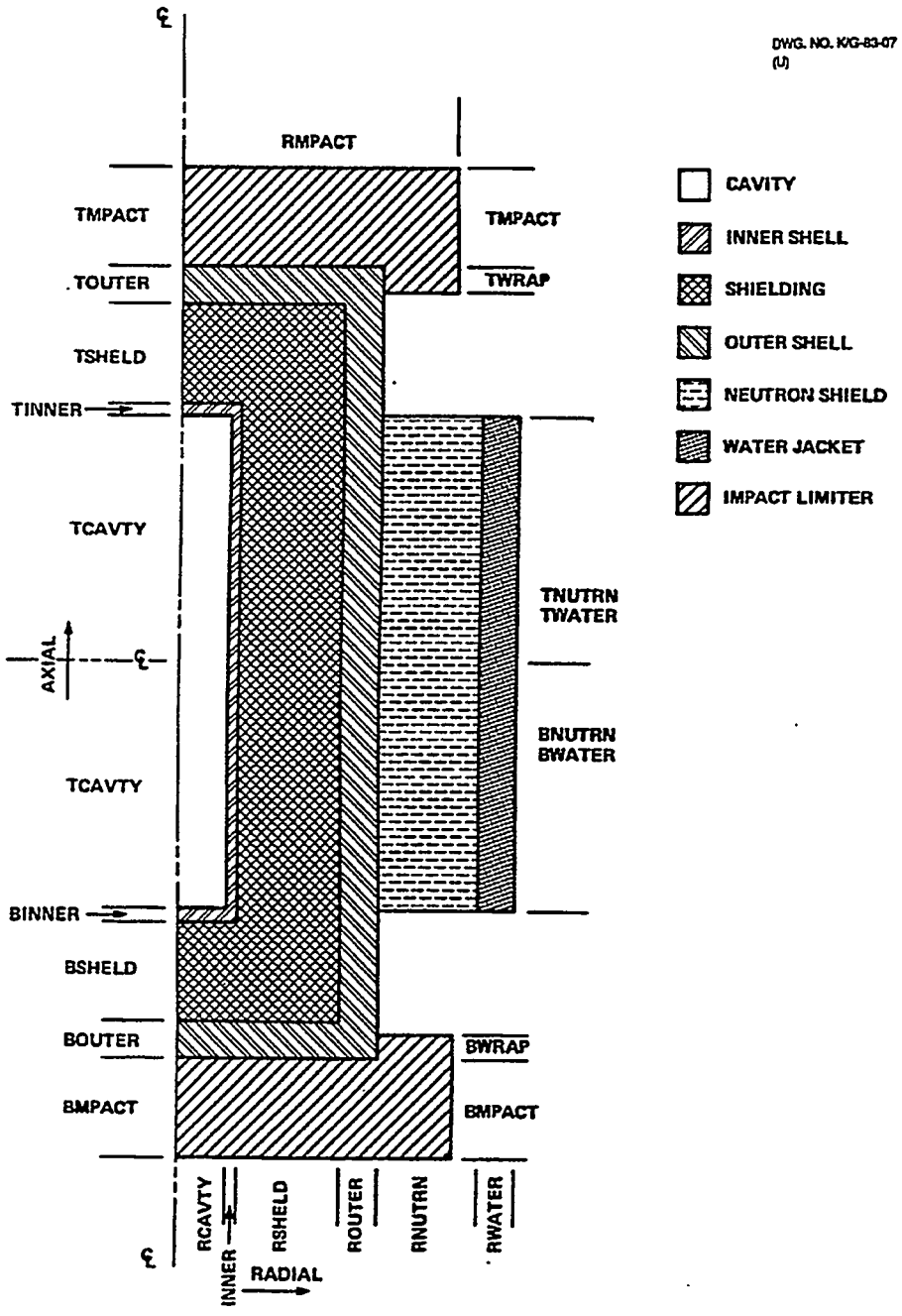



Figure H1.2.1 Zone configuration in HTAS1 general model with physical dimensional labels

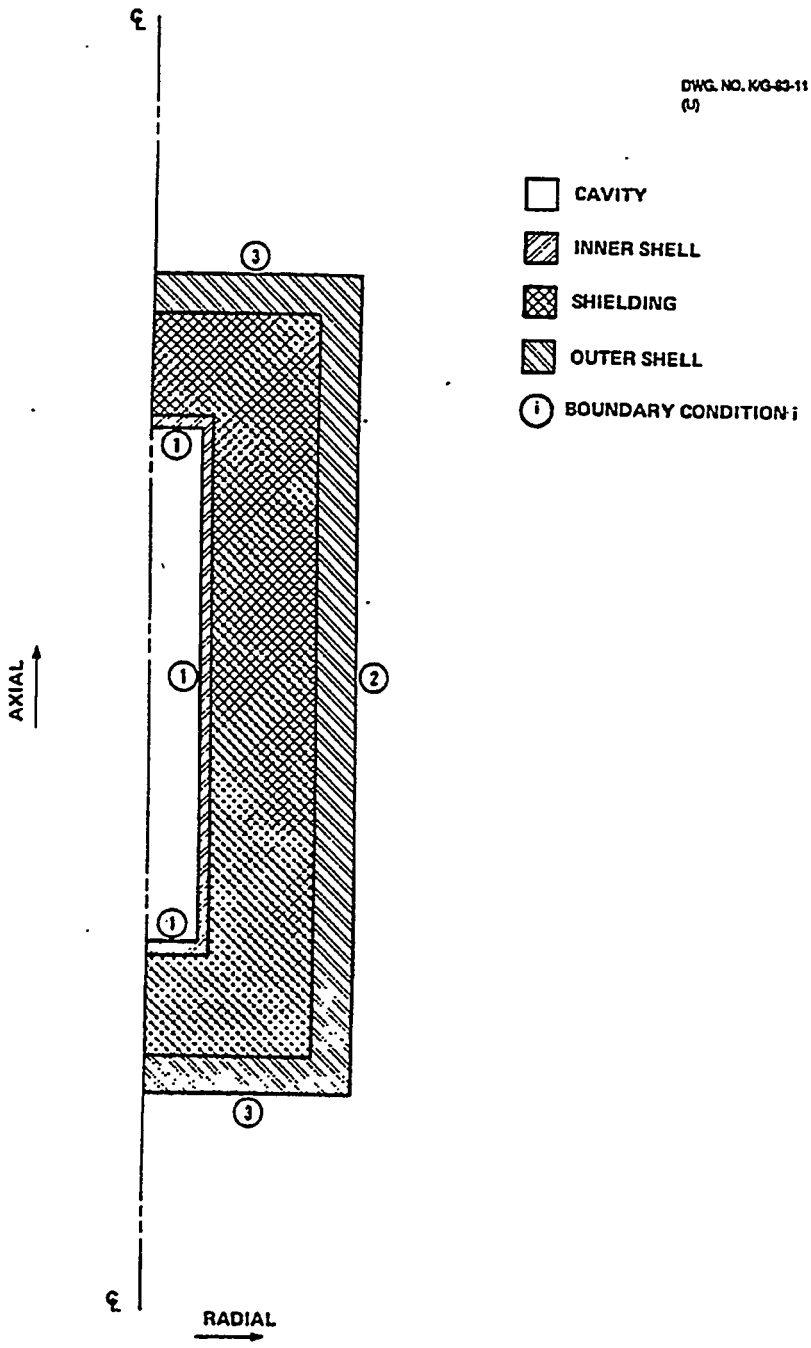



Figure H1.2.2 Location of boundary conditions in HTAS1 basic model (cavity, inner shell, shielding, outer shell)

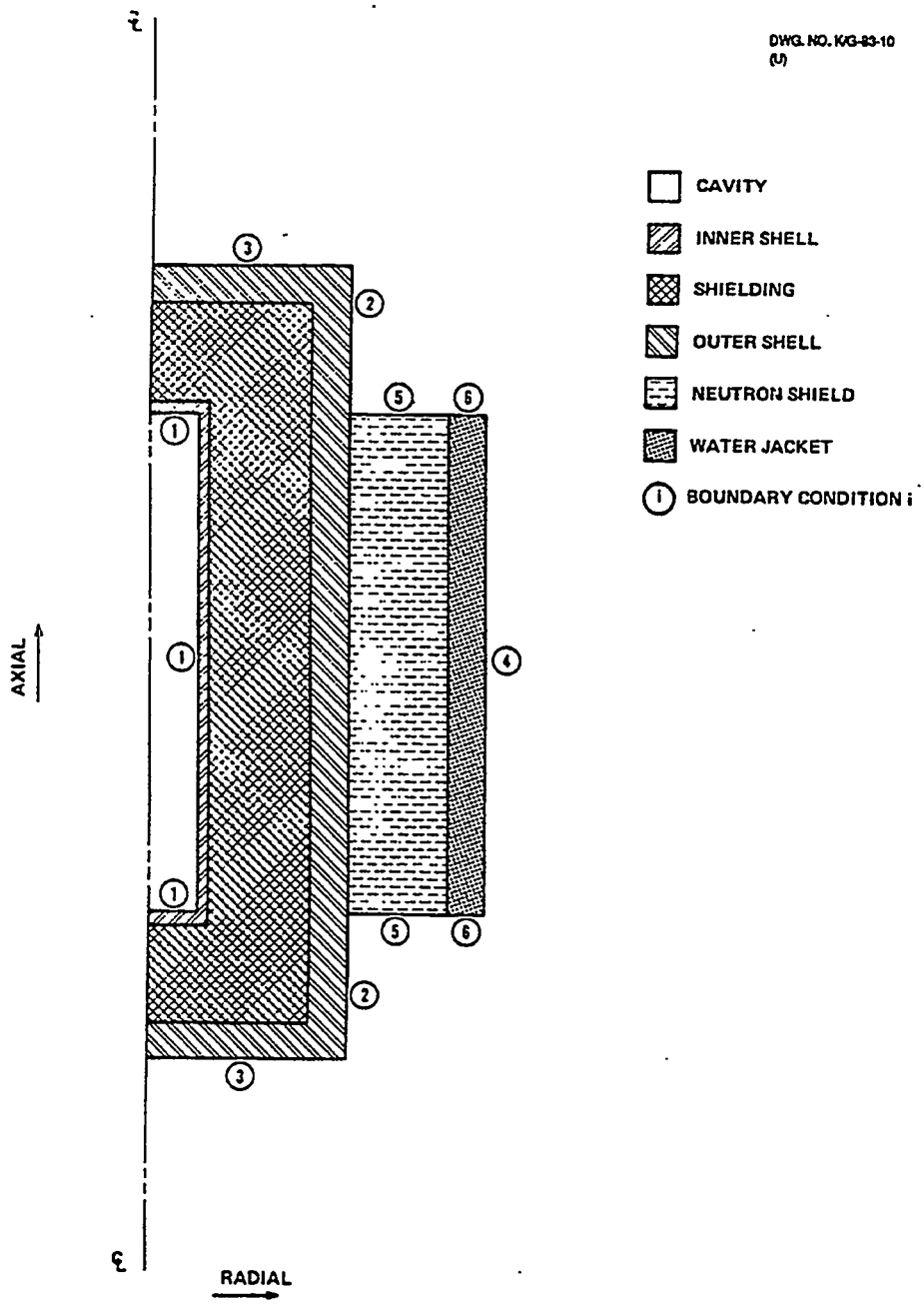



Figure H1.2.3 Location of boundary conditions in HTAS1 basic model with addition of neutron shield and water jacket

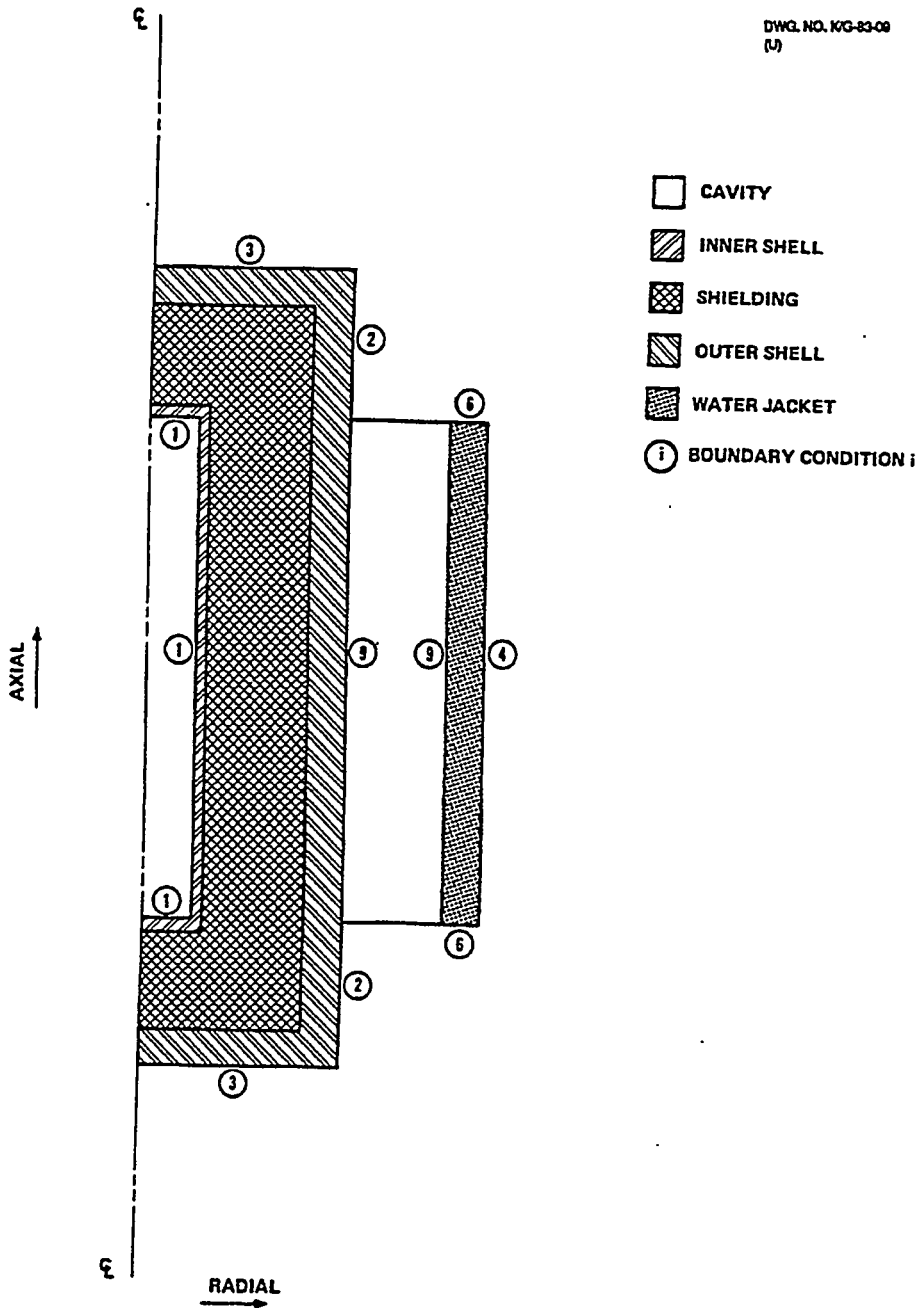



Figure H1.2.4 Location of boundary conditions in HTAS1 basic model with addition of neutron shield and water jacket after neutron shield has been deleted

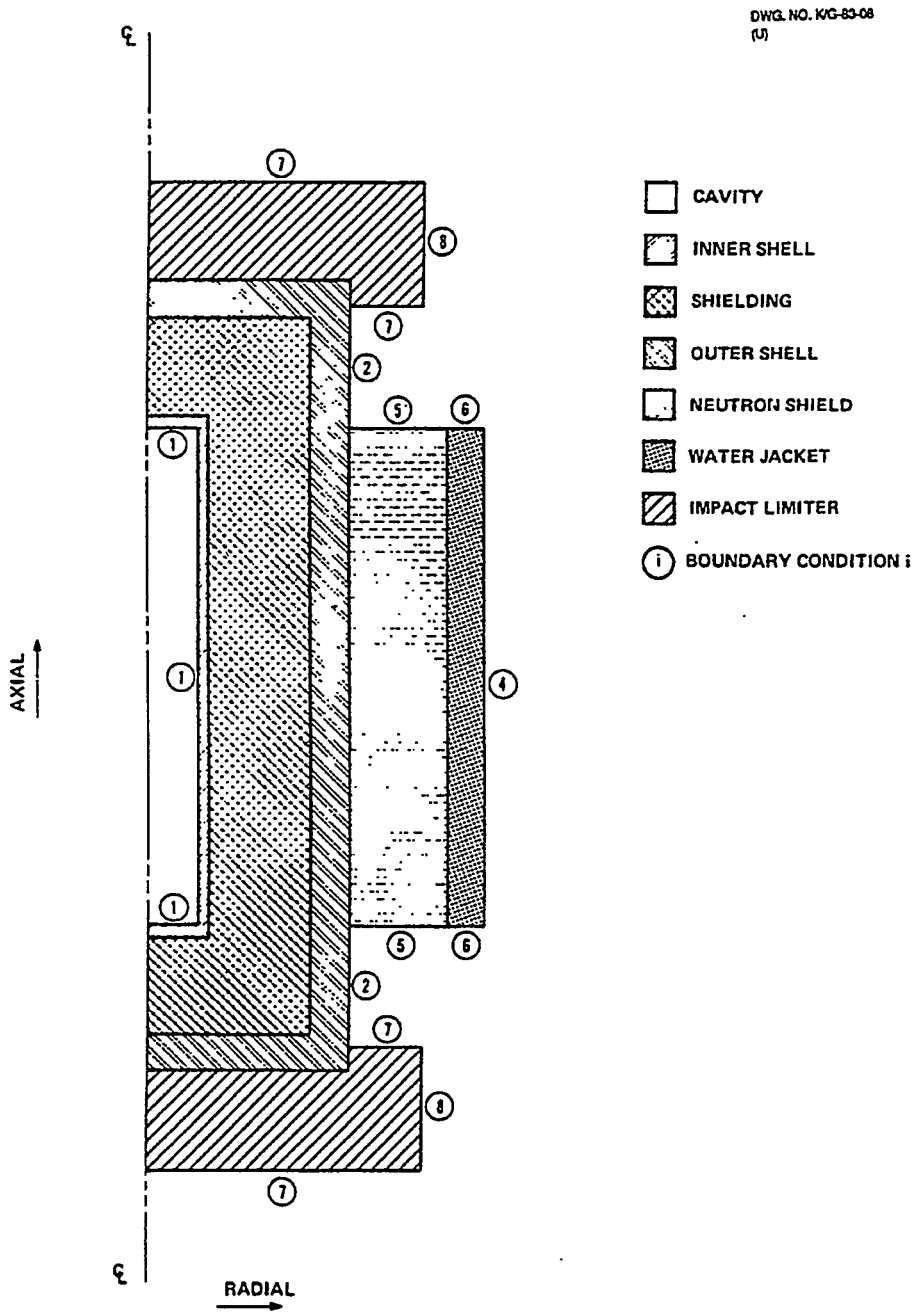



Figure H1.2.5 Location of boundary conditions in HTAS1 general model

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),

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 2 | BALSA[d] | | 0.0484 | 20.0 | | 0.55 | | | |
| 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.

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.

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

$$h_c = h_n \, |T_s - T_a|^{h_e}, \qquad \text{(H1.2.3)}$$

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)

$$h_r = \sigma \epsilon_s \,, \qquad \text{(H1.2.4)}$$

where

$\sigma$ is the Stefan-Boltzmann constant or $0.173 \times 10^{-8}$ Btu/(hr-ft$^2$-°R$^4$),

$\epsilon_s$ 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

$\epsilon_f$ 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 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 $\eta_f$ 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 $\eta$. 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,

$\psi$ = 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).

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

$$\psi = \frac{\tanh(\ell m)}{\ell m} \qquad m = \sqrt{\frac{h}{k\delta_B}}$$

$$R_{Sf} = (\ell + \delta_B)/\frac{S_1}{2}$$

h = convective heat transfer coefficient

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

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

$\mu_0 = 2\kappa\left[b_c + \delta_t(1 - \tan\gamma)/\tan\gamma\right]^{\frac{1}{2}}$

Table H1.2.4 (continued)

| Fin type | Description |
|---|---|

$$\mu_e = 2\kappa\left[\frac{\delta_t(1 - \tan\gamma)}{\tan\gamma}\right]$$

$$\kappa = \sqrt{\frac{h}{k\sin\gamma}}$$

$$\gamma = \tan^{-1}\left((\delta_B - \delta_t)/\ell\right)$$

$$b_c = \ell + \delta_t$$

$$R_{Sf} = (2\delta_t + 2\sqrt{\ell^2 + (\delta_B - \delta_t)^2})/S_1$$

$$R_{SW} = (S_1 - 2\delta_B)/S_1$$

$$R_{VA} = \ell\,(\delta_t + \delta_B)/S_1$$

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

$\psi = \psi$ *for FIN No.* 5

$$R_{Sf} = \pi\delta_B(2\ell + \delta_B)/(S_1S_2)$$

$$R_{SW} = (S_1S_2 - \pi\delta_b^2)/(S_1S_2)$$

$$R_{VA} = (\pi\delta_B^2\ell)/(S_1S_2)$$

Table H1.2.4 (continued)

| Fin type | Description |
|---|---|

7 SPINE, RECTANGULAR CROSS SECTION - TRIANGULAR PATTERN

$$\psi = \frac{1}{m\ell}\tanh(m\ell) \qquad m = \sqrt{\frac{hP}{kA}}$$

$$R_{SW} = (S_1S_2 - 2\delta_B\delta_t)/(S_1S_2) \qquad A = 4(\delta_B\delta_t) = \textit{cross-sectional area}$$

$$R_{VA} = (2\delta_B\delta_t\ell)/(S_1S_2)$$

$$R_{Sf} = 2[\ell(\delta_B + \delta_t) + \delta_B\delta_t]/(S_1S_2) \qquad P = 4(\delta_B + \delta_t) = \textit{perimeter}$$

8 SPINE, RECTANGULAR CROSS SECTION - RECTANGULAR PATTERN

$\psi = \psi$ *for FIN No. 7*

$$R_{Sf} = 4[\ell(\delta_B + \delta_t) + \delta_B\delta_t]/(S_1S_2)$$

$$R_{SW} = (S_1S_2 - 4\delta_B\delta_t)/(S_1S_2)$$

$$R_{VA} = (4\delta_B\delta_t\ell)/(S_1S_2)$$

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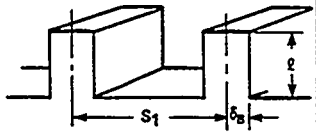
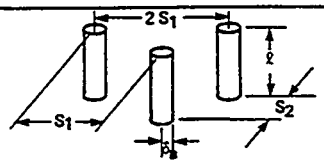
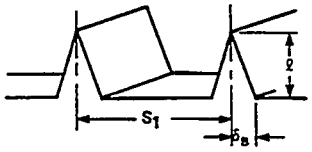
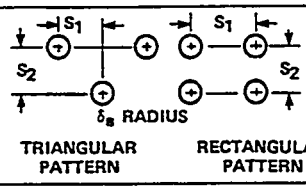
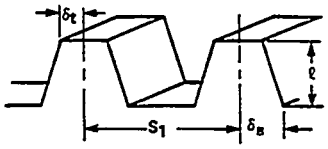
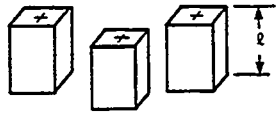
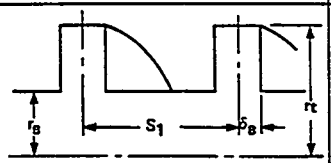
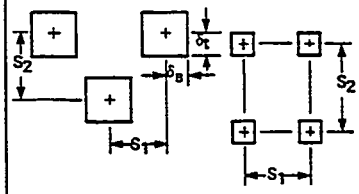
| FIN TYPE NO. | DESCRIPTION | FIGURE | FIN TYPE NO. | DESCRIPTION | FIGURE |
|---|---|---|---|---|---|
| 1 | STRAIGHT (LONGITUDINAL) RECTANGULAR CROSS SECTION |  | 7 | SPINE RIGHT CIRCULAR CYLINDER TRIANGULAR PATTERN |  |
| 2 | STRAIGHT (LONGITUDINAL) TRIANGULAR CROSS SECTION |  | 8 | SPINE RIGHT CIRCULAR CYLINDER RECTANGULAR PATTERN |  TRIANGULAR PATTERN RECTANGULAR PATTERN |
| 3 | STRAIGHT (LONGITUDINAL) TRAPEZOIDAL CROSS SECTION |  | 9 | SPINE RECTANGULAR CROSS SECTION TRIANGULAR PATTERN |  |
| 5 | CIRCULAR (ANNULAR) RECTANGULAR CROSS SECTION EXTERNAL FIN |  | 10 | SPINE RECTANGULAR CROSS SECTION RECTANGULAR PATTERN |  TRIANGULAR PATTERN RECTANGULAR PATTERN |

Figure H1.2.6 Fin effectiveness models, pictorial

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

$\eta$ = 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

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 |

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 be modified in a similar manner in the input data for the restart run. Since HTAS1 does not allow radiative heat 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 | $\frac{lb}{ft^3}$ | $\frac{lb}{in.}$ |
| 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, 1.733E-4, or .0001733 are the same as $1.733 \times 10^{-4}$; 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, if the input variable is an integer, 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 data for temperature profile plots. A REGP data block may be entered to generate summary region data. Each

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 |

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 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 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 50, 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 cylindrical shell. The inner shell encloses the central cavity. The water jacket may enclose an empty cylindrical shell (the neutron shield). All other shells are full and immediately adjacent to full shells. The shells 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$^n$), 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 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 $1.0 \times 10^{-5}$.

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 or conjugate gradient 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 must be chosen by setting the first entry to 1 for the SOR, 2 for the direct, or 3 for the conjugate gradient techniques. There is no default for this entry.

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 a default of 500 for the SOR technique and 20 for the direct and conjugate gradient techniques. 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 $\epsilon$ in Eq. (F10.2.14), which defines the steady-state convergence criterion. For the direct-solution and conjugate gradient techniques, 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 $\beta$ [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 $\beta$ is 1.9. This entry is not used for the direct-solution or conjugate gradient 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. 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 $1.0 \times 10^{-5}$.

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 or conjugate gradient 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 $\epsilon_1$ 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 $\epsilon_2$ 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 $\theta$ 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 [$\omega$ 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 $N_\omega$ 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 $I_\omega$ 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 $J_\omega$ 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 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 $1.0 \times 10^{-5}$.

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 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 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 HTAS1 input

TITLE
Job Title – up to 56 alphanumeric characters

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| MXCPU<br>Maximum number of CPU seconds allowed. | ITPIN<br>Unit number from which initial temperature distribution is to be read. | | | | | | | | | | Required |
| PRINTOUT TIMES | | --<br>At least two blanks. | First printout time. | Second printout time. | ... | Last printout time | | | | | Optional |
| CAVITY | | --<br>At least two blanks. | RCAVTY<br>Radius of the cavity in inches. | NRCAVT<br>Radial increments in the cavity. | TCAVTY<br>Distance from the midplane to the top of the cavity in inches. | NTCAVT<br>Axial increments between the midplane and the top of the cavity. | HEAT<br>Total heat load in the cavity in BTU/hr. | | | | Required |
| INNER SHELL | | --<br>At least two blanks. | RINNER<br>Radial thickness of the inner shell in inches. | NRINNE<br>Radial increments across the thickness of the inner shell. | TINNER<br>Axial thickness of the top of the inner shell in inches. | NTINNE<br>Axial increments across the inner shell top thickness. | BINNER<br>Axial thickness of the bottom of the inner shell in inches. | NBINNE<br>Axial increments across the inner shell bottom thickness. | | | Required |
| MATERIAL | | --<br>At least two blanks. | MZONE<br>Material index. | | | | | | | | Optional |
| ZONENM<br>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 Fin type for outer radial surface. | IFINZ 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 | --<br>At least two blanks. | RNUTRN<br>Radial thickness of neutron shield in inches. | NRNUTR<br>Radial increments across the neutron shield thickness. | TNUTRN<br>Axial distance from the midplane to the top of the neutron shield in inches. | BNUTRN<br>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 | --<br>At least two blanks. | ADELET<br>Neutron shield removal time keyword. | MZONE<br>Material index. | EMISIV(1)<br>Emissivity of the portion of the outer shell formerly covered. | EMISIV(2)<br>Emissivity of the portion of the water jacket formerly covered. | | | | | Optional |
| WATER JACKET | --<br>At least two blanks. | RWATER<br>Radial thickness of the water jacket in inches. | NRWATE<br>Radial increments across the water jacket thickness. | TWATER<br>Axial distance from the midplane to the top of the water jacket in inches. | BWATER<br>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 | --<br>At least two blanks. | ADELET<br>Water jacket removal time keyword. | | | | | | | | Optional |
| IMPACT LIMITER | --<br>At least two blanks. | RMPACT<br>Radius of both top and bottom impact limiters in inches. | NRMPAC<br>Additional radial increments needed to discretize the impact limiters. | TMPACT<br>Axial thickness of the top impact limiter in inches. | NTMPAC<br>Axial increments across the top impact limiter. | BMPACT<br>Axial thickness of the bottom impact limiter in inches. | NBMPAC<br>Axial increments across the bottom impact limiter. | TWRAP<br>Axial thickness of top impact limiter that wraps around the outer shell in inches. | BWRAP<br>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 | --<br>At least two blanks. | ADELET<br>Impact limiter removal time keyword. | ADELIM<br>Top, bottom or both. | | | | | | | Optional |
| INITIAL | --<br>At least two blanks. | DBDTP<br>Ambient temperature in °F. | DCONCR<br>Natural convection coefficient for radial surfaces. | DCONER<br>Natural convection exponent for radial surfaces. | DCONCA<br>Natural convection coefficient for axial surfaces. | DCONEA<br>Natural convection exponent for axial surface. | DFLUX<br>Solar heat load in BTU/hr-ft$^2$. | | | Optional |

Table H1.4.3 (continued)

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| NSSTYP<br>Steady-state technique flag<br>1 - SOR<br>2 - Direct<br>3 - CG | MAXIT<br>Maximum number of iterations for steady-state solution. | EPS<br>Steady-state convergence criterion. | BETA<br>Steady-state over-relaxation factor. | TDP<br>Number of iterations between property re-evaluation. | | | | | | | Optional |
| PREFIRE | | At least two blanks. | DBDTP<br>Ambient temperature in °F. | DCONCR<br>Natural convection coefficient radial surfaces. | DCONER<br>Natural convection exponent for radial surfaces. | DCONCA<br>Natural convection coefficient for axial surfaces. | DCONEA<br>Natural convection exponent for axial surfaces. | DFLUX<br>Solar heat load in BTU/hr-ft$^2$. | | | Optional |
| Can insert solution technique SS card as shown after the INITIAL block. | | | | | | | | | | | Optional |
| FIRE | | At least two blanks | DTIMEF<br>Duration of the fire transient in minutes. | DEMISF<br>Emissivity of the fire. | DBDTP<br>Temperature of the fire in °F. | DCONCR<br>Natural convection coefficient for radial surfaces. | DCONER<br>Natural convection exponent for radial surfaces. | DCONCA<br>Natural convection coefficient for axial surfaces. | DCONEA<br>Natural convection exponent for axial surfaces. | DFLUX<br>Solar heat load in BTU/hr-ft$^2$. | Optional |
| IMPLICIT | | | | | | | | | | | |
| RESDUL<br>Convergence criterion per time step. | NITREZ<br>Iterations between convergence tests. | ABSDIF<br>Convergence criterion per time step with temperature dependence. | THETA<br>Implicitness factor. | BETAT<br>Acceleration parameter. | NUPBTA<br>Iterations between attempts to optimize BETAT. | ITLRCO<br>Iterations between updates using Carre's technique. | ITLRCI<br>Change in number-of-iteration criterion. | | | | Optional |

Table H1.4.3 (continued)

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| DELTAT<br>Initial time step in minutes. | TSFACT<br>Time-step multiplication factor. | TSMAX<br>Maximum allowable time step in minutes. | TSCHGE<br>Not used. | TPCGMX<br>Maximum temperature change allowed at a node per time step in °F. | PDPCGM<br>Maximum percent of relative change in temperature allowed per time step. | TSMIN<br>Minimum time step allowed in minutes. | | | | | Optional |
| EXPLICIT | | | | | | | | | | | Optional |
| DELTAT<br>Initial time step in minutes. | KTMFCT<br>Levy factor. | | | | | | | | | | |
| POSTFIRE | | --<br>At least two blanks. | DTIMPF<br>Duration of the postfire transient in minutes. | DBDTP<br>Ambient temperature in °F. | DCONCR<br>Natural convection coefficient for radial surfaces. | DCONER<br>Natural convection exponent for radial surfaces. | DCONCA<br>Natural convection coefficient for axial surfaces. | DCONEA<br>Natural convection exponent for axial surfaces. | DFLUX<br>Solar heat load in BTU/hr-ft$^2$, | | Optional |
| Can insert solution technique description with IMPLICIT or EXPLICIT as shown above. | | | | | | | | | | | Optional |
| FINAL | | --<br>At least two blanks. | DBDTP<br>Ambient temperature in °F. | DCONCR<br>Natural convection coefficient for radial surfaces. | DCONER<br>Natural convection exponent for radial surfaces. | DCONCA<br>Natural convection coefficient for axial surfaces. | DCONEA<br>Natural convection exponent for axial surfaces. | DFLUX<br>Solar heat load in BTU/hr-ft$^2$. | | | Optional |
| Can insert solution technique SS card as shown after the INITIAL block | | | | | | | | | | | Optional |

Table H1.4.3 (continued)

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| PLOT | | --<br>At least two blanks. | MAXZVR<br>= 0, generate maximum temperature vs radial distance plots; = 1, suppress. | IVA<br>=0, generate volume-averaged temperature plots; =1, suppress. | ISEP<br>=0, temperature vs time curves are on same plot; =1 different plots. | IDELT<br>=0, temperature vs time curves are for actual temperature; =1, for temperature changes. | TIMMIN<br>Minimum time for plots in minutes. | TIMMAX<br>Maximum time for plots in minutes. | | | Optional |
| REGP | | | | | | | | | | | Optional |
| ITYPE<br>Type of plot. | XSCALE<br>Horizontal axis scaling factor. | YSCALE<br>Vertical axis scaling factor. | XREG1<br>Minimum r-value in inches. | XREG2<br>Maximum r-value in inches. | YREG1<br>Minimum z-value in inches. | YREG2<br>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
```

Table H1.5.2 (continued)

```
           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
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
```

Table H1.5.2 (continued)

```
     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
     material number                                          17
     material name                                       h20conv
          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
```

Table H1.5.2 (continued)

```
     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
          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
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
```

Table H1.5.2 (continued)

```
     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.
     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.
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
```

Table H1.5.2 (continued)

```
  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
  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
      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
```

Table H1.5.2 (continued)

```
   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
  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
```

Table H1.5.2 (continued)

```
      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
%
```

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11. ABSTRACT *(200 words or less)*

SCALE-a modular code system for Standardized Computer Analyses Licensing Evaluation- has been developed by Oak Ridge National Laboratory at the request of the U.S. Nuclear Regulatory Commission. The SCALE system utilizes well-established computer codes and methods within standard analysis sequences that (1) allow an input format designed for the occasional user and/or novice, (2) automated the data processing and coupling between modules, and (3) provide accurate and reliable results. System development has been directed at problem-dependent cross-section processing and analysis of criticality safety, shielding, heat transfer, and depletion/decay problems. Since the initial release of SCALE in 1980, the code system has been heavily used for evaluation of nuclear fuel facility and package designs. This revision documents Version 4.3 of the system.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

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