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**Least-Squares Dosimetry Unfolding:
The Program STAY'SL**

F. G. Perey

OAK RIDGE NATIONAL LABORATORY

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F. G. Perey

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ABSTRACT

A PDP-10 FORTRAN IV computer program STAY'SL, which solves the dosimetry unfolding problem by the method of least squares, is described. The solution (the output spectrum and its covariance matrix) is calculated by minimizing chi-square based on the input data (the activation data, the input spectrum, the dosimetry cross sections and their uncertainties given by covariance matrices). The solution reflects therefore the uncertainties in all of the input data and their correlations. The correlations among the various dosimetry cross sections are taken into account; however, the activation data, input spectrum and cross sections as classes are assumed to be uncorrelated with each other.

The code and sample problem are available from the Radiation Shielding Information Center (RSIC) at Oak Ridge National Laboratory.

I. Introduction

The computer program STAY'SL provides a solution to the dosimetry problem by the method of least squares. The output spectrum and its covariance matrix are obtained by minimizing chi-square based upon the activation data, the dosimetry cross sections, the input spectrum and their uncertainties characterized by non-diagonal covariance matrices. Therefore, the solution is the most likely value given the uncertainties in the input data and the important correlations in those uncertainties. We make the important simplification that the three different classes of input quantities (the activation data, the dosimetry cross sections, and input flux) have uncorrelated uncertainties. However, arbitrary correlations may exist among all of the activation cross sections.

Details of the formalism and the relationship of STAY'SL to other unfolding codes are given elsewhere.^{1,2} In Section II we provide an outline of the formalism and notation to assist in the understanding of the program solution. In Section III the method of computation is outlined to facilitate conversion of STAY'SL to other computers. Section IV describes the input to the code. Section V provides some comments on the output of the code. Section VI describes three utility programs which were developed in conjunction with the code and may prove useful to others, at least in the early stages of applications of STAY'SL. Finally, in Section VII we give a sample problem.

II. The Mathematical Formalism

A. Notation

We use capital letters to denote vectors and matrices with lower case letters bearing indices to denote the elements of these vectors and matrices.

Let V be a vector, we have:

$$V \equiv \begin{pmatrix} v_1 \\ v_2 \\ \vdots \end{pmatrix},$$

or we may write $V \equiv \{v_i\}$. Similarly for a matrix M we have:

$$M \equiv \begin{pmatrix} m_{11} & m_{12} & \cdots \\ m_{21} & m_{22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix},$$

or $M \equiv \{m_{ij}\}^{\sim}$

The transpose of a vector V or a matrix M is denoted by V^{\dagger} and M^{\dagger} .

We denote by \tilde{V} the diagonal matrix built from the vector V where:

$$\tilde{v}_{ii} = v_i,$$

and

$$\tilde{v}_{ij} = 0 \quad \text{for } i \neq j.$$

Matrix multiplications are denoted as follows:

$$A = B \cdot C$$

where

$$a_{ij} = \sum_k b_{ik} c_{kj}$$

We indicate the partition of a vector A into say the vectors B and C by:

$$A = \begin{pmatrix} B \\ C \end{pmatrix},$$

where, if B has the dimension k,

$$a_i = b_i \quad \text{for } i \leq k,$$

and

$$a_{k+i} = c_i.$$

Similarly, we indicate the partition of matrix M into submatrices by:

$$M = \begin{pmatrix} M_1 & M_2 \\ M_3 & M_4 \end{pmatrix},$$

where M_1 , M_2 , M_3 and M_4 are matrices of appropriate dimensions. When partitioning vectors and matrices often some subvectors or submatrices are null, i.e. all elements are zero, and we indicate this by the symbol 0.

B. Definitions

Let A° represent the measured saturated activities a_i° , $A^\circ \equiv \{a_i^\circ\}$.

Let M_{A° represent the relative covariance matrix of A° . Therefore, the covariance matrix of A° , N_{A° , is given by:

$$N_{A^\circ} = \tilde{A}^\circ \cdot M_{A^\circ} \cdot \tilde{A}^\circ.$$

Let ϕ represent the "group flux," i.e. $\phi \equiv \{\phi_j\}$, where the ϕ_j 's are the group fluxes over an appropriate neutron energy group structure for the problem. We often loosely refer to ϕ as the spectrum.

Let M_ϕ be the relative covariance matrix of ϕ and its covariance matrix, N_ϕ , is given by:

$$N_\phi = \bar{\phi} \cdot M_\phi \cdot \bar{\phi}^T .$$

Let Σ^i represent the cross sections σ_j^i for the activation a_i , $\Sigma^i \equiv \{\sigma_j^i\}$, where we have:

$$a_i \equiv \Sigma^{iT} \cdot \phi .$$

The σ_j^i 's are therefore the average cross section for activation i over the energy group j .

We define the cross section vector Σ as:

$$\Sigma \equiv \begin{pmatrix} \Sigma^1 \\ \Sigma^2 \\ \vdots \end{pmatrix} .$$

Note that we use a superscript to identify the various reactions and that Σ is a vector and not a matrix, i.e. $\Sigma \equiv \{\sigma_i\}$. If we have k energy groups, then:

$$\begin{aligned} \sigma_i &= \sigma_i^1 , \\ \sigma_{k+i} &= \sigma_i^2 , \\ \sigma_{2k+i} &= \sigma_i^3 , \quad \text{etc...., where } i \leq k. \end{aligned}$$

Let M_Σ be the relative covariance matrix of Σ which we may consider as partitioned into the submatrices $M_{\Sigma ij}$ as follows:

$$M_\Sigma = \begin{pmatrix} M_{\Sigma 11} & M_{\Sigma 12} & \cdots \\ M_{\Sigma 21} & M_{\Sigma 22} & \cdots \\ \vdots & \vdots & \ddots \end{pmatrix} ,$$

where $M_{\Sigma ij}$ is the relative covariance matrix of Σ^i and of Σ^j . The covariance matrix of Σ , N_{Σ} , is given by:

$$N_{\Sigma} = \overset{\sim}{\Sigma} \cdot M_{\Sigma} \cdot \overset{\sim}{\Sigma}$$

We define the parameter vector P as:

$$P \equiv \begin{pmatrix} \Phi \\ \Sigma \end{pmatrix},$$

and its covariance matrix N_P is therefore given by:

$$N_P = \begin{pmatrix} N_{\Phi} & 0 \\ 0 & N_{\Sigma} \end{pmatrix}.$$

Note that we assume there are no correlations of Φ and Σ since we have the "off diagonal" submatrices of N_P equal to zero.

We define the sensitivity matrix G as the matrix which transforms the changes in the parameters p_i , i.e. the vector ΔP , into the changes in the calculated activities a_j , i.e. the vector ΔA , we have:

$$\Delta A \equiv G \cdot \Delta P$$

More specifically the sensitivity matrix G is given by:

$$G = \begin{pmatrix} \Sigma^{1+} & \Phi^{\dagger} & 0 & 0 & \dots \\ \Sigma^{2+} & 0 & \Phi^{\dagger} & 0 & \dots \\ \vdots & \vdots & \vdots & \vdots & \dots \end{pmatrix}.$$

The covariance matrix of the calculated activities A, N_A , is therefore given by:

$$N_A = G \cdot N_P \cdot G^{\dagger}$$

Since the covariance matrix N_p is diagonal in the space of ϕ and Σ , the covariance matrix N_A is made up of two contributions, one from N_ϕ and one from N_Σ . We write them as N_A^ϕ and N_A^Σ and:

$$N_A = N_A^\phi + N_A^\Sigma ,$$

where

$$N_A^\phi = \{n_{Aij}^\phi\} = \{\Sigma^{i+} \cdot N_\phi \cdot \Sigma^j\} ,$$

and

$$N_A^\Sigma = \{n_{Aij}^\Sigma\} = \{\phi^\dagger \cdot N_{\Sigma ij} \cdot \phi\} .$$

C. The Least-Squares Solution

With the above definitions the χ^2 -function applicable to the dosimetry problem is:

$$\chi^2 = \begin{pmatrix} P & -\bar{P} \\ A^\circ & -\bar{A} \end{pmatrix}^\dagger \cdot \begin{pmatrix} N_p & 0 \\ 0 & N_{A^\circ} \end{pmatrix}^{-1} \cdot \begin{pmatrix} P & -\bar{P} \\ A^\circ & -\bar{A} \end{pmatrix} ,$$

where P and N_p are calculated from the input values of ϕ, Σ and M_ϕ, M_Σ respectively and \bar{A} is calculated from \bar{P} . Note that in our expression for the χ^2 -function we have assumed that P and A° were not correlated.

The value of \bar{P} which minimizes the χ^2 -function is P' and is given (see, for instance, reference 3) by:

$$P' - P = N_p \cdot G^\dagger \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A) .$$

The covariance matrix of P' is also given by:

$$N_{P'} - N_p = -N_p \cdot G^\dagger \cdot (N_A + N_{A^\circ})^{-1} \cdot G \cdot N_p^\dagger .$$

The minimum value of χ^2 is given by:

$$\chi_m^2 = (A^\circ - A)^\dagger \cdot (N_A + N_{A^\circ})^{-1} \cdot (A^\circ - A)$$

and has n_A degrees of freedom where n_A is the number of activation measurements.

The matrix $(N_A + N_{A^\circ})^{-1}$ is often called W the weight matrix and a solution can only be found if $N_A + N_{A^\circ}$ is nonsingular.

Through the use of $\Delta A \equiv G \cdot \Delta P$ we essentially have the capabilities of doing a nonlinear least squares. However, the code STAY'SL was written in such a way that iterations should not be done with the solution.¹

III. Method of Computation

The program STAY'SL solves only for the ϕ' and N_{ϕ} , components of P' and N_p , to solve the "dosimetry unfolding problem." The program TRY'SL, soon to be released, solves also for the Σ' and N_{Σ} , components of P' and N_p .

Although the mathematical formalism outlined above is written in terms of matrices whose dimensions may be very large, i.e. N_p , an analysis of the computational steps involved indicates that they may be handled one row at a time. Furthermore, as we have indicated, through proper partitioning of the large matrices, one need never handle more than one row at a time of the submatrices which have the dimensions of the number of groups in the flux ϕ .

We shall now indicate the flow of computation in STAY'SL:

1. The vector A° and its relative covariance matrix $M_{A^{\circ}}$ are read in. The covariance matrix $N_{A^{\circ}}$ is computed from:

$$N_{A^{\circ}} = \tilde{A}^{\circ} \cdot M_{A^{\circ}} \cdot A^{\circ} \quad .$$

2. The input assumed spectrum, in "group form," ϕ is read in.
3. The dosimetry cross sections Σ^i are read in one at a time and the "C-matrix" is computed where:

$$c_{ij} = \phi_j \sigma_j^i \quad .$$

4. The relative covariance matrix M_{ϕ} is read in one row at a time and the "U-matrix" is computed where:

$$u_{ij} = \sum_{\ell} m_{\phi j \ell} c_{i \ell} \quad ,$$

and \sum_{ℓ} means summation over ℓ .

5. The vector A is computed where:

$$a_i = \sum_j c_{ij}$$

6. The covariance matrix N_A^Φ is computed where:

$$n_{Aij}^\Phi = \sum_l c_{il} u_{jl}$$

7. The relative covariance matrices $M_{\Sigma ij}$ are read in one row at a time. It is convenient to label the element of the k^{th} row and l^{th} column of the matrix $M_{\Sigma ij}$ by $M_{\Sigma ij,kl}$. The covariance matrix N_A^Σ is computed where:

$$n_{Aij}^\Sigma = \sum_{k,l} c_{ik} m_{\Sigma ij,kl} c_{jl}$$

8. The W matrix is computed by inverting the matrix $N_A^\Sigma + N_A^\Phi + N_{A^0}$.

9. The minimum value of χ^2 , χ_m^2 is computed from:

$$\chi_m^2 = \sum_{i,j} (a_i^0 - a_i) w_{ij} (a_j^0 - a_j)$$

10. The output group fluxes ϕ'_j are computed from:

$$\phi'_j = \phi_j [1 + \sum_{i,k} u_{ij} w_{ik} (a_k^0 - a_k)]$$

11. The output relative covariance matrix M_Φ is computed where:

$$m_{\Phi'kl} = m_{\Phi kl} - \sum_{i,j} w_{ij} u_{ik} u_{jl}$$

Coding: The code listed in Appendix C consists of:

1. A main program.
2. A subroutine TITLE to read in the names of the input files.

It is through TITLE that the PDP-10 program is interactive.

3. A subroutine SCALE to scale each row of the matrix $N_A^\phi + N_A^\Sigma + N_{A^0}$ prior to inversion.
4. A subroutine PIVOT to invert the scaled matrix.
5. A subroutine RESCAL to scale the inverted matrix and obtain W.

Limitations: STAY'SL is currently dimensioned to accommodate 20 activation measurements and 200 group fluxes ϕ_j .

- Computation in PIVOT will stop if the matrix $N_A^\phi + N_A^\Sigma + N_{A^0}$ approaches singularity. The program types out the matrix before terminating prematurely the computation.

- As in all least squares procedures, STAY'SL is capable of producing a solution even when the input data are highly unlikely. However, as in all least squares procedures, there is a way to test the statistical consistency of the input data through the minimum value of χ^2 . Although the calculation will proceed regardless of how unlikely are the input data, a warning will be given on the output when χ^2 per degrees of freedom is less than 0.3 or greater than 2 where the output should be viewed with great caution.

IV. Input Description

The input to STAY'SL is in six files which are read sequentially. The subroutine TITLE is used to provide at execution time the names of these files. The names of the files with their extension are read in an A10-format.

A. Activation Data File

The description of the input files will be given by stating the FORTRAN list of the read statement and the format for ASCII files.

The activation data file is an ASCII file.

a. list: KA

format: I

KA is the number of activation measurements.

b. list: (AO(I),I=1,KA)

format: 10F

AO(I) is the saturation activity for the Ith reaction in units of DPS/target atom x 10²⁴.

Note: No provision is made in STAY'SL for cover foils.

B. Activation Covariance File

The activation covariance file is an ASCII file.

DØ 1 I=1,KA

1 List: (AOM(I,J),J=I,KA)

format: 10F

AOM(I,J) is the relative covariance of the Ith and of the Jth activity.

Note: A standard deviation of 1% corresponds to a relative variance of: 0.0001.

C. Flux Data File

The flux data file is an ASCII file.

a. list: KG, AK, VAK, NOR

format: I, 2F, I

KG is the number of group fluxes.

AK is an optional normalization constant.

When the group fluxes in the file are to be considered as properly normalized, $AK = 1$.

AK is a convenience facility in case the group fluxes in this file need to be renormalized prior to execution in STAY'SL.

STAY'SL considers the input flux to the least squares to be the renormalized flux.

VAK is an optional relative variance constant.

When the relative covariance matrix of the fluxes is to be considered as incorporating the component describing the relative uncertainty in the absolute normalization of the group fluxes, $VAK = 0$.

VAK is a convenience facility in case the relative covariance matrix of the fluxes in the flux covariance file did not include the component due to the relative uncertainty in the absolute normalization. VAK is added to every element of the flux covariance matrix read from the file prior to input to the least squares.

NOR is an option on normalization of the input group fluxes when $AK = 0$. If $AK \neq 0$, NOR is ignored. When $AK = 0$, the group fluxes will be renormalized prior to the least squares. The method of normalization depends upon the value of NOR.

NOR = 0 the input flux is normalized to minimize the sum of the square of the relative difference in the measured and computed activities calculated with the group fluxes read in.

NOR \neq 0 the input flux is normalized to minimize the sum of the square of the difference between the measured and computed activities calculated with the group fluxes read in.

Note: We emphasize that STAY'SL works with absolute group fluxes and will produce a normalized output flux consistent with all of the input data. AK, VAK and NOR are merely convenience features which were incorporated in the code to avoid regenerating the input group flux file and covariance matrix file if these had been generated on the basis of some arbitrary normalization.

b. list: (F(I),I=1,KG)

format: 10F

F(I) is the group flux in group I. F(I) is in neutrons $\text{sec}^{-1}\text{cm}^{-2}$.

c. list: (EL(I),I=1,KG)

format: 10F

EL(I) is the lower energy of the boundary of group I.

Note: EL(I) is not used by the code in any calculation, but merely used to make the output listing more readable.

D. Dosimetry Cross Section File

The dosimetry cross section file is an ASCII file.

```

DØ  1  I=1,KA
1   list: (S(I,J),J=1,KG)
      format: 10F

```

$S(I,J)$ is the dosimetry cross section for reaction I in group J.

The $S(I,J)$'s are in units of barns.

Note: The cross sections are average cross sections. The contribution to the activity $A(I)$ of neutrons in group J is given by $F(J)*S(I,J)$.

E. Flux Covariance File

The flux covariance file is a binary file.

```

DØ  1  I=1,KG
1   list: (FM(I,J),J=1,KG)

```

$FM(I,J)$ is the relative covariance of group flux I and group flux J.

F. Cross Section Covariance File

The cross section covariance file is a binary file.

The relative covariance matrix of the cross sections M_{Σ} is partitioned in the file into the matrices $M_{\Sigma ij}$. Each element of the matrix M_{Σ} in the file has associated with it four indices — I and J to denote the reactions and K and L to denote the groups.

The relative covariance matrix is read as:

```

DØ  2  I=1,KA
DØ  2  J=I,KA
list: FC
IF(FC.NE.1.) GO TO 2
DØ  1  K=1,KG
1   list: (SM(I,J,K,L),L=1,KG)
2   CONTINUE.

```

FC is a flag.

FC=1 when it precedes a full covariance matrix in the file.

FC≠1 indicates a "flat" covariance matrix, i.e. one where all the elements are equal to FC, in which case the matrix is not explicitly written in the file.

SM(I,J,K,L) is the relative covariance of the cross section for the reaction I in group K and of the cross section for the reaction J in group L.

V. Code Output

During execution of the code two scratch files, units 3 and 4 are used as storage for intermediate quantities (matrix elements of a KG by KG matrix).

STAY'SL generates two output files;

- A. STAYSL.CAL is a binary file which may be used by the FORTRAN coding:

```

      READ  KG
      READ  (F(I),I=1,KG)
      DØ    1    I=1,KG
1      READ  (FM(I,J),J=I,KG)
      READ  (FP(I),I=1,KG)
      DØ    2    I=1,KG
2      READ  (FMP(I,J),J=I,KG)

```

KG is the number of groups.

F(I) is the normalized input group flux in group I.

FM(I,J) is the relative covariance matrix of the input group flux I and input group flux J.

FP(I) is the output group flux in group I.

FMP(I,J) is the relative covariance matrix of the output group flux I and output group flux J.

- B. STAYSL.OUT is an ASCII file which is the annotated listable output of the code STAY'SL. We shall make a few comments on the output of the code. The contents of five input files are given in STAYSL.OUT, although often not in the input format.

The covariance matrices of the activation data and the input group fluxes are given in terms of the standard deviations and correlation matrices. The content of the cross section covariance file is not reproduced.

Page 1. χ_m^2 is given. As an assist in understanding the various contributions to it a quantity CHI, associated with each activation, is printed. The computation of χ_m^2 involves a double summation (see Section III.g.). The values of CHI are the terms contributing to the second summation. Since the W matrix is nondiagonal, χ_m^2 cannot be broken down into components which are uniquely associated with each dosimetry data. A large value of CHI for a given activation indicates some level of improbability associated with the activation in question.

When χ_m^2 per degree of freedom is less than 0.3 or more than 2, a message is printed out as a word of caution since this should be an unlikely statistical occurrence.

Under the heading of Dosimetry Activities is presented the measured input values and their standard deviations. The next column gives the calculated activities from the input group fluxes and dosimetry cross sections. The "difference" column indicates the percentage deviations of these calculated numbers with the measured activities.

The "after" column is a very peculiar quantity since it represents the calculated activities on the basis of the output group fluxes, but the input dosimetry cross sections!! This quantity has no real meaning in the context of the least squares procedure unless the cross sections were so well known that their output values are essentially the same as the input values. This occurs when all of the covariance matrix elements

of N_A^Σ are small compared to those of N_A^Φ . In such circumstances then mostly the group fluxes have been adjusted and very little change was made in the parameters Σ . The "difference" column indicates the percentage deviation of these values from the measured ones. The meaning of the CHI column has been explained above.

Page 2. The covariance matrix $N_A^\Sigma + N_A^\Phi$ is first given in the form of standard deviations and correlation matrix. The individual covariance matrices N_A^Φ and N_A^Σ are also given. It is always instructive to compare the three covariance matrices N_{A0} , given in the first page, and the two covariance matrices N_A^Φ and N_A^Σ since these provide in a nutshell the clue to the whole "dosimetry unfolding problem" and what has been learned from the dosimetry measurement.^{1,2}

Page 3. The input dosimetry cross sections are listed.

Page 4. The input and output group fluxes are printed as well as their standard deviations, followed by the integrals of the spectra with their standard deviations.

Page 5. The correlation matrix of the input group fluxes is listed.

Page 6. The correlation matrix of the output group fluxes is listed.

Note: All correlation matrices on the output have their elements multiplied by 1000.

VI. Utility Programs

Three utility programs are released with the code STAY'SL — one to prepare average cross sections and two to prepare covariance files.

Preparation of the input files for the activation data, group fluxes and dosimetry cross sections should present no particular problems to users of STAY'SL familiar with other dosimetry unfolding codes since the same information is required in very similar format. It is therefore assumed that their current utility programs to prepare such input may be easily adapted to create the input to STAY'SL. The utility program GROUP is nevertheless provided to assist in running the sample problem, though it may not be too generally useful.

Preparation of the input covariance files for STAY'SL may be more difficult since other unfolding codes do not require such specific input. The two utility programs FCOV and XCOV, which generate group fluxes and dosimetry cross section covariance files, are intended to fill a gap in the early stages of use of STAY'SL since such information is often not readily available. These programs create relatively crude covariance matrices which nevertheless should be useful to communicate to STAY'SL the major features of the covariance matrices in the absence of a detailed analysis. Ultimately dosimetry cross section evaluators should provide the covariance information as an integral part of the evaluations as is now possible in ENDF/B. This information should then be processed to obtain the covariance files needed by STAY'SL. The creation of group flux covariance matrices should be specific to the problems being solved and information based on sensitivity analysis and/or other information about the flux analyzed to obtain a credible covariance matrix.

A. The Program GROUP

1. General Description

The interactive PDP-10 FORTRAN IV program GROUP was primarily written to average cross sections which were tabulated over a certain energy mesh and varied linearly as a function of energy between tabulated values. The output energy mesh was a subset of the input tabulated mesh. A group flux file option was added to generate group fluxes based upon a fission spectrum or a 1/E plus fission spectrum above an input energy.

The input to the program is mostly in an energy grid file which specifies the input and output energy mesh structure and in files which contain the tabulated individual dosimetry cross sections. The output is in two files – the group flux file, if the flux option is used, and a cross section file. Both of these files may be read directly by STAY'SL.

The interactive part of the program consists mostly of providing to the code, at execution time, names of input and output files as well as whether to generate the group flux file and when it does the "normalization data option."

2. Input

a. The E-GRID File

The E-GRID file provides the description of the input and output energy mesh structure. It is read as follows:

i) list: NGS,NGU

format: 2I

NGS is the number of energies where the input cross sections are tabulated.

NGS \leq 611

NGU is the number of energy intervals for the output averaged cross sections.

NGU \leq 200

ii) list: (E(I),I=1,NGS)

format: 10F

E(I) is the energy in MeV at which the Ith cross section is given in the input files.

The last point, i.e. E(NGS), must be 18 MeV.

iii) list: (ID(I),I=1,NGU)

format: 10I

ID(I) is the number of energy intervals, defined by the input energy mesh, which are used to provide the Ith averaged output cross section. The sum of the ID(I)'s must equal NGS.

b. The Flux Option

After the E-GRID file is read, the code tries to exercise the flux option before processing the dosimetry cross sections. The code types:

FLUX OPTION: NF,EØE

It then waits for NF and EØE to be given (format: I,F). If:

NF = 0, the flux option is not exercised.

\neq 0, a group flux file, to be used as input to STAY'SL, will be generated based upon a normalized FRYE spectrum calculated at the midpoint of the output energy grid times the width of the group in MeV.

EØE, a matching energy in MeV below which the FRYE spectrum is replaced by a 1/E spectrum. The 1/E component is normalized to the FRYE spectrum at the energy EØE.

If the group flux file option is exercised, a file name must be provided at the query, GROUP FLUX FILE?, in A10 format. The normalization data required by STAY'SL are typed in at the query, ANORM, REL.VAR, IØP?, in 2F,I format.

c. The Cross Section Processing

The code requests a file name for the output cross section file to be used as input to STAY'SL. It is provided after the query, AVERAGED X-SECTION ØUTPUT FILE?, in A10 format. Then the code requests the names of the individual input cross section files which must be provided in A10 format. The input cross section files are read in the format 10F. Input to the code is terminated by a blank file name.

B. The Program FCOV

1. General Description

The interactive PDP-10 FORTRAN IV program FCOV may be used to provide a group flux covariance matrix file as input to STAY'SL. FCOV was written as a convenience to users of STAY'SL in the absence of a detailed analysis based on sensitivity studies and/or other information concerning the spectrum being analyzed which would provide a more credible and realistic relative covariance matrix.

FCOV may generate covariance matrices having three features:

1. A diagonal component, which therefore allows a statement to be made of how well the individual input group fluxes are known.
2. Fully correlated components which span several groups. A statement can therefore be made about correlations of group fluxes over a variable energy range. A serious limitation of FCOV as released is that

a particular group may only lie within one of these energy ranges and the various groups in the different energy ranges are uncorrelated.

3. A long-range component which spans the full energy range allowing a statement to be made about how well the overall normalization is known.

In ENDF/B-V language FCOV can presently process only 3, LB=1 type sub-subsections of file MF=33.

B. Input

The program FCOV is interactive only in the sense that the subroutine IØ is used to obtain the names of the input and output files which are read in A10 format.

The input file is read as follows:

a. The Control Record

list: KG, KD, KB, F

format: 3I, F

KG is the number of groups ($KG \leq 200$)

KD is a flag which controls the input for the diagonal components.

($KD < 100$)

KD < 0: there is no diagonal component to the relative covariance matrix.

KD=0. The diagonal components are specified for every group and will be read in.

KD > 0. A "short form" will be used to specify the diagonal component to be read.

KB is a flag which controls the input for the broad range component.

($KB < 100$)

$KB \leq 0$ there are no broad range components to the relative covariance matrix.

$KB > 0$ specifies the number of broad range components which span the full energy range.

F is the flat covariance matrix component of the relative covariance matrix.

Note: i) Each component given by KD, KB and F is added to obtain the relative covariance matrix.

ii) A value of $F=0.01$ means a standard deviation for the overall normalization of 10% since $0.01=(0.1)^2$.

b. The Diagonal Component

If $KD \geq 0$, the control record is followed by a specification of the diagonal component. The format will be a function of the value of KD.

$KD = 0$ FCOV will read:

list: (D(I),I=1,KG)

format: 10F

D(I) is the relative standard deviation for the diagonal component of group flux I. A 10% standard deviation is read in as: 0.1.

$KD > 0$ a "short form" will be used to read the diagonal component since many consecutive groups have the same relative standard deviation.

FCOV will read:

list: (ILD(I),I=1,KD)

format: 10I

list: (DS(I),I=1,KD)

format: 10F

ILD(I) is the lowest group index having the relative standard deviation DS(I).

Note: The "short form" specification is useful when many successive groups are assigned the same relative standard deviation for the diagonal component. FCOV will assign to the groups ILD(I) to ILD(I+1)-1 the value DS(I).

Therefore the value of ILD(1) is always 1 and the last value of ILD(KD) is less than KG. The code assumes that ILD(KD+1) which is not read in is KG+1. Example of list ILD and DS with a KG=200 and KD=3:

ILD list: 1 20 40

DS list: .10 .15 .20

Groups 1 through 19 have a 10% standard deviation.

20 through 39 have a 15% standard deviation.

40 through 200 have a 20% standard deviation.

c. The Broad Range Component

If KB > 0, KB specifies the number of broad range components which will be read after the diagonal components. FCOV will read:

list: (ILB(I),I=1,KB)

format: 10I

list: (B(I),I=1,KB)

format: 10F

ILB(I) is the lowest group index correlated with the broad range component having relative standard deviation B(I).

Note: The component B(I) spans the groups ILB(I) to ILB(I+1)-1. The first value of ILB, i.e. ILB(1), is 1. The last value of ILB, ILB(KB), is < KG. FCOV assumes that ILB(KB+1), which is not read, is KG+1. Example of ILB and B list for KB=4 and KG=200:

ILB list: 1 20 30 51

B list: 0. 0.05 0.1 0.

Groups 1 through 19 have no broad range component since $B(1)=0$.

Groups 20 through 29 are fully correlated by a component having 5% standard deviation.

Groups 30 through 50 are fully correlated by a component having 10% standard deviation.

Groups 51 through 200 have no broad range component since $B(4)$ is 0.

Caution: The diagonal and broad range components are specified by relative standard deviations, but the flat background is denoted by the variance, i.e. the square of the relative standard deviation.

d. Output

The output of FCOV is a binary file containing KG records being the rows of the relative covariance matrix. The output file of FCOV can be read by STAY'SL as created.

c. The Program XCOV

1. General Description

The interactive PDP-10 FORTRAN IV program XCOV may be used to generate a dosimetry cross section relative covariance file as input to STAY'SL. XCOV was written as a convenience to users of STAY'SL pending the availability of evaluated cross section covariance files which could be processed to obtain credible and realistic covariance matrices. Since STAY'SL only solves for the group fluxes, the dosimetry cross section covariances are only required to establish the weight matrix through computation of what was defined in the description as N_A^Σ . Since N_A^Σ is added to N_{A_0} to obtain

the weight matrix W , the important point for the solution of STAY'SL is that the sum of N_A^Σ and N_{A^0} be approximately correct. However, in practice it may be difficult to estimate directly the matrix elements of N_A^Σ without using the covariance matrices of the cross sections.

The users of XCOV should realize that the covariance matrices will only be used to generate N_A^Σ . The program TRY'SL, which also solves for the cross sections, has much more stringent requirements upon the dosimetry cross section covariance matrices.

Given KA reactions, XCOV must generate $KA(KA+1)/2$ covariance submatrices. If we write symbolically $XM(I,J)$ as the covariance matrix of the average cross sections of reaction I and those of reaction J , these covariance matrices must be described in the file in the order given by the simple FORTRAN program

```

      DØ    1    I=1,KA
1      list: (XM(I,J),J=I,KA)

```

XCOV is patterned after FCOV to generate the "diagonal covariance matrices" $XM(I,I)$. However, for the "off diagonal matrices," i.e. $XM(I,J)$ with $I \neq J$, only fully correlated matrices are produced. It is therefore necessary for the user to think of them as "effective covariance matrices." It would have been easier to code XCOV to generate all covariance matrices, diagonal and off diagonal, in the same manner and seemingly provide greater capabilities. However, the burden on the user to prepare the input such that nonphysical covariance matrix elements are not generated was judged too great. Even with "effective off diagonal" covariance matrices the user must be careful since he may generate nonphysical covariance matrices. The most important factor here is not to make sure that all elements of the

matrices $XM(I,J)$ are physically possible, but that the covariance matrix N_A^Σ is physically possible, i.e. has positive eigenvalues. As a consequence, all elements of the correlation matrix of N_A^Σ must be between ± 1 , but this is not sufficient. XCOV cannot perform this check since the concept of "effective covariance matrix" has meaning only in the context of generating N_A^Σ which requires the group fluxes which are not available to XCOV.

B. Input

The program XCOV is interactive only in the sense that the subroutine IØ is used to obtain the names of the input and output files which are read in A10 format.

The input file is read as follows:

a) The Master Control Record

list: KA,KG

format: 2I

KA is the number of reactions.

KG is the number of groups. ($KG \leq 200$)

b) Covariance Matrices Control Record

Following the master control record XCOV requires information to generate each of the $XM(I,J)$ matrices. These must be provided in the order given by the above simple FORTRAN program since they will be written sequentially in the file. More specifically, the order is: $XM(1,1)$, $XM(1,2)$, ..., $XM(1,KA)$, $XM(2,2)$, $XM(2,3)$, ..., $XM(2,KA)$, $XM(3,3)$, $XM(3,4)$, etc.

The covariance matrices control records are of two types: those for the off-diagonal matrices, $XM(I,J)$, and those for the diagonal matrices, $XM(I,I)$.

i) Off-Diagonal Matrices Control Record

The off-diagonal effective matrices are generated by reading in the effective relative covariance of the cross sections as a control record:

list: EFF

format: F

ii) Diagonal Matrices Control Records

The diagonal matrices are generated in the same fashion as done in the program FCOV. The input is therefore identical to the one of FCOV except that since KG, the number of groups, has been read in from the master control record it is not read again from the diagonal matrices control record. See the description of FCOV for detailed explanations of the symbols:

list: KD,KB,F

format: 2I,F

KD is a flag which controls the input of the diagonal components

(KD < 100)

KD < 0 there are no diagonal components to the relative covariance matrix.

KD = 0 the diagonal components are specified for every group and will be read in.

KD > 0 a "short form" will be used to specify the diagonal components.

KB is a flag which controls the input of the broad range component

(KB < 100)

KB \leq 0 there are no broad range components to the relative covariance matrix.

KB > 0 specifies the number of broad range components to the relative covariance matrix which spans the full energy range.

F is the flat component to the relative covariance matrix.

- Note:
1. Each component will be added to obtain the relative covariance matrix of the averaged cross sections over the groups.
 2. A value of F=0.01 means a standard deviation for the overall normalization of 10% since $0.01 = (0.1)^2$.

c) Diagonal and Broad Range Components

For diagonal matrices if the control record has $KD \geq 0$ and/or $KB > 0$ the diagonal components and/or broad range components must be specified. If needed the diagonal components are specified first and then if needed the broad range components are specified.

i) The Diagonal Components

If $KD=0$, XCOV will read after the control record:

list: (D(I),I=1,KG)

format: 10F

D(I) is the relative standard deviation for the diagonal component of the average cross section in group I.

If $KD > 0$, XCOV will read a "short form" to describe the diagonal components:

list: (ILD(I),I=1,KD)

format: 10I

list: (DS(I),I=1,KD)

format: 10F

ILD(I) is the lowest group index having the standard deviation DS(I).

Note: See FCOV description for more complete explanation and example.

ii) The Broad Range Components

If $KB > 0$, following the diagonal matrix control record if $KD < 0$ or after the diagonal components when $KD \geq 0$, XCOV will read the broad range components:

list: (ILB(I),I=1,KB)

format: 10I

list: (B(I),I=1,KB)

format: 10F

ILB(I) is the lowest group index of the average cross section correlated with the broad range component having the relative standard deviation B(I).

Note: See FCOV description for more complete explanation and example.

C. Output

The output of XCOV is a binary file containing the description of the relative covariance matrices of the averaged cross sections for the different reactions.

VII. Sample Problem

The program STAY'SL sample problem is patterned after problem No. 1 of the "unfolding code subgroup" of the "Euratom Working Group on Reactor Dosimetry."⁴

The ASCII files to run the sample problem and the output file are available with the deck from RSIC. The two binary files, the group flux and dosimetry cross section covariance files, must be generated using the utility programs FCOV and XCOV. We shall briefly discuss the statement of the problem by describing the input files and how they were generated.

A. Activation Data File

KA=9

(A0(I),I=1,9) = .7807,.1837,.01595,.09788,.06775,.009821,.001232,
.0005813,.2881.

These are the activation data from the core of the reactor for the reactions Rh¹⁰³, In^{115A}, Ti²⁷, Ni⁵⁸, Fe⁵⁴, Ti⁴⁶, Mg²⁴, Al²⁷ and U²³⁸, respectively.

B. Activation Covariance File

Since the request was to fit every activity to 1%, the relative variance was set to 0.0001 for each activity measured and all off-diagonal elements set to zero:

AOM(I,I) = 0.0001 for I=1 through 9,

AOM(I,J) = 0 for I≠J.

This is a somewhat unrealistic covariance matrix for an actual set of measurements.

C. Flux Data File

The flux data file was generated using the flux option of the utility program GROUP using a 1/E + FRYE spectrum with a matching energy of 2 MeV.

This was not the originally specified input spectrum, but the one used by every participant in the reported set of results. A group structure with 75 groups was used to span the energy range 0.1275 to 18 MeV and consisted of a subset of the last 211 points of the SAND-II energy mesh. The E-GRID file for input to GROUP has:

NGS=211, NGU=75

(E(I),I=1,211) = the last 211 energy points of the SAND-II structure.

(ID(I),I=1,75) =

3	5	4	3	2	2	2	2	2	2
2	2	2	2	2	2	1	1	1	1
1	1	1	1	1	1	1	1	1	1
1	1	1	1	1	1	1	2	2	2
2	2	2	2	2	2	2	2	2	2
2	2	4	4	4	4	4	4	4	4
4	4	5	5	5	5	5	5	5	5
5	5	10	10	10					

NF=2

ANORM = 0., REL.VAR = .0009, IOP = 0.

D. Dosimetry Cross Section File

The dosimetry cross section file was generated using the program GROUP and the E-grid file above as input for the code. The various dosimetry cross sections used as input consisted of the last 211 points provided by the Unfolding Code Subgroup over the SAND-II energy mesh.

E. Flux Covariance File

The flux covariance file must be generated using the utility program FCOV. No information was provided by the Subgroup concerning this input,

and our choice was arbitrary. Since a 3% normalization uncertainty was provided from the flux file, i.e. REL.VAR = .0009, no provision was made for a flat background. A purely uniform diagonal component with a relative standard deviation of 24% in every group was arbitrarily chosen. The strongly diagonal relative covariance matrix therefore generated may approximate the algorithms of other codes used in the comparison.

The input to FCOV was:

$$KG = 75, KD = 1, KB = 0, F = 0.$$

$$ILD(1) = 1$$

$$D(1) = .24.$$

F. Cross Section Covariance File

Uncertainties in the dosimetry cross sections provided by the "Unfolding Code Subgroup" were not specified since these data are not used by the other unfolding code tested. Again, to approximate the results of other codes, artificially small relative covariance matrix elements were used. In order to minimize input to the code XCOV, used to generate the cross section covariance file, the decision was made to calculate completely flat matrices. The diagonal submatrices are given a covariance component of 0.000001, corresponding to an overall normalization of 0.1%, the off-diagonal submatrices are set to zero.

The input to the code XCOV was:

$$KA = 9, KG = 75.$$

Following this master control record, the covariance matrices control records were placed with diagonal matrices control records being:

$$KD = -1, KB = 0, F = .000001$$

off-diagonal matrices control records being:

$$EFF = 0.$$

The net result was the generation of a binary file having 45 records each having a single number being either 0.000001 or 0.

Summary

Programs

The following ASCII files are provided which contain FORTRAN programs:

STAYSL.F4 - STAY'SL main program with subroutines: TITLE, SCALE, RESCAL and PIVOT.

GROUP.F4 - group main program - no subroutines needed.

FCOV.F4 - FCOV main program and subroutine IØ.

XCOV.F4 - XCOV main program and subroutine IØ.

Sample Problem for STAY'SL

Six input files are required to run STAY'SL. The four ASCII files are provided.

ACTIT.DA - contains the activation data

ACTIT.CV - contains the activation covariances

FLUXT.DA - contains the flux data

DØSID.DA - contains the dosimetry cross sections.

The two binary files: the flux covariance file and the dosimetry cross section covariance file, must be generated using FCOV and XCOV.

Flux Covariance File: the program FCOV is executed with the ASCII input file FCOV.INP which is provided.

Dosimetry Cross Section Covariance File: the program XCOV is executed and the ASCII input file XCOV.INP is provided.

Utility Program GROUP

The utility program GROUP need not be run to execute the sample problem since the two output files, FLUXT.DA and DOSID.DA, are provided. For users who would like to exercise the program GROUP, the ASCII input file E-GRID called GROUP.INP is also provided. The file FLUXT.DA may be generated using NF=1 and EØE=2. The file DOSID.DA may be generated using the input ASCII files RH103.DRK, IN115.DRK, TI47.DRK, NI58.DRK, FE54.DRK, TI46.DRK, MG24.DRK, AL27.DRK, AL27.DRK, U238.DRK. The order in which they have been given is the one in which they must be processed to correspond to the activation file ACTIT.DA.

A copy of the teletype printout for execution of the programs, GROUP, FCOV, XCOV and STAY'SL for the sample problem is given in Appendix A.

Sample Run Output

The file STAYSL.OUT is provided and is listed in Appendix B.

ACKNOWLEDGEMENT

I wish to thank G. L. Morgan for providing the subroutine PIVOT.

REFERENCES

1. F. G. Perey, "Uncertainty Analysis of Dosimetry Spectrum Unfolding," Proceedings Second ASTM-EURATOM Symposium on Reactor Dosimetry, Palo Alto, California, October 3-7, 1977.
2. F. G. Perey, "Spectrum Unfolding by the Least-Squares Method," Proceedings IAEA Technical Committee Meeting on Current Status of Neutron Spectrum Unfolding, Oak Ridge, Tennessee, October 10-12, 1977.
3. J. B. Dragt, J. W. M. Dekker, H. Greeppelaar, and A. J. Janssen, Nucl. Sci. Eng. 62, 117 (1977).
4. R. Dierckx and V. Sangiust, "Unfolding Codes for Neutron Spectra Evaluation Possibilities and Limitations," ISPRA, June 1975, EUR/C/IS/365/75e.

APPENDIX A

TELETYPE OUTPUT FOR SAMPLE PROBLEM EXECUTION

EXECUTION OF PROGRAM GROUP*

.EX GROUP)
LINK: LOADING
[LNKXCT GROUP EXECUTION]
PROGRAM GROUP E-GRID FILE ? GROUP.INP)
FLUX OPTION: NF,EOE ? 1 2.)
GROUP FLUX FILE ? FLUXT.DA)
ANORM,REL.VAR,IOP ? 0. 0009 0)
AVERAGED X-SECTION OUTPUT FILE ? DOSID.DA)
X-SECTION NO. 1 FILENAME ? RH103.DRK)
X-SECTION NO. 2 FILENAME ? IN115.DRK)
X-SECTION NO. 3 FILENAME ? TI47.DRK)
X-SECTION NO. 4 FILENAME ? NI58.DRK)
X-SECTION NO. 5 FILENAME ? FE54.DRK)
X-SECTION NO. 6 FILENAME ? TI46.DRK)
X-SECTION NO. 7 FILENAME ? MG24.DRK)
X-SECTION NO. 8 FILENAME ? AL27.DRK)
X-SECTION NO. 9 FILENAME ? U238.DRK)
X-SECTION NO. 10 FILENAME ?)

END OF EXECUTION

CPU TIME: 5.48 ELAPSED TIME: 2:36.80

EXIT

EXECUTION OF PROGRAM FCOV

.EX FCOV ↓

FORTRAN: FCOV

MAIN.

IO

LINK: LOADING

[LNKXCT FCOV EXECUTION]

INPUT FILE FCOV.INP ↓

OUTPUT FILE FLUXT.CV ↓

END OF EXECUTION

CPU TIME: 3.42 ELAPSED TIME: 29.92

EXIT

EXECUTION OF PROGRAM XCOV

.EX XCOV

FORTRAN: XCOV

MAIN.

IO

LINK: LOADING

[LNKXCT XCOV EXECUTION]

INPUT FILE XCOV.INP ↓

OUTPUT FILE DOSID.CV ↓

END OF EXECUTION

CPU TIME: 0.42 ELAPSED TIME: 22.65

EXIT

EXECUTION OF STAY'SL

.EX STAYSL.F4)
FORTRAN: STAYSL
MAIN.
TITLE
SCALE
RESCAL
PIVOT
LINK: LOADING
[LNKXCT STAYSL EXECUTION]
ACTIVATION DATA ACTIT.DA)
ACTIVATION COV. ACTIT.CV)
FLUX DATA FLUXT.DA)
DOSI. X-SECTION DOSID.DA)
FLUX COVARIANCE FLUXT.CV)
X-SECTION COVARIANCES DOSID.CV)

END OF EXECUTION
CPU TIME: 54.18 ELAPSED TIME: 2:48.28
EXIT

* Underlined quantities are typed in by the user. The symbol) means a carriage return.

INPUT DOSIMETRY X-SECTIONS (ENDF/B LAW 1)

G	ENERGY	X-SECTIONS								
1	1.275E-01	3.006E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
2	1.500E-01	2.302E-02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
3	2.000E-01	4.444E-02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
4	2.400E-01	6.870E-02	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
5	2.800E-01	9.054E-02	1.520E-04	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
6	3.200E-01	1.011E-01	8.268E-04	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01
7	3.600E-01	1.146E-01	1.765E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.777E-04
8	4.000E-01	1.279E-01	2.897E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	5.278E-05
9	4.500E-01	1.397E-01	4.557E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.531E-04
10	5.000E-01	1.642E-01	6.953E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	3.177E-04
11	5.500E-01	2.117E-01	9.619E-03	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	7.360E-04
12	6.000E-01	2.797E-01	1.381E-02	1.615E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.090E-03
13	6.600E-01	3.666E-01	1.906E-02	3.132E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.179E-03
14	7.200E-01	4.801E-01	2.591E-02	4.491E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	2.137E-03
15	8.000E-01	5.756E-01	3.496E-02	6.079E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	5.335E-03
16	8.800E-01	6.180E-01	4.438E-02	8.197E-05	0.000E-01	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.076E-02
17	9.600E-01	6.269E-01	5.228E-02	1.063E-04	1.250E-04	0.000E-01	0.000E-01	0.000E-01	0.000E-01	1.389E-02
18	1.000E+00	6.397E-01	6.284E-02	1.520E-04	1.000E-03	3.913E-05	0.000E-01	0.000E-01	0.000E-01	2.008E-02
19	1.100E+00	6.659E-01	8.152E-02	2.467E-04	2.625E-03	4.223E-04	0.000E-01	0.000E-01	0.000E-01	3.341E-02
20	1.200E+00	6.927E-01	1.035E-01	3.895E-04	4.375E-03	1.602E-03	0.000E-01	0.000E-01	0.000E-01	5.918E-02
21	1.300E+00	7.149E-01	1.273E-01	5.987E-04	6.500E-03	3.556E-03	0.000E-01	0.000E-01	0.000E-01	8.000E-02
22	1.400E+00	7.345E-01	1.548E-01	9.361E-04	9.750E-03	6.005E-03	0.000E-01	0.000E-01	0.000E-01	2.432E-01
23	1.500E+00	7.572E-01	1.813E-01	1.505E-03	1.412E-02	8.827E-03	0.000E-01	0.000E-01	0.000E-01	3.513E-01
24	1.600E+00	7.844E-01	2.050E-01	2.470E-03	1.888E-02	1.171E-02	0.000E-01	0.000E-01	0.000E-01	4.225E-01
25	1.700E+00	8.132E-01	2.271E-01	3.938E-03	2.428E-02	1.435E-02	0.000E-01	0.000E-01	0.000E-01	4.738E-01
26	1.800E+00	8.396E-01	2.465E-01	6.188E-03	3.166E-02	1.677E-02	0.000E-01	0.000E-01	0.000E-01	5.162E-01
27	1.900E+00	8.621E-01	2.650E-01	9.554E-03	4.100E-02	1.913E-02	0.000E-01	0.000E-01	0.000E-01	5.474E-01
28	2.000E+00	8.824E-01	2.839E-01	1.409E-02	5.150E-02	2.198E-02	5.135E-06	0.000E-01	0.000E-01	5.683E-01
29	2.100E+00	9.022E-01	3.012E-01	1.935E-02	6.350E-02	2.586E-02	2.567E-05	0.000E-01	0.000E-01	5.804E-01
30	2.200E+00	9.217E-01	3.149E-01	2.429E-02	7.594E-02	3.059E-02	6.212E-05	0.000E-01	0.000E-01	5.816E-01
31	2.300E+00	9.407E-01	3.251E-01	2.836E-02	8.568E-02	3.592E-02	1.107E-04	0.000E-01	0.000E-01	5.747E-01
32	2.400E+00	9.596E-01	3.326E-01	3.161E-02	9.304E-02	4.182E-02	1.915E-04	0.000E-01	0.000E-01	5.653E-01
33	2.500E+00	9.785E-01	3.379E-01	3.420E-02	1.057E-01	4.835E-02	3.363E-04	0.000E-01	0.000E-01	5.563E-01
34	2.600E+00	9.975E-01	3.415E-01	3.635E-02	1.313E-01	5.563E-02	5.805E-04	0.000E-01	0.000E-01	5.483E-01
35	2.700E+00	1.014E+00	3.441E-01	3.824E-02	1.620E-01	6.383E-02	9.882E-04	0.000E-01	0.000E-01	5.425E-01
36	2.800E+00	1.024E+00	3.461E-01	3.991E-02	1.910E-01	7.320E-02	1.715E-03	0.000E-01	0.000E-01	5.403E-01
37	2.900E+00	1.030E+00	3.474E-01	4.119E-02	2.122E-01	8.409E-02	2.979E-03	0.000E-01	0.000E-01	5.405E-01
38	3.000E+00	1.034E+00	3.487E-01	4.271E-02	2.666E-01	1.050E-01	6.755E-03	0.000E-01	0.000E-01	5.442E-01
39	3.200E+00	1.041E+00	3.502E-01	4.457E-02	2.607E-01	1.411E-01	1.407E-02	0.000E-01	0.000E-01	5.506E-01
40	3.400E+00	1.047E+00	3.509E-01	4.637E-02	2.273E-01	1.854E-01	2.176E-02	0.000E-01	0.000E-01	5.550E-01
41	3.600E+00	1.054E+00	3.509E-01	4.809E-02	2.661E-01	2.331E-01	2.953E-02	0.000E-01	0.000E-01	5.586E-01
42	3.800E+00	1.060E+00	3.508E-01	4.975E-02	3.350E-01	2.736E-01	3.734E-02	0.000E-01	0.000E-01	5.600E-01
43	4.000E+00	1.074E+00	3.505E-01	5.127E-02	3.696E-01	3.069E-01	4.503E-02	0.000E-01	0.000E-01	5.604E-01
44	4.200E+00	1.098E+00	3.500E-01	5.254E-02	3.980E-01	3.407E-01	5.255E-02	0.000E-01	0.000E-01	5.612E-01
45	4.400E+00	1.124E+00	3.494E-01	5.377E-02	4.232E-01	3.747E-01	5.996E-02	0.000E-01	0.000E-01	5.624E-01
46	4.600E+00	1.149E+00	3.488E-01	5.495E-02	4.467E-01	4.034E-01	6.689E-02	0.000E-01	0.000E-01	5.652E-01
47	4.800E+00	1.179E+00	3.481E-01	5.610E-02	4.678E-01	4.228E-01	7.355E-02	0.000E-01	0.000E-01	5.684E-01
48	5.000E+00	1.212E+00	3.473E-01	5.727E-02	4.883E-01	4.392E-01	7.953E-02	0.000E-01	0.000E-01	5.720E-01
49	5.200E+00	1.247E+00	3.461E-01	5.847E-02	5.076E-01	4.554E-01	8.425E-02	0.000E-01	3.410E-06	5.760E-01
50	5.400E+00	1.282E+00	3.447E-01	5.966E-02	5.224E-01	4.718E-01	8.878E-02	1.040E-04	1.466E-04	5.805E-01
51	5.600E+00	1.317E+00	3.427E-01	6.086E-02	5.356E-01	4.893E-01	9.316E-02	5.643E-04	5.005E-04	5.874E-01
52	5.800E+00	1.349E+00	3.404E-01	6.206E-02	5.485E-01	5.073E-01	9.747E-02	1.538E-03	1.001E-03	6.096E-01
53	6.000E+00	1.371E+00	3.363E-01	6.350E-02	5.641E-01	5.324E-01	1.045E-01	5.424E-03	2.507E-03	7.079E-01
54	6.400E+00	1.389E+00	3.296E-01	6.497E-02	5.795E-01	5.607E-01	1.150E-01	3.209E-02	8.148E-03	8.540E-01
55	6.800E+00	1.390E+00	3.216E-01	6.622E-02	5.913E-01	5.787E-01	1.267E-01	4.192E-02	1.620E-02	9.441E-01
56	7.200E+00	1.380E+00	3.124E-01	6.734E-02	6.003E-01	5.879E-01	1.383E-01	5.609E-02	2.481E-02	9.827E-01
57	7.600E+00	1.364E+00	3.024E-01	6.841E-02	6.051E-01	5.923E-01	1.494E-01	9.114E-02	3.665E-02	1.002E+00

58	8.000E+00	1.341E+00	2.917E-01	6.924E-02	6.079E-01	5.946E-01	1.600E-01	1.139E-01	4.645E-02	1.014E+00
59	8.400E+00	1.319E+00	2.782E-01	6.974E-02	6.082E-01	5.954E-01	1.705E-01	1.215E-01	6.193E-02	1.020E+00
60	8.800E+00	1.293E+00	2.648E-01	7.019E-02	6.061E-01	5.925E-01	1.828E-01	1.225E-01	7.385E-02	1.019E+00
61	9.200E+00	1.250E+00	2.505E-01	7.062E-02	5.995E-01	5.892E-01	1.967E-01	1.237E-01	8.251E-02	1.012E+00
62	9.600E+00	1.202E+00	2.355E-01	7.101E-02	5.917E-01	5.838E-01	2.123E-01	1.299E-01	8.856E-02	1.004E+00
63	1.000E+01	1.148E+00	2.173E-01	7.123E-02	5.812E-01	5.717E-01	2.322E-01	1.500E-01	9.546E-02	1.000E+00
64	1.050E+01	1.054E+00	1.961E-01	7.124E-02	5.671E-01	5.524E-01	2.526E-01	1.570E-01	1.053E-01	1.000E+00
65	1.100E+01	9.265E-01	1.749E-01	7.125E-02	5.485E-01	5.262E-01	2.701E-01	1.634E-01	1.131E-01	1.000E+00
66	1.150E+01	7.939E-01	1.535E-01	7.126E-02	5.277E-01	4.925E-01	2.891E-01	1.856E-01	1.195E-01	1.000E+00
67	1.200E+01	6.466E-01	1.315E-01	7.126E-02	5.044E-01	4.620E-01	2.997E-01	1.969E-01	1.244E-01	1.005E+00
68	1.250E+01	5.002E-01	1.085E-01	7.127E-02	4.756E-01	4.347E-01	3.000E-01	2.023E-01	1.278E-01	1.025E+00
69	1.300E+01	4.092E-01	8.734E-02	7.128E-02	4.430E-01	4.100E-01	3.000E-01	2.021E-01	1.286E-01	1.060E+00
70	1.350E+01	3.389E-01	7.368E-02	7.128E-02	4.062E-01	3.876E-01	3.000E-01	1.954E-01	1.270E-01	1.112E+00
71	1.400E+01	2.929E-01	6.756E-02	7.128E-02	3.621E-01	3.673E-01	3.000E-01	1.858E-01	1.230E-01	1.177E+00
72	1.450E+01	2.625E-01	6.316E-02	7.128E-02	3.025E-01	3.488E-01	3.000E-01	1.752E-01	1.162E-01	1.240E+00
73	1.500E+01	2.227E-01	5.970E-02	7.128E-02	2.048E-01	3.216E-01	3.000E-01	1.581E-01	1.047E-01	1.314E+00
74	1.600E+01	1.682E-01	5.876E-02	7.128E-02	7.437E-02	2.784E-01	3.000E-01	1.363E-01	8.835E-02	1.370E+00
75	1.700E+01	1.143E-01	5.732E-02	7.128E-02	6.309E-04	2.290E-01	3.000E-01	1.190E-01	6.919E-02	1.381E+00

GROUP FLUXES INPUT NORMALIZED BY 0.9290

G	ENERGY	NEW	OLD	RATIO	STD DEV % NEW	OLD	RATIO
1	1.275E+01	7.192E-02	7.201E-02	0.999	24.10	24.19	0.996
2	1.500E+01	1.256E-01	1.269E-01	0.990	24.05	24.19	0.994
3	2.000E+01	7.972E-02	8.073E-02	0.987	24.04	24.19	0.994
4	2.400E+01	6.720E-02	6.831E-02	0.984	24.00	24.19	0.992
5	2.800E+01	5.814E-02	5.920E-02	0.982	23.98	24.19	0.991
6	3.200E+01	5.141E-02	5.224E-02	0.984	23.99	24.19	0.992
7	3.600E+01	4.609E-02	4.674E-02	0.986	23.99	24.19	0.992
8	4.000E+01	5.148E-02	5.224E-02	0.985	23.94	24.19	0.990
9	4.500E+01	4.624E-02	4.674E-02	0.989	23.95	24.19	0.990
10	5.000E+01	4.196E-02	4.229E-02	0.992	23.94	24.19	0.990
11	5.500E+01	3.830E-02	3.861E-02	0.992	23.90	24.19	0.988
12	6.000E+01	4.191E-02	4.229E-02	0.991	23.73	24.19	0.981
13	6.600E+01	3.828E-02	3.861E-02	0.991	23.59	24.19	0.975
14	7.200E+01	4.620E-02	4.674E-02	0.988	22.93	24.19	0.948
15	8.000E+01	4.203E-02	4.229E-02	0.994	22.77	24.19	0.941
16	8.800E+01	3.875E-02	3.861E-02	1.004	22.87	24.19	0.946
17	9.600E+01	1.826E-02	1.812E-02	1.008	23.78	24.19	0.983
18	1.000E+00	4.392E-02	4.229E-02	1.039	22.62	24.19	0.935
19	1.100E+00	4.107E-02	3.861E-02	1.064	22.76	24.19	0.941
20	1.200E+00	3.831E-02	3.552E-02	1.078	22.88	24.19	0.946
21	1.300E+00	3.484E-02	3.289E-02	1.059	23.10	24.19	0.955
22	1.400E+00	3.112E-02	3.062E-02	1.016	23.10	24.19	0.955
23	1.500E+00	2.817E-02	2.865E-02	0.983	22.78	24.19	0.942
24	1.600E+00	2.616E-02	2.691E-02	0.972	22.57	24.19	0.933
25	1.700E+00	2.464E-02	2.537E-02	0.971	22.53	24.19	0.932
26	1.800E+00	2.337E-02	2.401E-02	0.974	22.61	24.19	0.935
27	1.900E+00	2.233E-02	2.277E-02	0.981	22.80	24.19	0.942
28	2.000E+00	2.143E-02	2.166E-02	0.989	22.98	24.19	0.950
29	2.100E+00	2.055E-02	2.061E-02	0.997	23.09	24.19	0.955
30	2.200E+00	1.971E-02	1.957E-02	1.007	23.11	24.19	0.956
31	2.300E+00	1.881E-02	1.857E-02	1.013	23.09	24.19	0.955
32	2.400E+00	1.784E-02	1.760E-02	1.014	23.07	24.19	0.954
33	2.500E+00	1.704E-02	1.665E-02	1.024	23.10	24.19	0.955
34	2.600E+00	1.657E-02	1.575E-02	1.052	23.19	24.19	0.959
35	2.700E+00	1.611E-02	1.487E-02	1.083	23.23	24.19	0.960
36	2.800E+00	1.551E-02	1.404E-02	1.105	23.21	24.19	0.960
37	2.900E+00	1.470E-02	1.324E-02	1.111	23.23	24.19	0.961
38	3.000E+00	3.090E-02	2.421E-02	1.276	20.34	24.19	0.841
39	3.200E+00	2.429E-02	2.143E-02	1.133	22.34	24.19	0.924
40	3.400E+00	1.799E-02	1.892E-02	0.950	22.74	24.19	0.940
41	3.600E+00	1.550E-02	1.667E-02	0.930	22.79	24.19	0.942
42	3.800E+00	1.424E-02	1.465E-02	0.972	22.88	24.19	0.946
43	4.000E+00	1.243E-02	1.285E-02	0.967	22.88	24.19	0.946
44	4.200E+00	1.075E-02	1.124E-02	0.956	22.88	24.19	0.946
45	4.400E+00	9.292E-03	9.829E-03	0.945	22.89	24.19	0.946
46	4.600E+00	8.064E-03	8.572E-03	0.941	22.95	24.19	0.949
47	4.800E+00	7.038E-03	7.467E-03	0.943	23.03	24.19	0.952
48	5.000E+00	6.148E-03	6.496E-03	0.947	23.13	24.19	0.956
49	5.200E+00	5.364E-03	5.643E-03	0.951	23.25	24.19	0.961
50	5.400E+00	4.659E-03	4.896E-03	0.952	23.37	24.19	0.966
51	5.600E+00	4.039E-03	4.242E-03	0.952	23.48	24.19	0.971
52	5.800E+00	3.500E-03	3.672E-03	0.953	23.59	24.19	0.975
53	6.000E+00	5.369E-03	5.903E-03	0.910	22.82	24.19	0.944
54	6.400E+00	4.343E-03	4.396E-03	0.988	19.32	24.19	0.799
55	6.800E+00	3.170E-03	3.262E-03	0.972	22.22	24.19	0.919
56	7.200E+00	2.359E-03	2.413E-03	0.978	22.35	24.19	0.924
57	7.600E+00	1.802E-03	1.779E-03	1.013	21.57	24.19	0.892

58	8.000E+00	1.332E-03	1.308E-03	1.019	21.95	24.19	0.908
59	8.400E+00	9.579E-04	9.597E-04	0.998	22.26	24.19	0.920
60	8.800E+00	6.922E-04	7.019E-04	0.986	22.18	24.19	0.917
61	9.200E+00	5.036E-04	5.124E-04	0.983	22.51	24.19	0.931
62	9.600E+00	3.679E-04	3.733E-04	0.986	23.07	24.19	0.954
63	1.000E+01	3.226E-04	3.260E-04	0.990	23.29	24.19	0.963
64	1.050E+01	2.162E-04	2.182E-04	0.991	23.59	24.19	0.975
65	1.100E+01	1.446E-04	1.457E-04	0.993	23.80	24.19	0.984
66	1.150E+01	9.661E-05	9.699E-05	0.996	23.96	24.19	0.990
67	1.200E+01	6.428E-05	6.444E-05	0.997	24.02	24.19	0.993
68	1.250E+01	4.264E-05	4.272E-05	0.998	24.06	24.19	0.995
69	1.300E+01	2.822E-05	2.826E-05	0.998	24.08	24.19	0.995
70	1.350E+01	1.864E-05	1.866E-05	0.999	24.09	24.19	0.996
71	1.400E+01	1.229E-05	1.230E-05	0.999	24.09	24.19	0.996
72	1.450E+01	8.082E-06	8.090E-06	0.999	24.10	24.19	0.996
73	1.500E+01	8.597E-06	8.606E-06	0.999	24.10	24.19	0.996
74	1.600E+01	3.686E-06	3.689E-06	0.999	24.10	24.19	0.996
75	1.700E+01	1.572E-06	1.573E-06	0.999	24.10	24.19	0.996

INTEGRALS OF SPECTRA

OLD SPECTRUM	1.586E+00 +0R-	5.086 %
NEW SPECTRUM	1.592E+00 +0R-	3.636 %

OUTPUT FLUX CORRELATION MATRIX (BY ROW FROM DIAGONAL)

1	1000	7	7	6	6	6	6	6	6	6	5	4	3	0	-1	0	4	-2	-1	-1	0	0	0	0	0	0
	0	0	0	1	1	1	1	1	1	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17
	3	4	0	1	-1	-2	-1	0	-1	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
2	1000	4	3	2	2	2	1	1	1	0	-2	-4	-12	-13	-12	-1	-13	-10	-8	-5	-3	-1	0	0	1	
	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	3	
	3	0	1	-1	-2	-1	0	0	0	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	
3	1000	2	1	1	1	0	0	0	0	-4	-6	-15	-16	-15	-2	-16	-13	-10	-6	-3	-1	0	1	1	2	
	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	2	3	
	-1	1	-1	-1	0	0	0	0	1	2	3	4	5	5	6	6	6	6	6	6	6	6	6	6	7	
4	1000	0	0	0	-1	-1	-1	-2	-7	-9	-20	-22	-20	-4	-21	-16	-12	-9	-5	-2	0	1	2	3		
	3	3	3	2	2	2	2	2	2	-2	-2	-1	0	0	0	0	0	1	1	1	2	2	2	-1		
	1	-1	-1	0	0	0	0	1	2	2	4	4	5	6	6	6	6	6	6	6	6	6	6	7		
5	1000	0	0	-2	-2	-2	-3	-8	-11	-23	-25	-23	-6	-24	-19	-14	-10	-6	-2	0	1	2	3	3		
	3	3	3	2	2	2	2	2	2	-2	-1	0	0	0	0	0	1	1	1	2	2	2	-1	1		
	-1	-1	0	0	0	0	1	2	2	3	4	5	6	6	6	6	6	6	6	6	6	6	6	7		
6	1000	0	-2	-1	-2	-3	-8	-11	-22	-24	-22	-6	-23	-19	-15	-10	-6	-2	0	1	2	3	3	3		
	3	2	2	2	2	2	2	-2	-1	0	0	0	0	0	1	1	1	2	2	2	2	-1	1	-1		
	-1	0	0	0	0	1	2	2	3	4	5	6	6	6	6	6	6	6	6	6	6	6	6	7		
7	1000	-2	-1	-2	-3	-8	-11	-22	-24	-22	-6	-24	-19	-15	-11	-6	-2	0	1	2	3	3	3	3		
	2	2	2	2	2	2	-2	-1	0	0	0	0	1	1	1	2	2	2	2	2	2	-1	1	-1		
	0	0	0	0	1	2	2	3	4	5	5	6	6	6	6	6	6	6	6	6	6	6	6	7		
8	1000	-3	-4	-5	-11	-14	-28	-30	-28	-8	-30	-25	-20	-14	-8	-3	0	1	2	3	3	4	3	2		
	2	2	1	1	1	-2	-1	-1	0	0	0	0	1	1	1	1	2	2	2	-1	1	-1	-1	0		
	0	0	0	1	2	2	3	4	5	5	6	6	6	6	6	6	6	6	6	6	6	6	6	7		
9	1000	-3	-5	-10	-14	-27	-29	-29	-29	-25	-20	-15	-8	-4	-1	0	2	3	3	3	3	3	2	2		
	1	1	1	1	-2	-1	-1	0	0	0	0	1	1	1	1	2	2	2	2	0	1	0	-1	0		
	0	0	1	2	3	4	5	5	5	6	6	6	6	6	6	6	6	6	6	6	6	6	6	7		
10	1000	-5	-11	-15	-28	-30	-29	-9	-31	-27	-22	-16	-10	-4	-1	0	2	3	3	3	3	3	2	1		
	1	1	1	-2	-1	-1	0	0	0	0	1	1	1	1	2	2	2	2	0	1	0	-1	0	0		
	0	1	2	3	4	5	5	5	5	6	6	6	6	6	6	6	6	6	6	6	6	6	6	7		
11	1000	-14	-18	-33	-36	-34	-11	-37	-32	-26	-20	-12	-5	-1	0	2	3	3	4	3	3	2	1	1		
	1	1	-2	-1	-1	0	0	0	1	1	1	1	1	1	2	2	2	2	1	0	-1	0	0	0		
	0	2	2	3	4	4	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	5	6		
12	1000	-28	-48	-52	-49	-19	-53	-46	-39	-29	-17	-8	-2	0	2	4	5	5	4	3	2	1	1	0		
	0	-1	-1	-1	0	0	1	1	0	1	0	0	0	1	1	0	1	0	0	0	0	0	0	0		
	1	1	2	3	3	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	5		
13	1000	-58	-63	-59	-24	-64	-56	-48	-36	-21	-10	-3	0	3	5	6	6	5	4	2	1	0	0	0		
	-1	0	0	0	1	1	1	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1		
	1	2	2	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	3	4		
14	1000	-102	-97	-42	-104	-91	-78	-59	-35	-17	-6	0	4	7	8	8	7	5	3	1	0	-1	-1	0		
	0	0	1	2	2	1	1	0	0	0	0	-1	-1	-1	-1	0	1	1	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	0	0	0	0	0		
15	1000	-104	-47	-113	-100	-86	-66	-40	-20	-8	-1	3	6	8	8	7	4	2	0	0	-1	-1	-1	0		
	0	1	3	3	2	1	0	0	0	-1	-1	-1	0	0	1	1	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	0	0	0	0	0	0	0		
16	1000	-45	-110	-98	-86	-67	-42	-22	-11	-4	0	3	5	6	5	3	1	0	-1	-1	-1	0	1	0		
	1	3	3	2	1	0	0	0	-1	-1	-1	-1	0	1	1	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	0	0	0	0	0	0	0	0		
17	1000	-51	-46	-41	-32	-20	-11	-5	-2	0	1	2	2	2	1	0	0	0	0	0	0	0	0	0		
	1	1	1	0	1	0	1	1	1	1	1	1	1	1	0	1	0	0	0	0	0	1	1	0		
	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	4	5		
18	1000	-118	-105	-84	-54	-31	-18	-11	-5	-1	1	2	2	0	-1	-2	-3	-3	-2	-1	2	1	0	2		
	3	2	1	0	0	-1	-1	-2	-2	-1	1	1	3	2	0	0	0	0	0	0	0	0	0	-1		
	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1		
19	1000	-103	-84	-57	-35	-24	-17	-11	-7	-4	-1	-1	-1	-3	-3	-4	-3	-2	-1	0	0	0	2	3		
	2	1	0	0	0	-1	-1	-1	2	2	3	2	0	-1	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	0	0	0	0	0	0	0	0	0		
20	1000	-84	-61	-43	-33	-27	-22	-16	-12	-8	-6	-5	-5	-5	-4	-3	-2	-1	1	1	0	1	3	2		

APPENDIX C

STAY'SL SOURCE PROGRAM LISTING

```

C      PROGRAM STAYSAIL
      DIMENSION A0(20),A0M(20,20),F(200),C(20,200),A(20),DA(20),
1      IU(20,200),TS(20),TB(200),AFM(20,20),ASM(20,20),AN(20,20),
2      W(20,20),Y(20),DF(200),AP(20),SC(20),BS(20),EL(200),
3      PPF(200),FP(200),TC(200),TD(200),PFP(200),IC(200)
      DOUBLE PRECISION DW(20,20),AT(6)
200   FORMAT (' ORNL F.G.PEREY STAYSAIL RUN OUTPUT ')
      TYPE 99
99    FORMAT (' ACTIVATION DATA ', $)
      CALL TITLE(AT(1))
      READ (1,100) KA
100   FORMAT (1,2F,1)
      READ (1,101) (A0(I),I=1,KA)
101   FORMAT (10F)
      TYPE 98
98    FORMAT (' ACTIVATION COV. ', $)
      CLOSE (UNIT=1)
      CALL TITLE(AT(2))
      DO 1 I=1,KA
      READ (1,101) (A0M(I,J),J=I,KA)
1     CONTINUE
      DO 2 I=1,KA
      DO 2 J=I,KA
      A0M(I,J)=A0M(I,J)*A0(I)*A0(J)
2     A0M(J,I)=A0M(I,J)
      CLOSE (UNIT=1)
      TYPE 97
97    FORMAT (' FLUX DATA ', $)
      CALL TITLE(AT(3))
      READ (1,100) KG,AK1,VAK,NOR
      AK=AK1
      READ (1,101) (F(I),I=1,KG)
      READ (1,101) (EL(I),I=1,KG)
      CLOSE (UNIT=1)
      TYPE 96
96    FORMAT (' DOSI. X-SECTION ', $)
      CALL TITLE(AT(4))
      DO 3 I=1,KA
      READ (1,101) (C(I,J),J=1,KG)
      A(I)=0.
      DO 3 J=1,KG
      C(I,J)=C(I,J)*F(J)
3     A(I)=A(I)+C(I,J)

```

```

IF (AK.NE.0.) GO TO 31
C1=0.
C2=0.
DO 4 I=1,KA
IF (NOR.EQ.0) C3=A0(I)*A0(I)
C1=C1+A0(I)*A(I)/C3
4 C2=C2+A(I)*A(I)/C3
AK=C1/C2
31 CONTINUE
DO 5 I=1,KA
A(I)=A(I)*AK
DA(I)=A0(I)-A(I)
TS(I)=DA(I)/A0(I)
DO 5 J=1,KG
5 C(I,J)=C(I,J)*AK
DO 6 I=1,KG
6 F(I)=F(I)*AK
CLOSE (UNIT=1)
TYPE 95
95 FORMAT (' FLUX COVARIANCE ',S)
CALL TITLE(AT(5))
DO 7 I=1,KA
DO 7 J=1,KG
7 U(I,J)=0.
KP=1
S=0.
SV=0.
DO 8 J=1,KG
S=S+F(J)
READ (1) (TB(L),L=1,KG)
DO 32 L=1,KG
32 TB(L)=TB(L)+VAK
DO 56 L=1,KG
56 SV=SV+TB(L)*F(J)*F(L)
PF(J)=SQRT(TB(KP))
WRITE (3) (TB(L),L=KP,KG)
KP=KP+1
DO 8 I=1,KA
DO 8 L=1,KG
8 U(I,J)=U(I,J)+TB(L)*C(I,L)
CLOSE (UNIT=3)
OPEN(UNIT=3,FILE='FOR03.DAT')

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DO 10 I=1,KA
DO 10 J=I,KA
AFM(I,J)=0.
DO 9 L=1,KG
9 AFM(I,J)=AFM(I,J)+C(I,L)*U(J,L)
10 AFM(J,I)=AFM(I,J)
DO 12 I=1,KA
DO 11 J=I,KA
11 TS(J)=AFM(I,J)/(A(I)*A(J))
12 CONTINUE
CLOSE (UNIT=1)
TYPE 94
94 FORMAT (' X-SECTION COVARIANCES ', $)
CALL TITLE(AT(6))
DO 16 I=1,KA
DO 16 J=I,KA
ASM(I,J)=0.
READ (1) FC
IF (FC.EQ.0.) GO TO 15
IF (FC.NE.1.) GO TO 600
DO 14 K=1,KG
READ (1) (TB(L),L=1,KG)
CI=0.
DO 13 L=1,KG
13 CI=CI+TB(L)*C(J,L)
14 ASM(I,J)=ASM(I,J)+CI*C(I,K)
GO TO 15
600 ASM(I,J)=FC*A(I)*A(J)
15 CONTINUE
16 ASM(J,I)=ASM(I,J)
DO 18 I=1,KA
DO 17 J=I,KA
17 TS(J)=ASM(I,J)/(A(I)*A(J))
18 CONTINUE
DO 19 I=1,KA
DO 19 J=I,KA
AN(I,J)=A0M(I,J)+AFM(I,J)+ASM(I,J)
19 AN(J,I)=AN(I,J)
CALL SCALE (AN,BS,KA)
DO 40 I=1,KA
DO 40 J=1,KA
40 DW(I,J)=AN(I,J)
KD=KA
CALL PIVOT (DW,KD)
IF (KD.NE.0) GO TO 34
TYPE 1000
1000 FORMAT (' RUN ABORTED !! N-MATRIX ')
DO 33 I=1,KA
33 TYPE 1001,(AN(I,J),J=I,KA)
1001 FORMAT (1P20E12.3)
CALL EXIT

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```

34  CONTINUE
    DO 21 I=1,KA
      DO 21 J=1,KA
21  W(I,J)=DW(I,J)
      CALL RESCAL (W,BS,KA)
      DO 22 I=1,KA
        Y(I)=0.
        DO 22 J=1,KA
22  Y(I)=Y(I)+W(I,J)*DA(J)
          DO 23 L=1,KG
            DF(L)=0.
            DO 23 I=1,KA
23  DF(L)=DF(L)+Y(I)*U(I,L)
              CHI=0.
              DO 24 I=1,KA
                SC(I)=DA(I)*Y(I)
24  CHI=CHI+SC(I)
                DO 25 I=1,KG
                  TB(I)=1.+DF(I)
25  FP(I)=TB(I)*F(I)
                  DO 26 I=1,KA
                    AP(I)=0.
                    DO 26 J=1,KG
26  AP(I)=AP(I)+C(I,J)*TB(J)
                      SP=0.
                      SVP=0.
                      DO 28 K=1,KG
                        SP=SP+FP(K)
                        DO 27 L=K,KG
                          TB(L)=0.
                          DO 27 I=1,KA
                            DO 27 J=1,KA
27  TB(L)=TB(L)-W(I,J)*U(I,K)*U(J,L)
                              READ (3) (TC(KP),KP=K,KG)
                              DO 30 M=K,KG
30  TD(M)=TC(M)+TB(M)
                                SVP=SVP+TD(K)*FP(K)*FP(K)
                                IF (K.EQ.KG) GO TO 58
                                DO 57 M=K+1,KG
57  SVP=SVP+TD(M)*FP(K)*FP(M)
58  CONTINUE
          PFP(K)=SQRT(TD(K))
          WRITE (4) (TD(KP),KP=K,KG)
28  CONTINUE
      CLOSE(UNIT=4)
      OPEN(UNIT=4,FILE='FOR04.DAT')
      CLOSE(UNIT=1)
      OPEN(UNIT=1,FILE='STAYSL.OUT')

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WRITE (1,200)
WRITE (1,300)
300 FORMAT(1H0,' INPUT FILES')
WRITE (1,301) AT(1),AT(2),AT(3),AT(5),AT(4),AT(6)
301 FORMAT (1X,A10,5X,A10)
WRITE (1,310) AK1,VAK,NOR
310 FORMAT (1H0,' INPUT NORMALIZATION DATA'/
11X,'AK1=',F10.4,' VAK=',F10.5,' NORM=',I2)
WRITE (1,302) AK,CHI
302 FORMAT (1H0,'INPUT FLUX NORMALIZED BY ',F10.4,
13X,'CHI-SQUARE',F10.4)
WRITE (1,303)
303 FORMAT (1H0,'DOSIMETRY ACTIVITIES'/,
11H0,5X,'MEASURED +OR- %',7X,'BEFORE DIFF %',8X,
2'AFTER DIFF %',5X,'CHI'/)
DO 50 I=1,KA
C1=(A0(I)-A(I))/A0(I)
C2=(A0(I)-AP(I))/A0(I)
TS(I)=SQRT(A0M(I,I))
C3=TS(I)/A0(I)
50 WRITE(1,304) I,A0(I),C3,A(I),C1,AP(I),C2,SC(I)
304 FORMAT (I3,1PE12.3,2PF8.2,1PE14.3,2PF8.2,1PE14.3,2PF8.2,0PF8.3)
C1=CHI/KA
IF (C1.LT..3.OR.C1.GT.2.) WRITE (1,318)
WRITE (1,319)
319 FORMAT (1H0,'DOSIMETRY DATA INPUT CORRELATION MATRIX',/)
DO 64 I=1,KA
DO 63 J=1,I
63 IC(J)=1000.*A0M(I,J)/(TS(I)*TS(J))+.5
64 WRITE (1,324) I,(IC(J),J=1,I)
324 FORMAT (2I15)
WRITE (1,323)
323 FORMAT (1H1,'RELATIVE COV. MATRIX OF ACTIVITIES'/,
11H0,9X,'% ',10X,'CORRELATION MATRIX'/)
DO 65 I=1,KA
65 TS(I)=SQRT(AFM(I,I)+ASM(I,I))
DO 67 I=1,KA
Y(I)=TS(I)/A(I)
DO 66 J=1,I
66 IC(J)=1000.*(AFM(I,J)+ASM(I,J))/(TS(I)*TS(J))+.5
67 WRITE (1,320) I,Y(I),(IC(J),J=1,I)
320 FORMAT (I3,2PF8.2,4X,20I5)
WRITE (1,321)
321 FORMAT (/1H0,'CONTRIBUTION DUE TO INPUT FLUX COV. MATRIX'/,
11H0,9X,'% ',10X,'CORRELATION MATRIX'/)
DO 68 I=1,KA
68 TS(I)=SQRT(AFM(I,I))

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DO 70 I=1,KA
Y(I)=TS(I)/A(I)
DO 69 J=1,I
69 IC(J)=1000.*AFM(I,J)/(TS(I)*TS(J))+.5
70 WRITE (1,320) I,Y(I),(IC(J),J=1,I)
WRITE (1,322)
322 FORMAT (/1H0,'CONTRIBUTION DUE TO INPUT X-SEC. COV. MATRIX'/,
11H0,9X,'% ',10X,'CORRELATION MATRIX'/)
DO 71 I=1,KA
71 TS(I)=SQRT(ASM(I,I))
DO 73 I=1,KA
Y(I)=TS(I)/A(I)
DO 72 J=1,I
72 IC(J)=1000.*ASM(I,J)/(TS(I)*TS(J))+.5
73 WRITE (1,320) I,Y(I),(IC(J),J=1,I)
DU 20 I=1,KA
DO 20 J=1,KG
20 C(I,J)=C(I,J)/F(J)
WRITE (1,314)
314 FORMAT (1H1,' INPUT DOSIMETRY X-SECTIONS (ENDF/B LAW 1)',
1/1H0,' G ENERGY',10X,'X-SECTIONS',/)
IF (KA.GT.10) GO TO 59
DO 29 I=1,KG
29 WRITE (1,315) I,EL(I),(C(K,I),K=1,KA)
315 FORMAT (1X,I3,1P11E10.3)
GO TO 60
WRITE (1,316)
316 FORMAT (1H0,50X,'1 THROUGH 10')
59 DO 61 I=1,KG
61 WRITE (1,315) I,EL(I),(C(K,I),K=1,10)
WRITE (1,314)
WRITE (1,317) KA
317 FORMAT (1H0,50X,'11 THROUGH',I3)
DO 62 I=1,KG
62 WRITE (1,315) I,EL(I),(C(K,I),K=11,KA)
60 CONTINUE
318 FORMAT (/1H0,20X,' CHECK INPUT IT IS RATHER UNLIKELY !!! ',
11H0,20X,'***** BEWARE OF OUTPUT !!!!!!!!!!!!! *****',/)
WRITE (1,305) AK
305 FORMAT (1H1,'GROUP FLUXES INPUT NORMALIZED BY ',F10.4/
11H0,' G',6X,'ENERGY',11X,'NEW',11X,'OLD',3X,'RATIO',
22X,'STD DEV % NEW OLD',3X,'RATIO'/)
OPEN (UNIT=20,FILE='STAYSL.CAL')
WRITE (20) KG
WRITE (20) (F(I),I=1,KG)

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DO 51 I=1,KG
C1=FP(I)/F(I)
C2=PFP(I)/PF(I)
51 WRITE(1,306) I,EL(I),FP(I),F(I),C1,PFP(I),PF(I),C2
306 FORMAT (I4,1PE12.3,2E14.3,0PF8.3,10X,2PF5.2,3X,2PF5.2,0PF8.3)
C1=SQRT(SV)/S
C1P=SQRT(SVP)/SP
WRITE (1,311) S,C1,SP,C1P
311 FORMAT (1H0,'INTEGRALS OF SPECTRA'/
11H0,' OLD SPECTRUM ',1PE12.3,' +OR- ',2PF7.3,' Z'/
21H0,' NEW SPECTRUM ',1PE12.3,' +OR- ',2PF7.3,' Z')
WRITE (1,307)
307 FORMAT (1H1,'INPUT FLUX CORRELATION MATRIX',
1' (BY ROW FROM DIAGONAL)',/)
CLOSE (UNIT=3)
DO 53 I=1,KG
READ (3) (TB(L),L=I,KG)
WRITE (20) (TB(L),L=I,KG)
DO 52 J=I,KG
52 IC(J)=1000.*TB(J)/(PF(I)*PF(J))+.5
53 WRITE (1,308) I,(IC(L),L=I,KG)
308 FORMAT (1X,I3,1X,25I4/10(5X,25I4/))
WRITE (1,309)
309 FORMAT (1H1,'OUTPUT FLUX CORRELATION MATRIX',
1' (BY ROW FROM DIAGONAL)',/)
WRITE (20) (FP(I),I=1,KG)
DO 55 I=1,KG
READ (4) (TB(L),L=I,KG)
WRITE (20) (TB(L),L=I,KG)
DO 54 J=I,KG
54 IC(J)=1000.*TB(J)/(PFP(I)*PFP(J))+.5
55 WRITE (1,308) I,(IC(L),L=I,KG)
CALL EXIT
END
SUBROUTINE TITLE(A)
DOUBLE PRECISION A
ACCEPT 1,A
1 FORMAT (A10)
OPEN(UNIT=1,FILE=A)
RETURN
END
SUBROUTINE SCALE (A,B,KA)
DIMENSION A(20,20),B(20)
DO 1 I=1,KA
B(I)=A(I,1)
DO 1 J=2,KA
IF (B(I).GT.A(I,J)) GO TO 1
B(I)=A(I,J)
1 CONTINUE
DO 2 I=1,KA
DO 2 J=1,KA
2 A(I,J)=A(I,J)/B(I)
RETURN
END

```

```

SUBROUTINE RESCAL (A,B,KA)
DIMENSION A(20,20),B(20)
DO 1 I=1,KA
DO 1 J=1,KA
1 A(I,J)=A(I,J)/B(J)
RETURN
END

SUBROUTINE PIVOT (S,N)
DIMENSION NC(20), NR(20)
DOUBLE PRECISION S(20,20), BIG, AIJ, TEMP
DO 457 I = 1, N
NC(I) = 0
457 NR(I) = 0
DO 600 KEEP = 1, N
BIG = 0.0D0
DO 500 NS = 1, N
IF (NR(NS)) 500, 460, 500
460 AIJ = 0.0D0
NX = 1
DO 480 K = 1, N
IF (DABS(S(NS,K)) - AIJ) 480, 480, 470
470 IF (NC(K)) 480, 475, 480
475 AIJ = DABS(S(NS,K))
NX = K
480 CONTINUE
IF (AIJ - BIG) 500, 500, 490
490 BIG = AIJ
I = NS
J = NX
500 CONTINUE
IF (BIG - 1.0D-8) 710, 710, 510
510 L = 0
515 L = L + 1
IF (L - J) 520, 515, 520
520 IF (L - N) 530, 530, 540
530 S(I,L) = -S(I,L)/S(I,J)
GO TO 515
540 CONTINUE
S(I,J) = 1.0D0/S(I,J)
K = 0
550 K = K + 1
IF (K - I) 555, 550, 555
555 IF (K - N) 560, 560, 590
560 L = 0
565 L = L + 1
IF (L - J) 570, 565, 570
570 IF (L - N) 575, 575, 580
575 S(K,L) = S(K,L) + S(I,L)*S(K,J)
GO TO 565
580 CONTINUE

```

```
585 S(K,J) = S(K,J)*S(I,J)
    GO TO 550
590 CONTINUE
    NR(I) = J
    NC(J) = I
600 CONTINUE
    DO 660 NY = 1, N
    DO 660 K = 1, N
    IF (NY - NR(K)) 630, 610, 630
610 NR(K) = NR(NY)
    NR(NY) = NY
    DO 620 NV = 1, N
    TEMP = S(NY, NV)
    S(NY, NV) = S(K, NV)
620 S(K, NV) = TEMP
630 CONTINUE
    IF (NY - NC(K)) 660, 640, 660
640 NC(K) = NC(NY)
    NC(NY) = NY
    DO 650 NV = 1, N
    TEMP = S(NV, NY)
    S(NV, NY) = S(NV, K)
650 S(NV, K) = TEMP
660 CONTINUE
    GO TO 700
710 N = 0
700 CONTINUE
    RETURN
    END
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