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SAVANNAH RIVER LABORATORY

DPST-83-510

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DEVELOPMENT OF A NEW SHIELDING MODEL FOR JB-LINE DOSE RATE CALCULATIONS

1. INTRODUCTION AND SUMMARY

This report describes the shielding model developed for the JB-Line Upgrade project. The product of this effort is a simple-to-use but accurate method of estimating the personnel dose expected for various operating conditions on the line. The current techniques for shielding calculations use transport codes such as ANISN, which, while accurate for geometries which can be accurately approximated as one dimensional slabs, cylinders or spheres, fall short in calculating configurations in which two- or three-dimensional effects (e.g. streaming) play a role in the dose received by workers.

The new technique is a composite model built from separate calculations of the radiation emitted by slab and cylinder sources, the transport of this radiation through parallel slab shields, and the transport of the radiation through empty space. When the pieces of the model are put together, the user can get a three dimensional view of the radiation field in the work area.

*These copies include only the INTRODUCTION AND SUMMARY of DPST-83-510.

The model is built up of four modular parts:

1. Source strength calculation: In this step, the source materials are analyzed to determine the spontaneous particle emission rates for neutrons and gammas.

2. Spatial source calculation: The previously calculated material particle sources are used in a 1D calculation of the source configuration. The resulting particle leakage from the outside of the source is determined and used as a boundary source in subsequent calculations.

3. Void transport to shield: The source emission particles are transported across the essentially empty space from the outside of the source to the inside of the shield.

4. Spatial shield calculations: The particles which reach the inside of the shield are transported through the material shields. The penetration rate of uncollided particles is determined from a 3D exponential attenuation model; this is coupled with a one-dimensional slab adjoint transport calculation of the collided particle penetration rate. (This combination is the core of the model and will be discussed in detail below.)

5. Void transport from shield to detector: The transport of collided particles from the outside of the shield to the desired detection points in the room is calculated.

The model has been validated by calculations of effects of feed composition on current exposure doses in the JB-line precipitator room.[4] Additional sample problems are given in Reference 5.

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2. DESCRIPTION OF NEW MODEL

2.1 Source Strength Calculation

The first step of the shielding problem is the definition of the radiation sources. In our case, the particles that contribute to the total exposure of workers are neutrons and gamma photons. Both arise in the JB-Line primarily from nuclide decay.

2.1.1 Gamma Ray Sources

The primary source of gammas in the processing areas is from decay of the plutonium isotopes and the fission products and daughters still present in the feed material. For the calculation of these sources, the RADSOR module of the SHIELD system[1] is used; RADSOR calculates the gamma emission rate in particles/cc/sec due both to nuclide decay (primarily alpha disintegration) and to spontaneous fission.

2.1.2 Neutron Sources

The primary source of neutrons in the feed mixture is from (α,n) reactions of decay alphas with light materials such as fluorine, oxygen, carbon and nitrogen present in the feed material. To determine the neutron emission rate, this model depends on experimental data for pure materials obtained from the literature,[2] coupled with a simple alpha slowing down model to adjust the data for the presence of other isotopes in the mixtures. (Appendix A describes this model.) The result of the (α,n) model is a neutron emission rate in particles/cc/sec which is added to the spontaneous fission neutron source.

2.2 Source Spatial Calculation

Once the neutron and gamma volumetric production rates have been determined, the next step in the calculation is to determine the particle leakage rate from the source region. This is accomplished by use of a forward discrete ordinate transport calculation of a one dimensional approximation to the source geometry. The SHIELD module SNONE is used for the calculation; this module was modified to save the angular outgoing boundary fluxes.

The use of a 1D source calculation results in a single emission rate from the outside of the source, instead of a more realistic shape which would be expected to drop off at the edges of the source. For most sources, in which the internal particle generation rate is uniform, this is probably not a very severe restriction, as the spatial dependence of the emitted particle rate is usually fairly uniform up to the edge.

2.3 Dose Rate Calculations at Detector Points

The calculation of the dose rates at the user-specified detector points is divided into two components - (1) the contribution from particles that penetrate the shielding without interaction and (2) the contribution from particles that penetrate the shielding despite collisions with shielding material.

2.3.1 Uncollided Particle Dose Contribution

The effect of particles that penetrate the shields without interaction can be calculated using the exact system geometry. For a point source, $S(\vec{\Omega},E)$, of particles of given energy E (in particles emitted per second), in direction $\vec{\Omega}$, the resulting flux contribution a distance R away is simply $S(\vec{\Omega},E)e^{-\mu(\vec{\Omega},E)}/4\pi R^2$ (particles/area/sec) where μ is the number of interaction mean free paths of shield between source and detector.

The dose rate from a finite slab or cylindrical source at a detector location is modelled by dividing the source boundary into a set of point sources and summing the dose rate contributions of the individual points. In this way the dose contribution from uncollided particles, which is often an important proportion of the total dose rate, can be accurately determined without geometric simplification.

2.3.2 Collided Particle Dose Contribution

The determination of the contribution to the dose rate from particles that penetrate the shield system despite undergoing one or more collisions within the shielding constitutes a much more difficult problem. To take account of particle collisions, one must know not only the overall collision probabilities (which was all we needed for the uncollided calculation), but also the individual probabilities for the types of collisions (absorption, scattering, etc.) and the type, energy distribution and angular distribution of any particles that are emitted from the interaction.

Rather than follow the particles directly from source to detector as for the uncollided calculation, the model computes the collided portion by following the particles to the inside edge of the shield, transmitting them through the shield, and then tracing them from the outside of the shield to the detectors. The transmission from the source to the inside shield wall and the transmission from the outside shield wall to the detectors are treated as void transport problems. The source and shield boundaries are divided into area segments which, like the detector positions, are considered points. The void transport is thus reduced to many point-to-point $1/R^2$ particle transport problems.

The calculation of the transport of the particles through the shield is accomplished with a 1-D adjoint discrete ordinates calculation. In the normal forward mode of discrete ordinates, the particles incident on the inside boundary of the shield are used as the source and the emerging dose is determined from integrating the calculated outer boundary flux of the system with the flux-to-dose response function. An alternate, and in this case preferable, method is to use the flux-to-dose response function as an adjoint boundary source on the outside boundary and to calculate the emerging adjoint flux on the inside boundary of the shield. The integration of this adjoint boundary flux with the forward boundary source also determines the emerging dose rate. For a single problem, either of these two methods of calculating the dose can be used; the choice between them for multiple calculations of a single shield is dictated by the following considerations:

a. The forward mode is better when the boundary source is the same for the calculations but the dose response will change (i.e. same source, different detector types).

b. The adjoint mode should be used when a constant dose response is used in the calculations, but the values of the boundary source will change (i.e. same detector type, different sources).

The shielding problems being considered for this model are in the second category. In the 3-D configuration of sources, shields, and detector points in this model, the number of particles incident on the inside edge of the shields will vary by position on the shield. A single adjoint calculation for each shield segment will give us the shield transfer properties, from which we can determine the emerging dose rate as a function of position on the shield given the number of incident particles at that position. One adjoint calculation used in this way can deliver as much information as running a forward calculation on each of the spatial divisions of the shield configuration.

2.4 *Uncollided Transport*

In the composite model we have developed, there are three stages in which uncollided particle transport is used. The first of these is the uncollided flux calculation in which the particles leaving the source region are transported to the detector positions, subject to material and distance attenuation. The other two occur as void transport steps of the collided flux calculation in which the source particles are transported to the inner shield wall and then the particles penetrating the shields are transported to the detector points.

In all three cases the steps are the same:

(1) The initial point particle source is described as $S_o(\vec{\Omega},E)$ particles/sec/unit solid angle, where E is the particle energy and $\vec{\Omega}$ is the direction from source to target;

(2) The attenuation environment between source and target is described in terms of distance between the points, R, and the number of attenuation mean free paths between the points, $\mu(\vec{\Omega},E)$; and

(3) The flux at the target is then given by

$$\Psi(\vec{\Omega},E)=S_o(\vec{\Omega},E)\frac{e^{-\mu(\vec{\Omega},E)}}{4\pi R^2} \text{ particles/sec/cm}^2 \text{ unit solid angle.}$$

The point source $S_o(\vec{\Omega},E)$ from a given surface element of the source (or outer shield boundary) is obtained from the surface flux by the relationship

$$S_o(\vec{\Omega},E) = \vec{n}\cdot\vec{\Omega}\ \Psi_o(\vec{\Omega},E)\Delta A$$

where $\Psi_o(\vec{\Omega},E)$ = surface flux in particles/cm^2/sec/unit solid angle

ΔA = area in cm^2 of surface element

$\vec{n}$ = outward vector normal to surface element

The $\vec{n}\cdot\vec{\Omega}$ is necessary because the flux is given per unit area perpendicular to direction of flight, $\vec{\Omega}$, whereas the direction $\vec{n}$ is perpendicular to surface area ΔA. The total flux is obtained by summing the target fluxes from all source area segments.

3. SHIELD INPUT AND OUTPUT DESCRIPTION

There are six calculational steps involved in a complete analysis using the new model:

(1) Calculation of the neutron volumetric sources;

(2) Calculation of the gamma volumetric sources;

(3) Generation of macroscopic cross sections for all materials in the problem;

(4) Calculation of particle angular leakage rates from each of angle the source regions;

(5) Calculation of shield penetration characteristics for each shield segment using adjoint transport calculations; and,

(6) Calculation of dose rate profile. This step implements the new model and delivers a three dimensional dose rate profile in the room.

A flow chart of the calculation steps and intermediate records are shown in Figure 1. Some of these steps can be omitted if similar calculations are being run together.

In this section, the JOSHUA input for each of these steps will be discussed. (These descriptions borrow heavily from Reference 1 to avoid excessive cross-reference.)

3.1. General Considerations on Execution of a SHIELD Job

The model developed for this project has been implemented in the SHIELD system of codes.[1] This subsection will describe the conventions used to execute a problem with the SHIELD system. Detailed input for the various calculations will be described in later subsections; the emphasis here will be the overall organization of the input and selected output from each calculational step.

3.1.1 Problem Organization

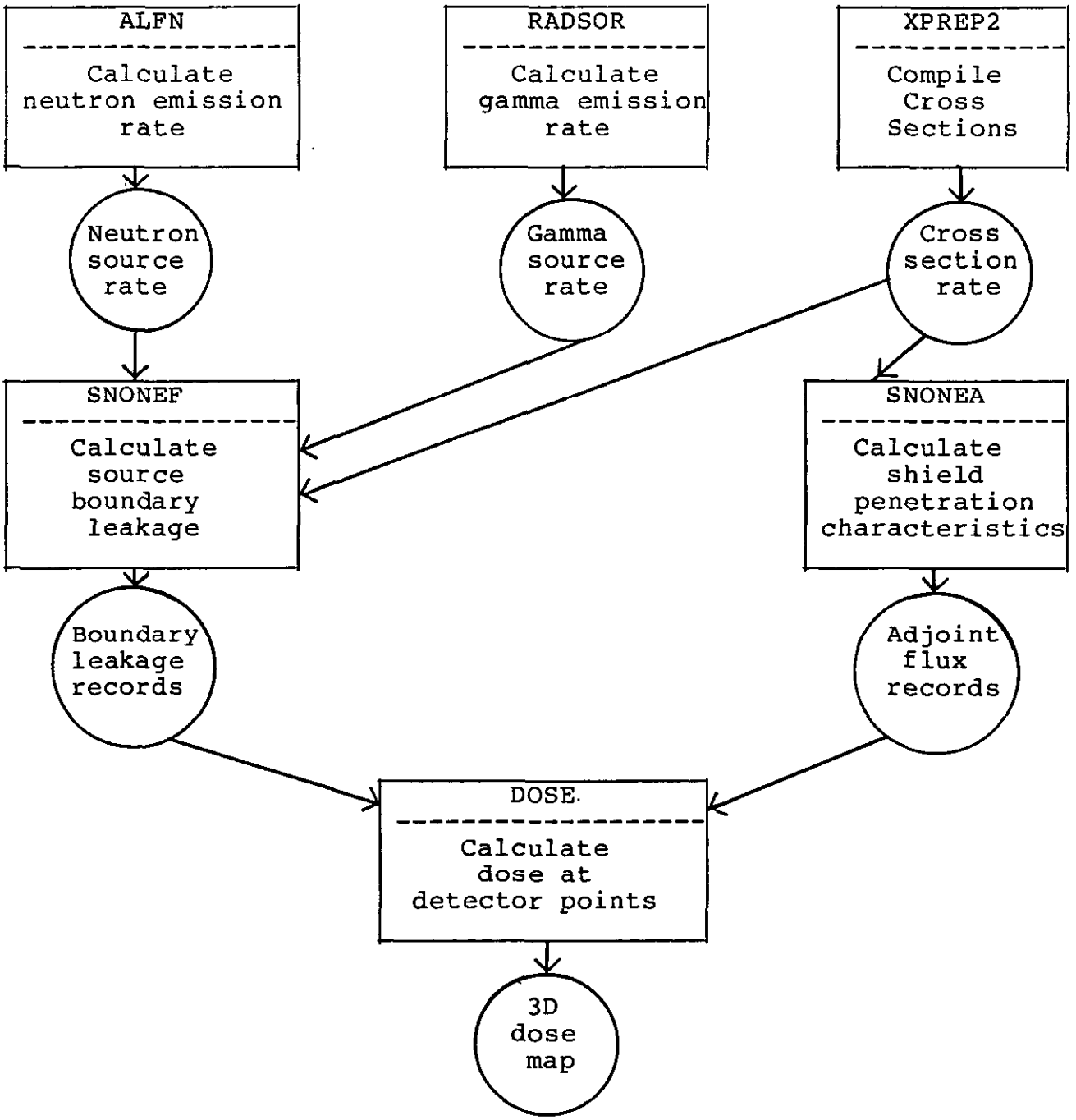
The SHIELD system uses a hierarchal naming convention to enable the user to break his problem into a series of calculational steps with full identification of input and output for each step. The naming conventions used in the SHIELD system are the following:

A. The user assigns a Problem Name to his problem. This Problem Name must be a single word of 8 or less alphanumeric characters. In all of the following discussion the mnemonic PROB will be used to identify this problem name. All input for any calculation will utilize the name PROB in the JOSHUA records.

B. The user breaks his problem (designated by name PROB) into one or more processes, each of which identifies a specific stage in the calculation. To each process the user assigns a unique Process Name. This Process Name must be a single word of 8 or less alphanumeric characters.

FIGURE 1

FLOW CHART OF CALCULATION STEPS AND INTERMEDIATE RECORDS



of the following discussion the mnemonic PROC will be 8 or less alphanumeric characters used to identify this process name. All input for any calculations associated with each process will utilize the name PROC in the JOSHUA records for that process.

3.1.2 Specification of Calculational Steps

In a given process (mnemonic PROC) in a problem (mnemonic PROB), one or more calculational steps will be required to obtain the desired resuts. These calculations are performed step by step within a process by specifying an eight-character calculation type name (mnemonic CALC) and an eight-character method name (mnemonic METH) for each step. There are several calculation types corresponding to the types of calculations for the typical problems plus editing and logic control calculation types. The calculation types used in the new model are listed in Table 1. The modules which were written or modified for this project are executed using the SPECIAL type.

Each calculation type has one or more calculation methods used to generate the results. These calculation methods are different mathematical algorithms for performing the calculation. One method may be more applicable to a given problem, but in some cases alternative methods will give equally valid results. The recommended calculation methods (mnemonic METH) for each calculation type (mnemonic CALC) used in the new model are also shown in Table 1.

3.1.3 Job Control Input Record

The calculational sequence for a problem is specified to the SHIELD system by an input record of name

SHIELD.INPUT.JOB.$JOB

This record contains two types of input

- Names of standard data sets to be used in the problem
- Specification of each calculational and control step in the problem

$JOB is the job name assigned to this JOSHUA Job.

An example of this record is given in Figure 2 for a typical problem.

TABLE 1

SHIELD CALCULATION TYPES USED

CALC	METH	DESCRIPTION
SOURCE	RADSOR	Photon spontaneous energy-dependent source calculation for a composition of nuclides
XSECTION	XPREP2	Creation of mixture cross sections for S_N transport modules
EDIT	RADSOR XSECTION RADFIELD	Editing the results of these calculations
SPECIAL	SNONEF	Forward S_n calculation of particle leakage from source.
	SNONEA	Adjoint S_n calculation of shield penetration characteristics.
	ALFN	Neutron spontaneous energy-dependent source calculation for a composition. Includes (α,n) and spontaneous fission of plutonium isotopes.
	EXPOSE	Implements new model by determining dose rate in 3D configuration of sources, shields, and dose points.

```
4579.SHIELD.INPUT.JOB.DOSE4579

****   SHIELD COMPUTATION SYSTEM CALCULATION STEPS RECORD   ****

          PROBLEM NAME FOR THIS CALCULATION  :SAMP1

VERSION OF FISSPROD DATA SET TO BE USED IN THIS CALC    :ENDFB4

VERSION OF MULTIGRP DATA SET TO BE USED (NEUTRON DATA) :ANISN58
VERSION OF MULTIGRP DATA SET TO BE USED (PHOTON DATA)  :ANISN58

NEUTRON GROUP STRUCTURE NAME FOR XSECTION CALCULATION  :ANISN58
PHOTON GROUP STRUCTURE NAME FOR XSECTION CALCULATION   :ANISN58

NUMBER OF CALCULATION STEPS TO FOLLOW   (MAX 250)  .   : 13
```

**** SHIELD COMPUTATION SYSTEM CALCULATION STEPS RECORD ****

STEP NO	PROCESS NAME	CALCULATION TYPE	CALCULATION METHOD
1	:SOUR1	:SPECIAL	:ALFN
2	:SOUR1	:SOURCE	:RADSOR
3	:	:EDIT	:
4	:XSEC1	:XSECTION	:XPREP2
5	:FORW1	:SPECIAL	:SNONEF
6	:	:EDIT	:
7	:FORW2	:SPECIAL	:SNONEF
8	:	:EDIT	:
9	:ADJT1	:SPECIAL	:SNONEA
10	:	:EDIT	:
11	:ADJT2	:SPECIAL	:SNONEA
12	:	:EDIT	:
13	:DOSE1	:SPECIAL	:EXPOSE

FIGURE 2

SHIELD.INPUT.JOB.?JOB RECORD

3.1.4 Calculation Step Input Records

Each calculational step in a control sequence has an input record. The name of the input record for any calculation step is always

SHIELD.INPUT.?PROB.?PROC.?NAME

where ?PROB, ?PROC, and ?NAME are the Problem Name, Process Name, and a calculation identifier.

3.1.5 Executing the SHIELD System

The SHIELD system is executed as a standard JOSHUA Job using the following parameters:

Module Name - SHIELD
PDS1 - JOS. GSASSLIB
GOSIZE - 500K (or more if required.)

Sample JCL is shown in Figure 3. Note that the JOB=DOSE4579 tells the code to look in SHIELD.INPUT.JOB.DOSE4579 for the problem parameters.

3.2 Problem Set-Up

The new model is designed for 3-D shielding problems composed of any combination of cylindrical or slab sources, slab shields, and point detector locations. Each cylindrical source can be characterized by a finite height of rings of material around a central core, as illustrated in Figure 4; as shown in the figure a physical source with several height "layers" should be modelled as one source per layer. Each slab source and shield can be characterized by finite height and width "sheets" of material of varying thicknesses, as also shown in Figure 4; again, more complicated slab configurations should be built up from this type of unit. The geometry can be built up from any number of sources and shields in this pattern, and the detector points can be located anywhere outside the sources and shields.

3.3 Calculation of the Neutron Volumetric Sources

The neutron sources from (α,n) and spontaneous fission are calculated using CALC = SPECIAL and METH = ALFN. The main calculational scheme in this step is the (α,n) mixture method described in Appendix A. At the present time the ALFN calculation can handle Pu-238, Pu-239, Pu-240, Pu-241, Pu-242, and Am-241 sources and (α,n) reactions with oxygen, carbon, fluorine, and beryllium mixtures.

```
//SAM14579 JOB (8532-1M,T4579,L034,002,10),
//       'SHIELD ',MSGLEVEL=1,CLASS=0,MSGCLASS=T,NOTIFY=T4579
//SI   EXEC JOSHUA,USER=4579,GTIME=002,BUFNO=10,SSPACE=015,
//     GOSIZE=2000K,JOB=DOSE4579,DISP=NEW,RLSE=NO,MEMBER=SHIELD,
//     SPACE=35,GOUT='SYSOUT=*',
//     PDS1='JOS.GSASSLIB'
//STEPLIB DD DSN=&PDS1,DISP=SHR
//         DD DSN=&PDS2,DISP=SHR
//         DD DISP=SHR,DSN=JOS.PGMS01
//         DD DISP=SHR,DSN=JOS.BATCH
//         DD DISP=SHR,DSN=JOS.SYSTEM3
//GO.JOSIN DD *

DATASET= DOSE4579,4579,STD,DOSE4579

SCRATCH= DOSE4579

/*

//
```

FIGURE 3

SAMPLE JCL FOR NEW MODEL

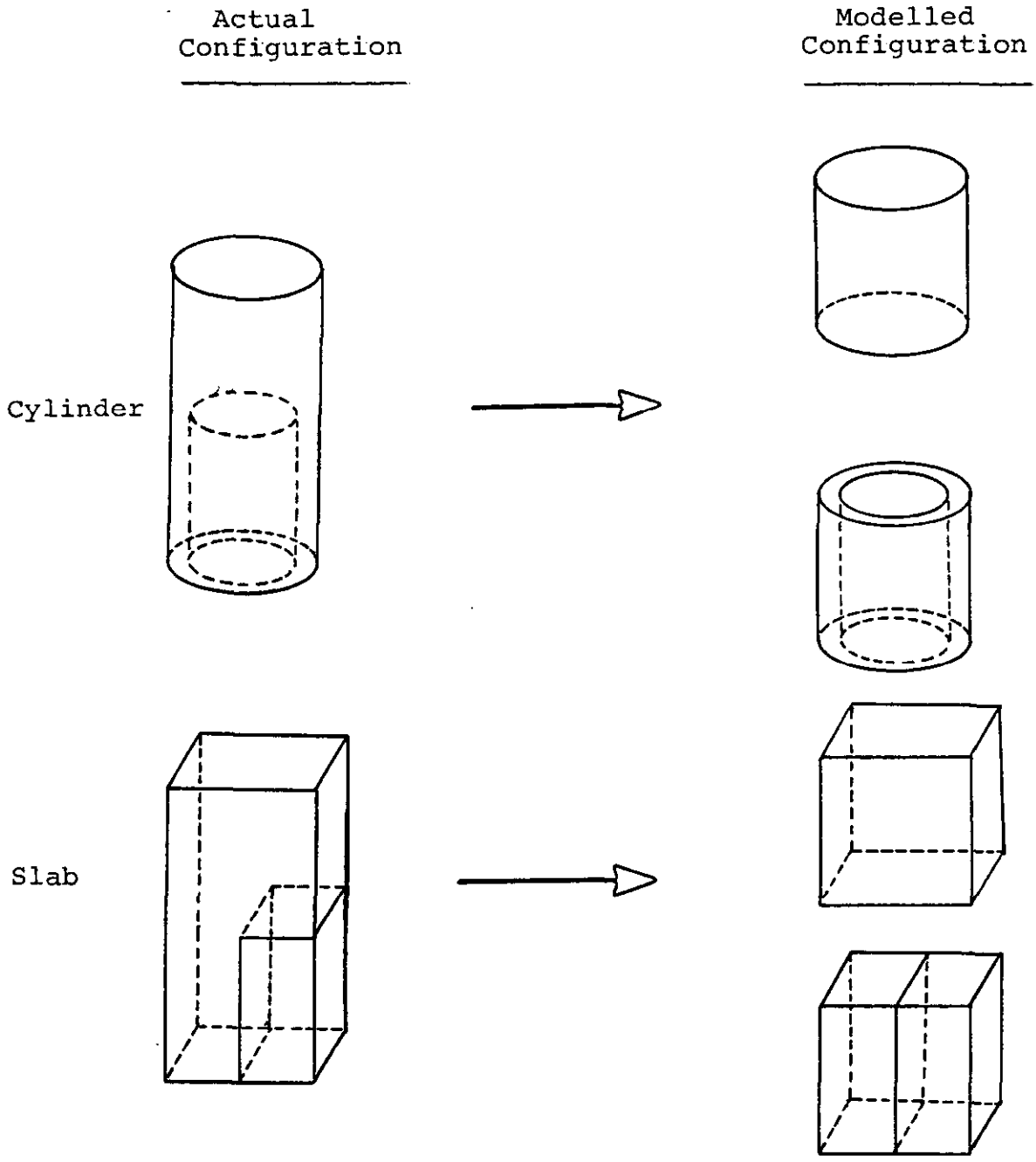


FIGURE 4

GEOMETRIC ARRANGEMENTS - SLAB OR CYLINDRICAL SOURCES, SLAB SHIELDS

The input to the ALFN consists of two records. The first, named

SHIELD.INPUT.?PROB.?PROC.ALFN

(an example is shown in Figure 5), specifies the source materials by name and version number.

For each material and version listed in the above record a material record named

SHIELD.?PROB.?PROC.ATOMDENS.?AMAT.?IMAT

is required where AMAT and IMAT are the material name and version number. The composition of each material version is listed by nuclide IZAS number (i.e., atomic number * 1000 + atomic weight) and density in atoms/barn/cm. An example of this record is shown in Figure 6.

It should be noted that the composition as listed in these records should represent the alpha particle slowing down medium. As an example, in a recent problem the principal neutron source was from (α,n) reaction for a PuF_3 suspension in a nitrate solution. In this problem because the alpha particles emitted by the Pu isotopes would primarily slow down in the PuF_3 suspension, the composition of the medium for the ALFN calculation was represented as a sparse PuF_3 medium; the actual density of Pu nuclides (in atoms/barn/cm) was necessary to accurately determine the number of alphas emitted per cm^3 per second and the density of F was three times the Pu density to properly determine the number of neutrons emitted in (α,n) reactions per alpha particle (see Appendix A). The product of the two is the neutron source per cc per second.

The output from ALFN is a series of

SHIELD.?PROB.?PROC.SOURCE.?AMAT.?IMAT.NEUTRON

records which contain the neutron source by energy group. These records are the neutron equivalent of the gamma SOURCE records produced by the RADSOR module. The printed output of the module gives the above source as well as the total spontaneous fission and (α,n) neutron production rates.

4579.SHIELD.INPUT.SAMP1.SOUR2.ALFN

NUMBER OF MATERIAL DESCRIPTIONS THIS RUN : 2

NUMBER	MATERIAL
1	:SLURRY . : 1
2	:PUF3 . : 1

FIGURE 5

SHIELD.INPUT.?PROB.?PROC.ALFN RECORD

4579.SHIELD.SAMP1.SOUR2.ATOMDENS.SLURRY.1

NO. OF VALUES : 6

	IZAS	DENSITY	UNIT
1	:94238	:10.0269E-09	ATOMS/BARN/CM
2	:94239	:67.2668E-06	ATOMS/BARN/CM
8	:94240	:89.5347E-07	ATOMS/BARN/CM
4	:94241	:82.0145E-08	ATOMS/BARN/CM
5	:94242	:28.6483E-09	ATOMS/BARN/CM
6	: 9019	:21.4862E-05	ATOMS/BARN/CM

FIGURE 6

SHIELD.?PROB.?PROC.ATOMDENS.?AMAT.?IMAT RECORD

3.4 Calculation of the Gamma Volumetric Sources

The gamma source is calculated using the calculation type (CALC) SOURCE and method (METH) RADSOR.

A SOURCE calculation is designed to calculate the gamma source in multigroup form that arises from a homogeneous composition. The calculation is performed by summing over the individual isotopes in a composition using predefined multigroup spontaneous production spectra for each mode of decay.

All input to the SOURCE calculation is given in record

SHIELD.INPUT.?PROB.?PROC.SOURCE

where ?PROB and ?PROC are the Problem Name and Process Name in the current computation step. If an ALFN step is also used in the procedure, the ALFN step must precede the RADSOR step and the ?PROB and the ?PROC names should be the same.

An example of SOURCE calculation input is shown in Figure 7. This record is typical of the SOURCE calculations performed in a computational sequence.

Each line of input in Figure 7 contains names which point to an additional record (input composition record) to define each composition for which a SOURCE calculation is to be performed. The required data on each line is the following:

Process Name => Process name in the input composition record
Composition Name => Composition name in the input composition record
State Number => Integer identifier of different versions of same composition
Time => Time identifier not used in static problems (use 0.00)

Each composition is then defined in a record

SHIELD.INPUT.?PROB.?PROC.COMPOSIT.?COMPS.?NSTS

4579.SHIELD.INPUT.SAMP1.SOUR1.SOURCE

********** SHIELD SOURCE CALCULATION INPUT RECORD **********

NUMBER OF COMPOSITION-TIMES AT WHICH SOURCES ARE REQUIRED

(MAX 250) : 2

********** SHIELD SOURCE CALCULATION INPUT RECORD **********			
PROCESS NAME	COMPOSITION NAME	STATE NO.	TIME (HRS)
:SOUR1	:SLURRY	: 1	: 0.000
:	:PUF3	: 1	: 0.000

FIGURE 7

SHIELD.INPUT.?PROB.?PROC.SOURCE RECORD

shown in Figure 8, where

?PROB => Problem name of this problem
?PROC => Process name of input composition record
?COMPS => Composition name of input composition record
?NSTS => Cataloged state number of this source

The Problem Name in the input composition records is assumed to be the Problem Name of the problem being executed. A state number or a time is required, but only one will be used. If both are specified the state number will be used. If only time is specified the input composition is obtained from adjacent cataloged time-states by linear interpolation.

The group structure of the calculated multigroup source is specified in the SHIELD.INPUT.JOB.?JOBNAME record. Versions of the MULTIGRP data set for neutron data and photon data are specified. If either is omitted a source for that particle will not be computed. Failure to specify either version name will give an error message. The recommended MULTIGRP data set for the new model is ANISN58, which has 37 neutron energy groups and 21 gamma groups.

The resultant composite source is stored in record

SHIELD.?PROB.?PROC.SOURCE.?COMPS.?NSTS.PHOTON

A catalog of all sources for a composition is given in record

SHIELD.?PROB.?PROC.SOURCE.?COMPS.STATES

3.5 Compilation of Cross-Section Data

The cross-section data used in the transport calculations are created using CALC = XSECTION, METH = XPREP2. The XSECTION calculation forms multigroup macroscopic cross sections for homogenous mixtures of isotopes. Cross sections can be prepared for neutron only, photon only, and coupled neutron-photon problems. Energy group structure can be the same as the MULTIGRP version from which microscopic cross sections for each isotope in a mixture are taken, or may be a collapsed subset of that MULTIGRP

4579.SHIELD.SAMP1.SOUR1.COMPOSIT.SLURRY.1

********** ISOTOPIC COMPOSITION AT A TIME STATE **********

NUMBER OF ISOTOPES IN THIS COMPOSITION . . . . . .: 11

FLUX HISTORY NAME USED TO GENERATE THIS COMPOSITION. .:

PROBLEM NAME OF INITIAL COMPOSITION. . . . . .:SAMP1

PROCESS NAME OF INITIAL COMPOSITION. . . . . .:SOUR1

COMPOSITION NAME OF INITIAL COMPOSITION. . . . . .:SLURRY

TIME STATE NUMBER OF INITIAL COMPOSITION . . . . . .: 1

TIME (HRS) FOR THIS COMPOSITION-STATE. . . . . :00.0000E-01

********** ISOTOPIC COMPOSITION AT A TIME STATE **********

IZAS	CONC (ATM/B-CM)	IZAS	CONC (ATM/B-CM)
942380	10.0269E-09	942400	89.5347E-07
942420	28.6488E-09	10010	63.1868E-08
942390	67.2668E-06	942410	82.0145E-08
90190	75.0909E-05	80160	84.7086E-08
70140	18.8649E-04	160320	10.1789E-05
60120	17.5631E-05		

FIGURE 8

SHIELD.?PROB.?PROC.COMPOSIT.?COMPS.?NSTS RECORD

version. Cross sections for each mixture may be collapsed using different collapsing weights corresponding to different neutron and/or photon energy spectra.

All cross sections generated by the XSECTION calculations are written to SHIELD.SNXSECT...records for permanent retrieval in the JOB data set of the problem.

3.5.1. Energy Group Specifications

In the XSECTION calculation isotopic microscopic cross sections are taken from a version of the JOSHUA MULTIGRP dataset, combined with the number density for that isotope, and added into the composite cross sections in an energy group structure specified in input records to the XSECTION calculation. The MULTIGRP version names and output group records are input in the SHIELD.INPUT.JOB.?JOBNAME record.

An example of specifications of cross section energy group structure record name is shown in Figure 2. In this example the neutron cross section data is taken from MULTIGRP data set version ANISN58 and photon cross section data is taken from MULTIGRP.PHOTON version ANISN58. Omission of a MULTIGRP version name for the neutron data will generate photon cross sections only and omission of a MULTIGRP version name for the photon data will generate neutron cross sections only. The specifications shown in Figure 2 will generate a coupled neutron-photon set of data because both MULTIGRP version names are given.

The names of the energy group structure records in which the output SHIELD.SNXSECT...cross sections will be generated are also specified in the SHIELD.INPUT.JOB.?JOBNAME record. The neutron group structure is specified in record

```
SHIELD.XSECTION.GROUPS.?NEUTGRPS.NEUTRON
```

where ?NEUTGRPS is the neutron group structure name specified in the SHIELD.INPUT.JOB.?JOBNAME record. Similarly the photon energy group structure is specified in record

```
SHIELD.XSECTION.GROUPS.?PHOTGRPS.PHOTON
```

where ?PHOTGRPS is the photon group structure name specified in the SHIELD.INPUT.JOB.?JOBNAME record.

It is recommended that the user specify NEUTGRPS = PHOTGRPS = ANISN58 and use the default standard 58 group structure.

The final energy group structure is output to record

SHIELD.SNXSECT.?SNVER.GROUPS

where ?SNVER always has the name

FG*?NN*?MM

where ?NN = number of neutron energy groups in structure
?MM = number of photon energy groups in structure.

3.5.2 XSECTION Calculation Input Record

The basic XSECTION Calculation Input Record is

SHIELD.INPUT.?PROB.?PROC.XSECTION

where ?PROB and ?PROC are the problem name and process name respectively for the calculation step being executed. An example of this record is shown in Figure 9. The content of this record is a series of case names (?CASE) each describing a mixture of isotopes that constitute a material of interest.

For each case name (?CASE) in the XSECTION calculation input record a material is described in a record with name

SHIELD.XSECTION.?CASE

where ?CASE was defined above. An example of this record is shown in Figure 10. Four types of input information are provided in the XSECTION case input record as follows:

- Material name and temperature under which the cross sections are to be stored.
- Specification of collapsing weights if group collapsing is to be performed.
- The highest Legendre order to which transfer matrices are to be generated.

```
4579.SHIELD.INPUT.SAMP1.XSEC1.XSECTION
********** SHIELD SYSTEM XSECTION CALCULATION INPUT **********

NUMBER OF CASE NAMES TO BE EXECUTED IN THIS STEP :  5

********* SHIELD SYSTEM XSECTION CALCULATION INPUT *********
:POLYETH    :LEXAN      :LUCITE     :PUF8       :SLURRY
```

FIGURE 9

SHIELD.INPUT.?PROB.?PROC.XSECTION RECORD

- Isotope names and number densities (or equivalent) of the mixture.

The name of the material (?MAT) and integer temperature (?ITC) in degrees C are entered on the first page of the XSECTION case input record, in Figure 10. The temperature also is used to retrieve data from the MULTIGRP data set.

Specifications of the optional collapsing weights is given on the second page of the XSECTION case input record, in Figure 10. If the standard group collapsing weights in the MULTIGRP data set are used a YES in the designated field will invoke use of these weights. If collapsing weights are to be derived from a geometrical zone in a RADFIELD calculation, the zone name and RADFIELD identification names are entered in the designated fields. It is recommended that no collapsing be done to the ANISN58 structure, and these lines left blank.

The highest Legendre order to be used in transfer matrices is specified on the first page of the XSECTION Case Input Record in Figure 10. If this specification exceeds the Legendre order available in MULTIGRP cross section data, the Legendre order in the mixture cross sections will be reduced to reflect this limitation. The recommended value is 3, the ANISN58 maximum order. Neither the material density nor temperature entries on the first page are used in this model and should be entered as 0's. The isotopes and number data are specified in the list on the third page of the XSECTION case input record in Figure 10. Isotopic content of the material can be specified in absolute units (ATM/B-CM,PPM, etc.) or relative units (WGT-PCNT,WGT-FRAC,BAL,etc.); the allowed units are listed on the record. If any isotope is specified in relative units a density for the material must be specified on the first page of the XSECTION case input record in Figure 10.

Isotope names that appear on the third page of the XSECTION case input record are specified as they appear in the ISOTOPES record for the MULTIGRP versions specified. If only neutron cross sections are being generated these names are taken from the MULTIGRP.?VERS.ISOTOPES record for the neutron data. If only photon cross sections are being generated these names are taken from the MULTIGRP.PHOTON.?VERS.ISOTOPES record for the photon data. If coupled neutron-photon cross sections are being generated the names should come from the MULTIGRP.?VERS.ISOTOPES record for the neutron data.

```
    4579.SHIELD.XSECTION.SLURRY

************   XSECTION CALCULATION CASE RECORD   ************

MATERIAL NAME FOR THIS CROSS SECTION SET              :SLURRY

NUMBER OF LINES OF ISOTOPES TO ADD IN THIS MATERIAL   :  8

MAXIMUM LEGENDRE ORDER IN THIS CROSS SECTION SET      :8

DENSITY OF MATERIAL (IF REQUIRED)                  :00.0000E-01

TEMPERATURE (DEG C) OF THIS MATERIAL                  :  0



************   XSECTION CALCULATION CASE RECORD   ************

ADD THE ISOTOPES TO THE CROSS SECTIONS IN RECORDS (OPTIONAL)
       SHIELD.SNXSECT.:         .:         .:   0 ...

     THE FOLLOWING OPTIONS ARE FOR GROUP COLLAPSING

     USE STANDARD COLLAPSING WEIGHTS (YES OR NO) :YES

OR

     GET COLLAPSING WEIGHTS FROM REGION :
            IN THE RADFIELD FLUX RECORDS
    SHIELD.:         .:         .RADFIELD.:         ...



************   XSECTION CALCULATION CASE RECORD   ************
INDEX    ISOTOPE    CONCENTRATION    UNIT NAME  | ALLOWED UNITS -
  1    :PU239       :67.5864E-06     :AB        | AB OR ATM/B-CM
  2    :PU240       :89.9215E-07     :AB        | AP OR ATM-PCNT
  3    :H           :63.1868E-03     :AB        | AF OR ATM-FRAC
  4    :F           :75.0909E-05     :AB        | AR OR ATM-RATO
  5    :O-CORR      :84.7086E-03     :AB        | WP OR WGT-PCNT
  6    :N-CORR      :13.8649E-04     :AB        | WF OR WGT-FRAC
  7    :S           :10.1789E-05     :AB        | WR OR WGT-RATO
  8    :C12         :17.5631E-05     :AB        | GM/CC,PPM, BAL
```

FIGURE 10

SHIELD.XSECTION.?CASE RECORD

3.5.3 XSECTION Calculation Output Records

The material cross sections generated in an XSECTION calculation are stored in a special set of SHIELD data set records that may be saved for later use at the users discretion. This permits cross sections for standard materials to be generated once and retained. Cross sections have been generated in ANISN58 group structure for the standard materials AIR, WEP, Aluminum, SS304, and SS316, and stored in the STANDARD SHIELD data set.

Within a SHIELD.SNXSECT version a catalog of all material names generated in this run is maintained in record

SHIELD.SNXSECT.FG*?NN*?MM.CONTENTS

where ?NN and ?MM are the number of neutron groups and photon groups respectively. An example of this record is shown in Figure 11.

The energy group structure of a SHIELD.SNXSECT version is given in record

SHIELD.SNXSECT.FG*?NN*?MM*.GROUPS

where NN and MM are the number of neutron groups and photon groups respectively. Neutron groups are always ordered first in a coupled neutron-photon group structure.

For each material-temperature pair in a SHIELD.SNXSECT version several records are output to store the cross section information. These records contain the following information:

- Isotopic content of the material
- Collapsing weights used to generate the material cross section (appears only if group collapsing is done).
- Smooth macroscopic cross sections for each energy group.
- Heat generation cross sections for each energy group
- Total transfer matrices to each energy group and all Legendre orders specified in the calculation

These records are catalogued under SHIELD.SNXSECT.FG*?NN*?MM....

SHIELD.SNXSECT.FG*87*21.CONTENTS

******** MATERIAL NAMES IN A SHIELD SNXSECT VERSION ********

NUMBER OF MATERIAL NAMES IN THIS SNXSECT VERSION : 5

******** MATERIAL NAMES IN A SHIELD SNXSECT VERSION ********

INDEX	MATERIAL NAME	TEMP (DEG C)
1	:AIR	: 0
2	:WEP	: 0
8	:ALUMINUM	: 0
4	:SS304	: 0
5	:SS316	: 0

FIGURE 11

SHIELD.SNXSECT.FG*NN*MM.CONTENTS RECORD

3.6. Calculation of the Particle Leakage Rates From the Source Regions

The determination of the outgoing angular flux values on the outside boundaries of the source regions are determined using CALC = SPECIAL and METH = SNONEF. The "source region" applies to the radioactive material itself plus any containers, packaging and local shielding which immediately surround the radioactive material.

The SNONEF module is a version of the standard SHIELD system SNONE module, modified to store the outgoing angular flux on the outside boundary and converge on leakage rate.

The calculation uses a 1-D S_N transport module to calculate the spatial flux distribution of neutrons and/or photons for a specified geometry having a fixed arrangement of homogeneous materials.

Input to the calculation modules can be divided into three groups:

- Specification of the required calculation and assignment of cross sections and sources to geometrical zones.
- Specification of problem geometry.
- Specification of options that permit input of

  -anisotopic fixed sources
  -boundary sources
  -a variety of eigenvalue searches
  -material density modification factors.

Specification of input will be described in the section to follow. No description of S_N transport theory is included in these sections. The user is referred to Reference 3 for a complete description of the theoretical methods.

3.6.1. SNONEF Calculation Specification Record

The record named

SHIELD.INPUT.?PROB.?PROC.SPECIAL

is used to name the boundary source being calculated. The basic calculation specifications are given in record

```
SHIELD.INPUT.?PROB.?PROC.RADFIELD
```

where ?PROB and ?PROC are the problem name and process name for the current calculation step. An example of this record is shown in Figure 12.

The record shown in Figure 12 specifies the following information to the S_N transport module (listed in order of occurrence in the record).

Radiation Field Name

This name is used to store all calculated results. These results will appear in records:

```
SHIELD.?PROC.?PROB.RADFIELD.?RNAME....
```

where ?PROB and ?PROC are the problem name and process name respectively, and ?RNAME is the radiation field name.

Type of Calculation

The type of calculation determines input record requirements and how the calculation is performed. For the new method, KEFF should be specified if fissile material is present and SOURCE specified otherwise.

Type of Fluxes

SHIELD system S_N modules are designed to calculate DIRECT fluxes, ADJOINT fluxes, or BOTH as the user specifies. For the new model, DIRECT should be specified.

QUADRATURE WEIGHTS NAME

The SHIELD system has many sets of S_N quadrature weights stored in standard SHIELD data set records. A complete description of these standard sets is given in Table 2 along with the record names. The recommended quadratures are S16CYL1D for cylindrical sources and S16SLB1D for slab sources.

```
    4579.SHIELD.INPUT.SAMP1.FORW1.RADFIELD

******  SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD  *****

RADIATION FIELD NAME TO BE CALCULATED. . . . . :SLURRY

TYPE OF CALCULATION TO PERFORM -- OPTIONS ARE
      SOURCE / KEFF / ALPHA / ZONEWIDE / OUTRAD / BUCKLING

                        :KEFF

TYPE OF FLUXES TO BE CALCULATED (DIRECT, ADJOINT, OR BOTH)

                        :DIRECT

QUADRATURE WEIGHTS FOR THIS SN CALCULATION ARE TAKEN FROM RECORD

                SHIELD.QUADCOEF.:S16SLB1D

CROSS SECTIONS FOR THIS PROBLEM WILL BE TAKEN FROM

                SHIELD.SNXSECT.?VERSION . . .:FG*37*21



******  SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD  *****

            GEOMETRY OF PROBLEM TAKEN FROM-RECORD

             SHIELD.GEOMETRY.:ONED      .:M3BOT

THE INITIAL FLUX GUESS (OPTIONAL) IS TAKEN FROM RECORDS

      SHIELD.:          .:          .RADFIELD.:          ....

THE FISSION SPECTRUM USED IN THE CALCULATION WILL BE TAKEN FROM
THE MATERIAL IN ZONE NAME

                        :SOL        IN THE GEOMETRY RECORD
```

FIGURE 12

SHIELD.INPUT.?PROB.?PROC.RADFIELD RECORD

```
    4579.SHIELD.INPUT.SAMP1.FORW1.RADFIELD
******   SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD   *****

ANISOTROPIC SOURCES WILL BE TAKEN FROM RECORD
                SHIELD.RADFIELD.ANSOURCE.:
BOUNDARY SOURCES WILL BE TAKEN FROM RECORD
                SHIELD.RADFIELD.BDSOURCE.:
SEARCH PARAMETERS WILL BE TAKEN FROM RECORD
                SHIELD.RADFIELD.SEARCH.:
DENSITY FACTORS WILL BE TAKEN FROM RECORD
                SHIELD.RADFIELD.DENFACT.:


******   SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD   *****
MAXIMUM LEGENDRE SCATTERING ORDER. . . . . .:3
CONVERGENCE CRITERIA ON EIGENVALUE AND FLUXES. . . .:10.0000E-03
MAXIMUM INNER ITERATIONS ALLOWED . . . . . .: 50
MAXIMUM OUTER ITERATIONS ALLOWED . . . . . .: 20
LEAKAGE BUCKLING (1/CM**2) . . . . . .:00.0000E-01


NUMBER OF GEOMETRY ZONES WITH CROSS SECTION AND/OR SOURCE SPECS
                : 8
```

FIGURE 12 (CONTD)

****** SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD *****

ZONE NAME IN THE GEOMETRY DESCRIPTION RECORD :PREC

(ZONE NAME 'REST' REFERS TO ALL UNSPECIFIED ZONES)

CROSS SECTIONS FOR THIS ZONE ARE TAKEN FROM RECORDS

SHIELD.SNXSECT.?VERSION.:PUF3 .: 0 ...

ISOTROPIC DISTRIBUTED SOURCE FOR THIS ZONE IS TAKEN FROM RECORD

SHIELD.:SAMP1 .:SOUR1 .SOURCE.:PUF3 ...

AT STATE NUMBER : 1 OR AT TIME :00.0000E-01 HRS

—

****** SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD *****

ZONE NAME IN THE GEOMETRY DESCRIPTION RECORD :SOL

(ZONE NAME 'REST' REFERS TO ALL UNSPECIFIED ZONES)

CROSS SECTIONS FOR THIS ZONE ARE TAKEN FROM RECORDS

SHIELD.SNXSECT.?VERSION.:SLURRY .: 0 ...

ISOTROPIC DISTRIBUTED SOURCE FOR THIS ZONE IS TAKEN FROM RECORD

SHIELD.:SAMP1 .:SOUR1 .SOURCE.:SLURRY ...

AT STATE NUMBER : 1 OR AT TIME :00.0000E-01 HRS

FIGURE 12 (CONTD)

```
    4579.SHIELD.INPUT.SAMP1.FORW1.RADFIELD
******   SHIELD SYSTEM RADFIELD CALCULATION INPUT RECORD   *****

    ZONE NAME IN THE GEOMETRY DESCRIPTION RECORD :POLY
     (ZONE NAME 'REST' REFERS TO ALL UNSPECIFIED ZONES)

CROSS SECTIONS FOR THIS ZONE ARE TAKEN FROM RECORDS
          SHIELD.SNXSECT.?VERSION.:POLYETH  .:   0 ...


ISOTROPIC DISTRIBUTED SOURCE FOR THIS ZONE IS TAKEN FROM RECORD
          SHIELD.:          .:          .SOURCE.:          ...
          AT STATE NUMBER :  0 OR AT TIME :00.0000E-01 HRS
```

FIGURE 12 (CONTD)

TABLE 2

QUADRATURE SETS IN STANDARD SHIELD DATA SET

SET NAME	ORDER AND GEOMETRY	COMMENTS
S2CYL1-D	S_2 1-D cylinder	Completely
S4CYL1-D	S_4 1-D cylinder	Symmetric quadrature
S6CYL1-D	S_6 1-D cylinder	sets satisfying an
S8CYL1-D	S_8 1-D cylinder	even moments condition
S12CYL1D	S_{12} 1-D cylinder	
S16CYL1D	S_{16} 1-D cylinder	
S2SLB1-D	S_2 1-D slab	Completely symmetric
S4SLB1-D	S_4 1-D slab	quadrature sets
S6SLB1-D	S_6 1-D slab	satisfying an
S8SLB1-D	S_8 1-D slab	odd moments
S12SLB1D	S_{12} 1-D slab	condition
S16SLB1D	S_{16} 1-D slab	

SHIELD.SNXSECT Version Name

To assure that all cross sections have the same group structure a single version name is entered for the cross sections to be used in the problem. These cross sections may be prepared by the XSECTION calculation (Section 3.5) or by direct input to **SHIELD.SNXSECT...** records. For the ANISN58 group structure, this value will be FG*37*21.

Geometry Description Record Name

The geometry for the calculations is specified in record

SHIELD.GEOMETRY.?GNAME1.?GNAME2

where ?GNAME1 and ?GNAME2 are identification names for the geometry. This record will be described in detail in Section 3.6.2

Initial Flux Guess (Optional)

An initial flux guess may be input provided the flux was calculated for the same geometry as the current problem. As such a flux guess seldom helps a source problem, it is recommended that these values be left blank.

Fission Spectrum Specification

For 2-D S_N calculations a fission spectrum is required for the problem, but a standard spectrum is used in 1-D. Therefore this entry can be left blank for our 1-D case here.

Anisotropic Source Record (Optional)

The use of this option should not be necessary, so should be left blank.

Boundary Source Records, Search Calculation Input Parameters, Density Factor Records

Legendre Scattering Order

This quantity is the maximum order Legendre polynominal to be used in the problem for treatment of anisotropic scattering. Any odd integer order or zero order (isotropic scattering) is permitted so long as cross sections are available for all orders. The recommended value is 3.

Convergence Criterion For Eigenvalue and Fluxes

This quantity provides the overall convergence criterion for the problem. Several other criteria are used within the S_N modules and are defined relative to this criterion. The default value is 1.0×10^{-4}, which is much tighter than we need. The recommended value is 0.001.

Maximum Inner Iterations

The number limits the flux solution iterations for a single energy group within an outer iteration. A recommended value for this number is 20. For very large problems a slightly larger number might be required, but should never exceed 50.

Maximum Outer Interations

This number is an upper limit for iteration of fission sources (outer iterations) in k_{eff} calculations. The number should never exceed 100 and usually converges with no more than 25 iterations.

Leakage Buckling

Leakage is entered into the problem using a DB^2 term added to the total and absorption cross sections. The diffusion coefficient (D) is computed from $1/3\Sigma_{tr}$ where Σ^{tr} is contained in the cross sections for each region separately. A region dependent leakage cannot be entered. If a buckling search is performed the value entered here is used as the initial value for the search.

Number of Geometry Zones With Source and Cross Sections

This number controls the number of pages to follow. Each page to follow will specify the cross sections and/or isotropic external sources to assign to each zone in the geometry record.

Cross Sections and Sources For Each Geometry Zone

Three quantities are entered on each page that specify the cross sections and optional isotropic external source to be assigned to each geometrical zone. These quantities are:

- The geometry zone name that appears in the specified geometry record for the problem. If the name REST is used it implies that the cross sections and sources here specified are to be used in all zones not explicitly specified elsewhere.

- The name of the cross sections to use in the zone with name specified above. These cross sections must be in SHIELD.SNXSECT records with version name as specified previously. The material name and integer temperature are specified here to identify the cross section. The mixture cross sections may be generated by a XSECTION calculation (see Section 3.5) or input by the user in SHIELD.SNXSECT records.

- The name of an optional isotropic external source to be uniformly distributed in the geometrical zone. The units of this source are particles/cc/sec. The name of the SHIELD...SOURCE record is entered to specify the source. These SOURCE records may be generated by the RADSOR or ALFN calculation (Section 3.3 & 3.4) or input independently by the user in SHIELD records.

Information on whether the problem is a neutron only, photon only, or a coupled neutron-photon calculation is obtained from the cross sections and sources input to the problem.

3.6.2 S_N Geometry Specification

S_N problem geometry is specified in a generalized record that permits use of slab, cylindrical, or spherical geometry. The record has the name

```
SHIELD.GEOMETRY.?GNAME1.?GNAME2
```

where ?GNAME1 and ?GNAME are user defined names. An example of this record is shown in Figure 13.

The information entered into this record is the following:

Number of Dimensions

For the new model this should be a 1.

Number of Spatial Zones

A zone is a region of homogeneous material in the geometry. Each zone is assigned a unique name and size later in this record. The number of zones in the geometry description is entered here.

```
    4579.SHIELD.GEOMETRY.ONED.M3BOT

**********   SHIELD SYSTEM GEOMETRY SPECIFICATIONS   **********

NUMBER OF DIMENSIONS IN THIS GEOMETRY (1,2, OR 3)    :1

NUMBER OF SPATIAL ZONES IN THIS GEOMETRY             :  2

TYPE OF GEOMETRY (SLAB/CYL/SPH/XY/RZ/RT/XYZ/RTZ/RTP) :SLAB
    CYL -> CYLINDER, SPH -> SPHERE, X -> X COORDINATE,
    Y -> Y COORDINATE, Z -> Z COORDINATE, R -> R COORDINATE,
    T -> THETA COORDINATE, P -> PHI COORDINATE

**************   BOUNDARY CONDITIONS ON GEOMETRY   **************

      SPECIFY APPLICABLE BOUNDARY CONDITIONS - OPTIONS ARE
          VACUUM / REFLECT / WHITE / PERIODIC / ALBEDO
LOW  COORDINATE BOUNDARY CONDITION FOR DIMENSION 1   :REFLECT
HIGH COORDINATE BOUNDARY CONDITION FOR DIMENSION 1   :VACUUM
LOW  COORDINATE BOUNDARY CONDITION FOR DIMENSION 2   :
HIGH COORDINATE BOUNDARY CONDITION FOR DIMENSION 2   :
LOW  COORDINATE BOUNDARY CONDITION FOR DIMENSION 3   :
HIGH COORDINATE BOUNDARY CONDITION FOR DIMENSION 3   :
```

FIGURE 13

SHIELD.GEOMETRY.?GNAME1.?GNAME2

4579.SHIELD.GEOMETRY.ONED.M3BOT

******** ZONE SPECIFICATIONS FOR ZONE NUMBER 1 **********

ZONE NAME :SOL

DIMENSION NO.	MIN. VALUE	MAX. VALUE	NO. SUBDIVISIONS
1 (X OR R)	:00.0000E-01	:42.4180E-01	: 15
2 (Y,Z, OR T)	:00.0000E-01	:00.0000E-01	: 0
8 (Z OR P)	:00.0000E-01	:00.0000E-01	: 0

******** ZONE SPECIFICATIONS FOR ZONE NUMBER 2 **********

ZONE NAME :POLY

DIMENSION NO.	MIN. VALUE	MAX. VALUE	NO. SUBDIVISIONS
1 (X OR R)	:42.4180E-01	:48.7680E-01	: 10
2 (Y,Z, OR T)	:00.0000E-01	:00.0000E-01	: 0
8 (Z OR P)	:00.0000E-01	:00.0000E-01	: 0

FIGURE 13 (CONTD)

Type of Geometry

For this problem specify either SLAB for slab sources or CYL for cylindrical sources.

Boundary Conditions

Boundary conditions are selected from the options shown in Table 3 for the low and high coordinate of each dimension. For 1-D geometry the boundary conditions are ignored for dimension 2 and 3 and may be left blank or set to any name. The dimension 1 HIGH (right) boundary should be VACUUM; the LOW (left boundary should also be VACUUM for a slab problem and REFLECT for a cylinder. (REFLECT may be used for a slab problem if the geometry is symmetric about a midplane.)

Zone Specifications

Information is entered for as many geometrical zones as specified earlier in this record. The geometry must be configured so that the outside of the source is to the right. The information required is the following:

- Coordinate values for the minimum and maximum value of each dimension for the zone. Spatial coordinates of X, Y, Z, or R are entered in centimeters (cm).
- The number of spatial segments into which the zone interval is subdivided is specified for each dimension separately. This subdivision should be done in such a way as to permit best resolution of angular fluxes in the zone intervals irrespective of any adjacent zone.

The input geometry description is processed by the S_N modules and written into record

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.GEOMETRY

3.6.3. SNONEF Calculation Output (Also Applies for SNONEA Output.)

The printed output of the SNONEF includes an iteration history, a groupwise leakage and dose listing, and group and region edits. The RADFIELD calculation normally writes a large number of output records to the JOB data set. These records are sometimes used as input to later calculations (e.g. DOSE

TABLE 3

BOUNDARY CONDITIONS FOR SNONE RUNS

Boundary Conditions	Description
VACUUM	Particles that leave the boundary never return. (All incoming fluxes are set to zero)
REFLECT	Reflecting boundary conditions in which particles leaving the boundary return with angle corresponding to the optically reflected angle.
WHITE	Particles returning through a boundary are set equal to the angular average flux leaving the boundary for all incoming angles. This boundary condition is not available for 1-D calculations or for the left boundary in 2-D calculations.
PERIODIC	Particles leaving the right boundary enter the left boundary at the same angle. Particles leaving the left boundary enter the right boundary at the same angle. This boundary condition is not available for top and bottom boundaries in a 2-D problem.
ALBEDO	This boundary conditions is not available for any S_N transport calculation.

calculations or XSECTION calculations) or as input to the EDIT calculation. The SNONEF version writes a special set of boundary flux records named

```
SHIELD.?PROB.?PROC.BOUND.?ASOUR.?IG
```

where ?ASOUR is the source name and ?IG is the energy group number.

The basic problem specification record is written to record

```
SHIELD.?PROB.?PROC.RADFIELD.?RNAME.CONTENTS
```

where ?PROB and ?PROC are the problem name and process name respectively, and ?RNAME is the field calculation name specified in the input.

The geometry of the RADFIELD calculation (described in Section 3.5.2) is written to record

```
SHIELD.?PROB.?PROC.RADFIELD.?RNAME.GEOMETRY
```

where ?PROB,?PROC, and ?RNAME are the same as described previously.

Any input fixed sources are written to records

```
SHIELD.?PROB.?PROC.RADFIELD.?RNAME.SOURCE.?L.?IG
```

where ?PROB, ?PROC and ?RNAME are described above and ?L is the Legendre order of the source and ?IG is the group number of the source. This source contains all isotropic and anisotropic sources for the problem. An index of groups, Legendre orders, and number of associated Legendre components is contained in record

```
SHIELD.?PROB.?PROC.RADFIELD.?RNAME.SOURCE.CONTENTS
```

The P_0 Legendre order fluxes are output into records of name

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.?FLUX.?IG

where ?PROB, ?PROC, and ?RNAME are described above and ?FLUX is either FLUX or AFLUX denoting direct and adjoint fluxes respectively. ?IG is the group number. A record of this type is output for each group with non-zero fluxes. A catalog of groups and spatial intervals in the records is given in record

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.?FLUX.CONTENTS

Legendre fluxes containing all P_ℓ^m components are output into records of name

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.?LFLUX.?L.?IG

where ?PROB, ?PROC, and ?RNAME were previously defined. ?LFLUX is either LFLUX or LAFLUX depending on whether the fluxes are direct (SNONEF) or adjoint (SNONEA) fluxes. ?L is the Legendre order and ?IG is the energy group number. A catalog record containing the highest Legendre order, number of groups and number of space points is written with name

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.?LFLUX.CONTENTS

A number of records are written (or rewritten) to store the result of searches performed. These will be described by type of search performed.

The k_{eff} from a K_{eff} type calculation is stored in record

SHIELD.?PROB.?PROC.RADFIELD.?RNAME.KEFF.?FLUX

where ?PROB, ?PROC, and ?RNAME are defined above and ?FLUX is FLUX or AFLUX depending on whether the calculation was for direct fluxes or adjoint fluxes. For most shielding problems, there will be an external source of neutrons and therefore k_{eff} will go to 1. (This does not indicate a critical configuration, but only a static flux field.)

3.7 Calculation of Shield Penetration Characteristics

The calculation of the shield penetration characteristics is performed using CALC = SPECIAL and METH= SNONEA. The calculation is a series of adjoint calculations in slab geometry, one for each backward direction in the angular quadrature. For each direction the outside (right) boundary source for the problem is taken as the groupwise flux-to-dose conversion function in the direction of interest with no source for the other directions. The resulting adjoint boundary flux on the inside (left) boundary of the shield is then interpreted as a transfer function between incoming (left) angular fluxes (particles/sec/cm^2) and outgoing (right) angular dose rates (mrem/hr).

The SNONEA module is a version of the SHIELD SNONE module, modified to deal with boundary fluxes and sources in this way. The input and output records for SNONEA are the standard RADFIELD records described in Section 3.4 for SNONEF. The differences in input will be treated in the following text.

3.7.1 Calculation Specification Record

The record named

SHIELD.INPUT.?PROB.?PROC.SPECIAL

is used to name the shield name for this run. This name (ASHLD) is used in the new model in putting the sources and shields together.

The specification record is given in

SHIELD.INPUT.?PROB.?PROC.RADFIELD

Because this form is exactly the same as for SNONEF, it is vital that the SNONEF and SNONEA records have different PROC names, preferably identifying the input as forward (F) or adjoint (A) in the name.

The following information differs from the corresponding record for the SNONEF runs (See Figure 12):

Types of Calculation

As shields will not contain fissile material (otherwise they would be classified as sources), this value should be SOURCE.

Type of Fluxes

ADJOINT should be specified.

Quadrature Weights Name

The choices of quadrature here are the same as for the SNONEF (see Table 2). This quadrature can be chosen independently of the source calculation quadrature.

Maximum Inner and Outer Iterations

For this SNONEA calculation without fissile material, there will be only one outer iteration. The values for the inner iterations should be 50 or 100.

3.7.2 S_N Geometry Specification

The following differences occur in the geometry records for SNONEA calculations versus SNONEF (see Figure 13):

Type of Geometry

The model can currently only handle SLAB shields.

Boundary Conditions

Both sides must be vacuum conditions. Even if the shield is symmetric about a center plane, the entire shield must be modeled. The left side must be the inside (side the sources are on) and the right side must be outside (where the detector points are located).

3.7.3 SNONEA Calculation Output

The output from the SNONEA consists of a set of shield penetration transfer matrices in the records

```
SHIELD.ADJOINT.?ASHLD.NEUTRON.?M
SHIELD.ADJOINT.?ASHLD.GAMMA.?M
```

where ?ASHLD is the shield name and M is the adjoint source angle.

The printed output includes a convergence history for each backward angle calculation, as well as group and region edits of sources and reaction rates.

3.8 Calculation of Dose Rate at Detector Points

This step of the calculation implements the new model to calculate the dose rates at specified points in the configuration from an assemblage of slab and cylindrical sources and slab shields. The input to this calculation is described in the record named

SHIELD.INPUT.?PROB.?PROC.EXPOSE

as shown in Figure 14. The data requested by this record are the dose factor used (FG*37*21 for the 58 group structure) and the keynames ?DECT, ?SOUR, and ?SHLD which point to the records containing the detector locations, source description and shield description, respectively. The input is divided into three parts: description of sources, description of shields, and definition of dose points desired.

In each of these an (x,y,z) coordinate system is used to position the problem elements (sources, shields, detector points). The origin of the coordinate system is left up to the user, but the orientation of the problem is not. The slab sources and shields must be bounded by planes perpendicular to the axes, and the cylindrical sources must be cylinders about an axis parallel to the z axis. The source regions are approximated by the model as either YZ finite plane surface sources (for slab sources) or outer radius cylindrical surface sources (for cylindrical sources).

```
4579.SHIELD.INPUT.SAMP1.DOSE1.EXPOSE

DOSE FACTOR VALUES BY ENERGY GROUP IN
    SHIELD.DOSEFACT.:FG*37*21

DETECTOR POSITIONING DESCRIBED IN
    SHIELD.DETECTOR.:SAMP2

SOURCE DESCRIBED IN
    SHIELD.SOURCE.:SAMP1

SHIELD SYSTEM DESCRIBED IN
    SHIELD.SHIELD.:SAMP1
```

FIGURE 14

SHIELD.INPUT.?PROB.?PROC.EXPOSE RECORD

3.8.1 Description of Sources

The sources are described using the record named

SHIELD.SOURCE.?SOUR

shown in Figure 15. The information required by this record are the dimensions and characteristics of the source. In the new model the sources are considered surface sources - for slab geometry, a rectangle perpendicular to the x-axis; for cylindrical geometry, a truncated cylinder surface with a z-axis centerline. For slab geometry, the x, y, and z geometrical data are self-explanatory. For cylindrical, the x-coordinate value is for the centerline of the cylinder, the y-coordinate values are the minimum and maximum y values. The outleakage data set entry should point to the results of an SNONEF run, and the quadrature entry should be the quadrature used in the SNONEF calculation.

3.8.2 Description of Shields

The shield configuration is described in the record

SHIELD.SHIELD.?SHLD

as shown in Figure 16. This record provides shielding information for use in calculating dose rate contributions from both uncollided and collided source particles.

The first page of the record gives the number of following pages in the record and the quadrature used in the adjoint calculation. Each succeeding page contains a description of a shield segment, which is a portion of the total shielding configuration, satisfying the following two conditions:

1. Composed of a single homogeneous material, and
2. Bounded by planes perpendicular to the x, y, and z axes.

For each shield segment, the record includes

1. the minimum and maximum x, y, and z values,
2. the number of divisions of each dimension to be used in discretizing the geometry,

```
NO. OF SOURCE DESCRIPTIONS :  2


X COORDINATE OF SOURCE :-5.1440E 01

    MINIMUM VALUE OF Y :13.0000E 01
    MAXIMUM VALUE OF Y :28.5410E 01
    NO. OF Y DIVISIONS : 21

    MINIMUM VALUE OF Z :51.0000E 00
    MAXIMUM VALUE OF Z :64.3100E 00
    NO. OF X DIVISIONS :  6

    GEOMETRY OF SOURCE 0/1-SLAB/CYL :0


    SOURCE OUT LEAKAGE IS IN SHIELD.BOUND. :BOTTOM

    SOURCE.QUADRATURE IS IN SHIELD.QUADCOEF.:S16SLB1D



X COORDINATE OF SOURCE :-5.1440E 01

    MINIMUM VALUE OF Y :17.5410E 01
    MAXIMUM VALUE OF Y :23.5410E 01
    NO. OF Y DIVISIONS :  6

    MINIMUM VALUE OF Z :64.3100E 00
    MAXIMUM VALUE OF Z :14.0400E 01
    NO. OF X DIVISIONS : 12

    GEOMETRY OF SOURCE 0/1-SLAB/CYL :0


    SOURCE OUT LEAKAGE IS IN SHIELD.BOUND. :TOP

    SOURCE.QUADRATURE IS IN SHIELD.QUADCOEF.:S16SLB1D
```

FIGURE 15

SHIELD.SOURCE.?SOUR RECORD

```
NUMBER OF SHIELDS :  2

SHIELD QUADRATURE IS IN SHIELD.QUADCOEF.:S16SLB1D


        MINIMUM X VALUE :-6.3500E-01
        MAXIMUM X VALUE :00.0000E-01
        NUMBER OF X DIVISIONS : 15

        MINIMUM Y VALUE :00.0000E-01
        MAXIMUM Y VALUE :47.2000E 01
        NUMBER OF Y DIVISIONS : 20

        MINIMUM Z VALUE :00.0000E-01
        MAXIMUM Z VALUE :32.0000E 01
        NUMBER OF Z DIVISIONS : 20

ADJOINT FOR SHIELD MATERIAL IS IN ADJOINT.:LEXAN

CROSS SECTIONS FOR MATERIAL ARE IN
        SHIELD.SNXSECT.:FG*37*21 .:LEXAN     .:   0


        MINIMUM X VALUE :63.5000E-01
        MAXIMUM X VALUE :11.4300E 00
        NUMBER OF X DIVISIONS : 10

        MINIMUM Y VALUE :11.5000E 01
        MAXIMUM Y VALUE :24.3000E 01
        NUMBER OF Y DIVISIONS : 15

        MINIMUM Z VALUE :18.0000E 00
        MAXIMUM Z VALUE :11.1000E 01
        NUMBER OF Z DIVISIONS : 15

ADJOINT FOR SHIELD MATERIAL IS IN ADJOINT.:LUCITE2

CROSS SECTIONS FOR MATERIAL ARE IN
        SHIELD.SNXSECT.:FG*37*21 .:LUCITE    .:   0
```

FIGURE 16

SHIELD.SHIELD.?SHLD RECORD

3. the name of the record that contains the adjoint fluxes (collided penetration information) for the outer YZ plane boundary of this segment, and

4. the name of the record that contains the cross-section information for this segment.

The third item, the adjoint flux for the collided particle penetration, depends not only on the shield segment being described, but also on any other segments that a particle would pass through in route from the source to the segment being described. This consideration can affect the definition of segments, as shown in the following example:

For the simplified 2-D source-shield configuration shown in Figure 17, a particle traveling from the source through the two shields normal to the shield surfaces could have three different path histories through the shielding:

(Path 1) It could pass through material 1 only,
(Path 2) It could pass through material 2 only, or
(Path 3) It could pass through both materials 1 and 2.

Each of these three paths needs its own adjoint and must be described as a separate shield segment. This shielding configuration would therefore need to be described in the following three segments:

(1) Composition of material 1 shield, full dimensions of shield 1, adjoint calculated from shield 1 only;

(2) Composition of material 2 shield, dimensions of portion of shield 2 above shield 1, adjoint calculated from shield 2 only; and

(3) Composition of material 2 shield, dimensions of overlapping region between two shields, adjoint calculated from back-to-back shields 1 and 2.

The reason that segment 1 would have the full dimensions of shield 1 (rather than just the part of shield 1 below shield 2) is that the hypothetical particle penetrating shield 1 is "unaware" of shield 2. The converse is not true of particles penetrating shield 2, thus the need for two segments covering shield 2.

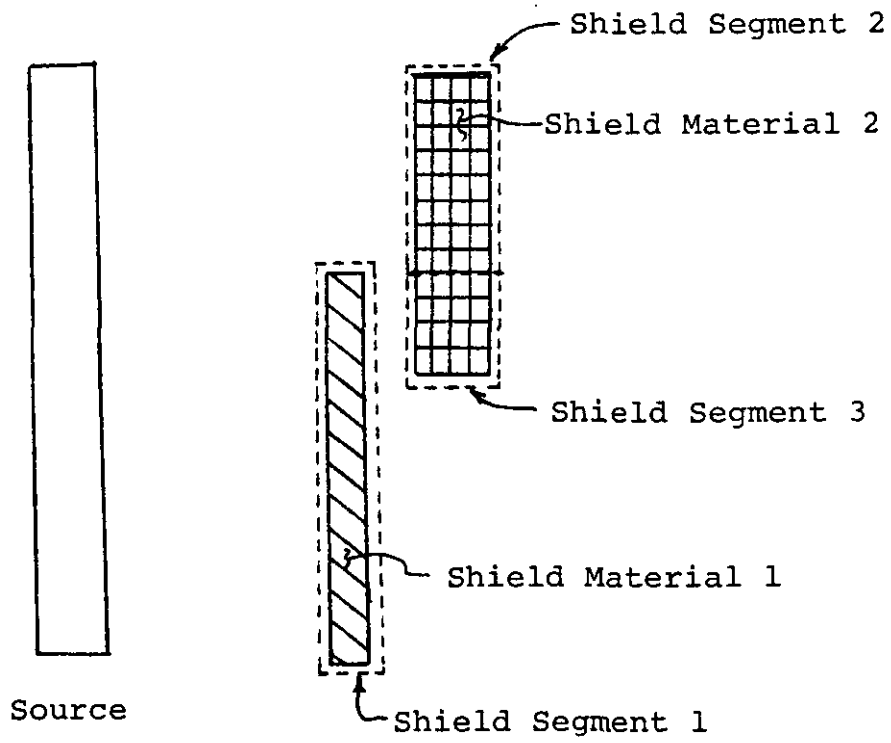


FIGURE 17

DIAGRAM OF SHIELD SEGMENT DIVISIONS

3.8.3 Description of Detector Positions

The location of detector points are given in the record

SHIELD.DETECTOR.?DTEC

as shown in Figure 18. The points are entered by the (x,y,z) coordinates.

4. General Considerations for Calculations With the New Model

The new shielding model has been structured in separate modules for efficiency in running multiple problems with the same sources and/or shields. This makes it especially well suited for parametric and design studies. Table 4 is a list of the input records which must be created by the user for a standard run of the new model using the ANISN58 energy group structure and one of the standard quadrature sets. For each record the page number of a sample figure is given. Table 5 lists the recommended values for some of the input parameters by input record name. Table 6 lists and describes selected intermediate output records.

Much calculational effort can be saved in some cases by taking advantage of the modularity of the system. For repeated calculations on the "same" sources, there is no reason to repeat the ALFN-RADSOR-XPREP2-SNONEF sequence again; the user can just reuse the SHIELD.?PROB.?PROC.BOUND.... records for that source. This is also true for saving repeated runs of the XPREP2-SNONEA sequence for the "same" shield in similar dose calculations.

The quotes were put around the word "same" in the preceding paragraph because SNONEF and SNONEA are one dimensional calculations. Once a source calculation has been run for a given radius (cylindrical geometry) or thickness (slab geometry) source the SHIELD.?PROB.?PROC.BOUND.... records will suffice for any height cylinder or for any width and height slab (described in SHIELD.SOURCE.?SOUR record). The same is true for the shield segments: the SHIELD.ADJOINT.... records apply to a given thickness of the shield material and any height or width can be specified in the SHIELD.SHIELD.?SHLD record.

The original geometric capabilities of the model (1-D cylinder and slab sources, slab shields) were designed for shielding problems on hand. If the capability is every desired to handle shielding problems involving spherical sources, cylindrical shield, or spherical shields, the model could be extended with a modest amount of additional coding.

NO. OF DETECTOR LOCATIONS : 18

POS.	X POSITION	Y POSITION	Z POSITION
1	:26.6700E 00	:20.5000E 01	:30.4800E 00
2	:26.6700E 00	:20.5000E 01	:60.9600E 00
3	:26.6700E 00	:20.5000E 01	:91.4400E 00
4	:26.6700E 00	:20.5000E 01	:12.1920E 01
5	:26.6700E 00	:20.5000E 01	:15.2400E 01
6	:26.6700E 00	:20.5000E 01	:18.2880E 01
7	:80.0000E 00	:18.3500E 01	:30.4800E 00
8	:80.0000E 00	:18.3500E 01	:60.9600E 00
9	:80.0000E 00	:18.3500E 01	:91.4400E 00
10	:80.0000E 00	:18.3500E 01	:12.1920E 01
11	:80.0000E 00	:18.3500E 01	:15.2400E 01
12	:80.0000E 00	:18.3500E 01	:18.2880E 01
13	:13.3400E 01	:18.3500E 01	:30.4800E 00
14	:13.3400E 01	:18.3500E 01	:60.9600E 00
15	:13.3400E 01	:18.3500E 01	:91.4400E 00
16	:13.3400E 01	:18.3500E 01	:12.1920E 01
17	:13.3400E 01	:18.3500E 01	:15.2400E 01
18	:13.3400E 01	:18.3500E 01	:18.2880E 01

FIGURE 18

SHIELD.DETECTOR.?DTEC RECORD

TABLE 4

LIST OF INPUT RECORDS
(Using ANISN58 and standard quadrature sets)

TABLE 5

RECOMMENDED VALUES FOR SELECTED INPUT PARAMETERS

RECORD	VARIABLE	RECOMMENDED VALUE
SHIELD.INPUT.JOB.?JOB	Version of FISSPROD data	ENDFB4
	Version of multigroup (n and α)	ANISN58
	Neutron group structure (n and α)	ANISN58
SHIELD.INPUT.?PROB .?PROC.SOURCE	State No.	1
	Time	0.000
SHIELD.?PROB.?PROC .COMPOSIT.?COMPS.?NTS	Flux history	(blank)
	Time State no.	1
	Time (hrs)	0.0
SHIELD.XSECTION.?CASE	Maximum Legendre order	3
	Density of material	0.0
	Temperature of material	0.0
	All second page input	(blank)
SHIELD.INPUT.?PROB .?PROC.RADFIELD	Quadrature wts	S16SLB1D or S16CYL1D
	Cross sections for problem	FG*37*21
	Initial flux guess	(blank)
	Fission spectrum	any material with fuel
	All third page	(blank)
	Maximum Legendre	3
	Convergence criterion	0.001
	Maximum inner iterations	50
	Maximum outer iterations	20
	Leakage Buckling	0.000
SHIELD.GEOMETRY .?GNAME1.?GNAME2	Low coordinate b.c.	VACUUM for slab, REFLECT for cyl.
	No. of subdivisions	At least 1 per cm thickness
SHIELD.INPUT.?PROB .?PROC.EXPOSE	Dose factor values	FG*37*21

TABLE 5 (Continued)

RECORD	VARIABLE	RECOMMENDED VALUE
SHIELD.SOURCE.?SOUR	Number of divisions	Enough so that the distance between divisions is 2 or 3 times less than distance from source to nearest shield
SHIELD.SHIELD.?SHLD	Number of divisions	Enough so that the distance between divisions is 2 or 3 times less than distance from shield to nearest dose point.

TABLE 6

INTERMEDIATE OUTPUT RECORDS

MODULE	RECORD	DESCRIPTION
ALFN	SHIELD.?PROB.?PROC.SOURCE.?AMAT .?IMAT.NEUTRON	Neutron source rate for material ?AMAT version ?IMAT
RADSOR	SHIELD.?PROB.?PROC.SOURCE.?AMAT .?IMAT.GAMMA	Gamma source rate for material ?AMAT version ?IMAT
XPREP2	SHIELD.SNXSECT.FG*?NN*?MM.?AMAT .?IMAT.XSECTION	Total cross sections for material ?AMAT version ?IMAT
	SHIELD.SNXSECT.FG*?NN*?MM.?AMAT .?IMAT.PLMATRIX.TOTAL.?IG	Scattering matrix for material ?AMAT version ?IMAT to group ?IG
SNONEF	SHIELD.BOUND.?AMAT.?IG	Boundary leakage records for material ?AMAT group ?IG
SNONEA	SHIELD.ADJOINT.?AMAT.NEUTRON .?IMS	Adjoint flux records for material ?AMAT neutron dose rate in angle ?IMS
DOSE	SHIELD.DOSE.COLLIDED.?SOUR	Collided dose rate for source ?SOUR
	SHIELD.DOSE.UNCOLLIDED.?SOUR	Uncollided dose rate for source ?SOUR
	SHIELD.DOSE.TOTAL.?PROC	Total dose rate for problem

REFERENCES

1. Finch, D. R., Chandler, J. R., and Church, J. P., "The SHIELD System," DP-MS-79-54, November 1977.

2. Zimmerman, M. G., "High Burn-Up Plutonium Isotopic Compositions Recommended for Use in Shielding Analysis," BNWL-2282, June 1977.

3. Engle, W. W., Jr., "A User's Manual for ANISN, A One-Dimensional Transport Code with Anisotopic Scattering," USAEC Report K-1693, Union Carbide Corporation, March 1967.

4. Pevey, R. E., "Effects of Feed Composition and Shielding on Radiation Doses in the JB-Line Precipitator Room," DPST-83-369, March 1983.

5. Pevey, R. E., "Verification of the JB-Line Shielding Model," DPST-83-826 (to be issued).

APPENDIX A

DETERMINATION OF (α,n) NEUTRON SOURCE IN MIXTURES

Although the neutron production rates from (α,n) reactions have been experimentally determined for many materials of interest to shielding analysts,[3] it is sometimes necessary to find the (α,n) production rate for mixtures not included in the data. In current studies, for example, we need the rate in PuF_3 knowing the rate in PuF_4. Unfortunately, the relationship between the two is not simple.

Mathematically, the total neutron yield, $Y(E_\alpha)$, from a single alpha particle of energy E is given by:

$$(A.1)\quad Y(E_\alpha) = \sum_i a_i \int_0^{E_\alpha} \sigma_i(E')\, S_m^{-1}(E')\, dE'$$

$$= \frac{\rho_m N_a}{A_m} \sum_i n_i \int_0^{E_\alpha} \sigma_i(E')\, S_m^{-1}(E')\, dE'$$

where $S_m(E)$ = stopping power, MeV/cm, in mixture

a_i = abundance of nuclide i, atoms barn/cm

n_i = no. of atoms of i per molecule of mixture

$\sigma_i(E)$ = (α,n) cross section in barns

N_a = Avogadro's number

$Y(E_\alpha)$ = neutrons/alpha of energy E_α

ρ_m = density of mixture g/cm^3

and A_m = atomic weight of mixture

To formally evaluate (A.1) would require knowledge of both the (α,n) cross section and the stopping power as a function of alpha particle energy. The relationship can be simplified, however, because the stopping power shape is practically independent of material if expressed in MeV-cm^2/g. Denoting

this shape as $S_H(E)$ normalized to a hydrogen medium, use of the Bethe formula[4] gives the relationship between the stopping power of element x to the stopping power of hydrogen as:

$$S_x(E_\alpha) \doteq \frac{\rho_x}{\rho_H} S_h(E_\alpha)\, Z_x\, (1. - k*\ln(Z_x))/A_x$$

where Z_x, A_x = atomic number, atomic weight of element x,

ρ_x = density of material x, grams/cm^3, and

k = 0.15 from a fit to experimental data.

If we define

$$K_x = Z_x\, (1 - 0.15*\ln(Z_x))/A_x,$$

then the ratio of stopping powers between materials x and hydrogen is:

$$\frac{S_x(E_\alpha)}{S_H(E_\alpha)} = \frac{\rho_x K_x}{\rho_H}.$$

For a mixture. this is: $\dfrac{S_m(E_\alpha)}{S_H(E_\alpha)} = \dfrac{\rho_m}{\rho_H} \sum_i n_i K_i \dfrac{A_i}{A_m}$

where i = constituent of mixture m,

n_i = no of atoms of i per molecule of mixture m.

Using this result in Equation (A.1) for mixture m yields

$$Y_m(E_\alpha) = N_a \sum_i n_i \int_0^E \frac{\sigma_i(E')\,\rho_H}{S_H(E')\sum_j n_j K_j A_j}\, dE'$$

$$= \left[\sum_i n_i \int_0^{E_\alpha} N_a \frac{\sigma_i(E')\rho_H}{S_H(E')}\, dE'\right] * \left[\frac{1}{\sum_j n_j K_j A_j}\right]$$

For a mixture of known composition, the only unknowns of the problem are in the integral, defined by

$$I_i(E_\alpha) = \int_0^{E_\alpha} N_a \frac{\sigma_i(E')\rho_H}{S_H(E')}\, dE'$$

and we have

$$(A.2)\quad Y_m(E_\alpha) = \sum_i n_i I_i(E_\alpha) / \sum_J n_j K_j A_j$$

Example 1: Given that for pure carbon Y_C (5.Mev) = 5.3×10^{-8} (Ref. 3) predict Y_{uc} (5.).

For pure carbon $n_C = 1$ and

$$Y_C(5.) = \frac{I_C(5.)}{K_C * A_C} = 5.3 \times 10^{-8}$$

$$K_C = Z_C\,(1 - 0.15\ \ln\ (Z_C))/A_C = 6(1 - 0.15\ \ln\ 6)/12 = 0.36562$$

$$\therefore I_C\ (5.) = (5.3 \times 10^{-8})(.36562)^{(12)} = 2.3253 \times 10^{-7}$$

For the mixture UC, $n_u = 1$, $n_C = 1$

$$K_C = 0.36562$$

$$K_u = 92\ (1 - 0.15\ \ln\ 92)/238 = 0.12437$$

$$I_u = 0.$$

$$Y_{uc} = \frac{2.3253 \times 10^{-7}}{(.36562)(12) + (.12437)\ (238)} = 6.8418 \times 10^{-9}$$

The Reference 3 value is 6.2×10^{-9}. (This was calculated using Equation A.1. with cross section data.)

In applying this procedure, one must know the number and energies of the emitted alphas. The total neutron source is given by:

$$(A.3)\quad Y_{total} = \sum_k S_k Y_m(E_k)$$

where k represents a given alpha source with emission rate S_k and energy E_k.

Substituting (A.2) into (A.3) yields

$$Y_{total} = \sum_k S_k \sum_i n_i I_i(E_k) \sum_j n_j K_j A_j$$

The value $I_i(E_k)$ is calculated by the relationship

$$I_i(E_k) = (EF)_{ik} I_i(5.\ MeV)$$

where $I_i(5.\ MeV)$ = neutron yield in isotope i from a 5. MeV alpha particle

$(EF)_{ik}$ = "effectiveness factor" of alpha source k in isotope i

$$= I_i(E_k)/I_i(5.)$$

$$Y_{total} = \sum_k S_k \sum_i n_i I_i(5)(EF)_{ik} / \sum_j m_j K_j A_j$$

Example 2: PuF_4 produces 2.04×10^6 neutrons/sec/g Pu-238 and 6.35×10^3 neutrons/sec/g Pu-239. What is the neutron production rate of PuF_3 which is 90 wt % Pu-239 and 10 wt % Pu-238?

For $Pu^{238} F_4$, (A.3) is

$$Y^{F48}_{total} = S_{48} (4 \times I_F(5)(EF)_{F48})/(K_{48} * 238 + 4 *_F K * 19)$$

$$K_{48} = 94 (1 - 0.15 \ln 94)/238 = 0.12580$$

$$K_F = 9 (1 - 0.15 \ln 9)/19 = 0.31757$$

$$Y^{F48}_{total} = \frac{S_{48} * I_F(5.) * (EF)_{F48}}{13.5186} = 2.04 * 10^6$$

$$S_{48} * I_F(5.) * (EF)_{F48} = 2.7578 * 10^7$$

For Pu^{238} F_4,

$$K_{49} = 94*(1 - 0.15 \ln 94)/239 = 0.12527$$

$$Y^{F49}_{total} = \frac{S_{49} * I_F(5.) * (EF)_{F49}}{13.5186} = 6.35 \times 10^3$$

$$S_{49} * I_F(5.) * (EF)_{F49} = 8.58433 \times 10^4$$

For the 90% - 10% PuF_3 mixture

$$Y^{PuF_3}_{total} = \left[S_{48} * 0.1 * 3 * I_i(5)(EF)_{F48} + S_{49} * 0.9 * 3 * I_F(5) * (EF)_{F49}\right] / (0.9 * K_{49} * 239 + 0.1 * K_{48} * 238 + 3K_F * 19)$$

$$= \left[0.3 * 2.7578 * 10^7 + 2.7 * 8.48433 * 10^4\right] / (0.9 * 0.12527 * 239 + 0.1 * 0.12580 * 238 + 3 * 0.31757 * 19)$$

$$= 1.77 * 10^5 \quad \text{neutrons/sec/g Pu}$$

Comparing this result with a 90%-10% PuF_4 mixture, which would produce $2.097 * 10^5$ neutrons/sec/g Pu, we see that PuF_3 is a neutron source about 85% as strong as PuF_4.