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A User's Guide for the JULIET Module of the FORSS Sensitivity and Uncertainty Analysis Code System

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A USER'S GUIDE FOR THE JULIET MODULE OF THE FORSS SENSITIVITY AND UNCERTAINTY ANALYSIS CODE SYSTEM

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ABSTRACT

JULIET is the FORSS module that calculates generalized sources, responses (e.g., criticality, reaction rate ratios, reactivity worths), normalization parameters and sensitivity coefficients. JULIET is organized into execution paths which are in effect submodules. This permits a problem to be segmented for solution at the user's discretion (i.e., multiple entry points). JULIET normally operates with fluxes generated by the FORSS version of ANISN; however, the execution path concept permits interaction with other neutronics codes such as DOT and VENTURE.

The proposed CCCC file MATXS is the cross-section data base for JULIET permitting the calculation of sensitivity coefficients with respect to partial cross sections. The sensitivity coefficients calculated by JULIET are placed in the proposed CCCC file SENPRO where they may be accessed by other modules in the FORSS system or transmitted to other installations.

I. INTRODUCTION

JULIET is the FORSS[1] module that calculates sources, responses (e.g., criticality, reaction rate ratios, reactivity worths), normalization parameters, and sensitivity coefficients. As a user's guide, this document presents the algorithms implemented in JULIET but does not include their theoretical development which is available in Ref. 2. JULIET optimizes and extends algorithms that were initially implemented in the SOURCE (see Ref. 2 for theoretical development) and SWANLAKE[3] codes.

JULIET is designed to execute as a module of the FORSS driver controlled system. It withdraws and deposits information in the FORSS repository which serves as an information exchange medium for FANISN[4] (the FORSS

version of ANISN) and JULIET. When FANISN has been selected as the neutronics code for a FORSS study, JULIET receives angular fluxes and computes generalized source data for subsequent steps in which FANISN is used to generate generalized[2] angular fluxes. JULIET is organized into execution paths which are in effect submodules. This permits a problem to be segmented for solution at the user's discretion (i.e., multiple points of entry into the system). The execution path concept also permits interaction with neutronics codes other than ANISN such as DOT[5] and VENTURE.[6] Additional information on this interaction is available in the FORSS user's guide.[7]

Sensitivity analysis requires access to partial cross sections. The proposed CCCC file MATXS[8] is the cross-section data base for JULIET. The preparation of a MATXS file is discussed in the FORSS user's guide.

The end product of JULIET is sensitivity coefficients (profiles). They are placed in a proposed CCCC[9] file, SENPRO.[10] A SENPRO Service Module[7] is available in the FORSS system which operates on a SENPRO file providing a number of functions such as listing, plotting, merging, etc. SENPRO files are input for sensitivity analysis modules such as SENTINEL,[11] CAVALIER,[12] and UNCOVER.[13]

II. EXECUTION PATHS

JULIET has four execution paths and the combination selected is problem-dependent.

A. Operator Definition

The path is selected by the word, MIX. This path prepares the cross-section operators required for the problem solution (these correspond to cross sections appearing in the response definition and/or cross sections in the terms of the Boltzmann equation). The MATXS cross-section file is the primary data base for operator definition. User input defines the operators required for the problem solution. An operator may be a single material-reaction type or it may be a mixture of many materials and include several reaction types.

B. Flux Preparation

The path is selected by the word FLUX. This path calculates moment fluxes from existing forward and adjoint angular fluxes for use in computing certain reactor parameters (e.g., worth). This path also prepares the $\langle \phi^* \phi \rangle$, $\langle \Gamma^* \phi \rangle$, or $\langle \Gamma \phi^* \rangle$ inner products needed for a sensitivity calculation.

C. Source Response Calculation

The path is selected by the word SOURCE. The path has the capability to calculate bilinear sources, linear sources, responses, and normalization parameters.

D. Sensitivity Coefficient Generation

The path is selected by the word SENSE. This path calculates sensitivity coefficients using the SWANLAKE algorithm expanded to include direct effects.

III. OPERATOR DEFINITION

The FORSS system is an attempt to provide a sensitivity analysis capability with respect to a response defined as:

for bilinear $R = \frac{\langle \phi^* H_1 \phi \rangle}{\langle \phi^* H_2 \phi \rangle}$, for linear $R = \frac{\langle H_1 \phi \rangle}{\langle H_2 \phi \rangle}$ with sensitivity coefficients defined as: $\frac{\partial R/R}{\partial \Sigma_x / \Sigma_x}$ where Σ_x is a cross section appearing in the Boltzmann equation or in the definition of H_1 or H_2. In the above equations ϕ and ϕ^* represent the forward and adjoint fluxes, the brackets denote integration over phase space, and the operators H_1 and H_2 can in general be arbitrary. However, the physical cases of most practical interest occur when either H_1 or H_2 is a macroscopic cross section, in which case R would represent a weighted reaction rate ratio. For example, the linear response $^{28}\delta$ would be defined as $R = \frac{\langle {}^{238}\Sigma_c \phi \rangle}{\langle {}^{235}\Sigma_f \phi \rangle}$; clearly H_1 is the ^{238}U capture reaction and H_2 is the ^{235}U fission reaction. Operators may also be linear combinations of any or all terms appearing in the Boltzmann equation. For example, the bilinear response for Na worth would be defined as:

$$R = \frac{-\left\langle \phi^* \left(\Sigma_T \phi - \sum_{g',\ell'} \Sigma_s^{\ell'} (g' \to g) \phi_\ell(g') \right) \right\rangle}{\left\langle \phi_0^* \left(\chi \sum \nu \Sigma_f \right) \phi_0 \right\rangle}$$

Here H_1 is the Boltzmann operator for Na, and H_2 is the fission operator for all fissionable materials in the system of interest.

IV. FLUX PREPARATION

A. Moment Fluxes

Angular fluxes are input to a JULIET calculation. Moment fluxes are prepared for use in source, response, and sensitivity calculations according to the following equation:

$$\phi(j,g,\ell') = \sum_{i=1}^{NOA} W_i Y_\ell^m(\mu_i)\phi(j,g,\mu_i) \qquad (1)$$

where

ISCT - order of scattering,

NMOM - maximum of (ISCT, ISN),

NOA - number of angles,

for slab and spherical geometry NOA = ISN + 1

for cylindrical geometry NOA = (ISN * (ISN + 4))/4

ISN - quadrature order,

LMOM - number of moments,

ℓ' - moment index which assumes values from 1 to LMOM. ℓ' is a function of m and ℓ. Equations 4, 6, and 7 illustrate the relationship of ℓ', ℓ, m as implemented in the code.

g - group index,

i - angle index,

W_i - quadrature weight (input, see Section VI, Block 1),

μ_i - discrete angle cosine (input, see Section VI, Block 1),

Y_ℓ^m - spherical harmonic,

$\phi(j,g,\mu_i)$ - angular flux calculated by FANISN,

$\phi(j,g,\ell')$ - angular flux moment calculated by FANISN.

B. $\langle\phi^*\phi\rangle$ Files

$\langle\phi^*\phi\rangle$ files are prepared for use in the sensitivity equations. $\langle\phi^*\phi\rangle$ is a symbolic term since the file may represent products of $\langle\Gamma^*\phi\rangle$ or $\langle\Gamma\phi^*\rangle$. A $\langle\phi^*\phi\rangle$ file is required for K and worth sensitivity analysis. A $\langle\Gamma^*\phi\rangle$ file is required for reaction rate ratio sensitivity analysis.

$\langle\phi^*\phi\rangle$ files are prepared in the ANISN cross-section format. For the 0th moment the total position of the $\langle\phi^*\phi\rangle$ file is calculated as:

$$PS(IHT,g,z,1) = -\sum_{j\varepsilon z} V(j) \sum_i \phi(j,g;\mu_i)\phi^*(j,g,\mu_i)W(i) \qquad (2)$$

where

IHT - position of total cross section in ANISN cross-section table,

g - group index,

z - zone index,

R - the radii by interval boundary,

V(j) - volume of spatial interval j,

= R(j+1) - R(j) for slab,

= $(R^2(J+1) - R^2(j))$ for cylinder,

= $\frac{4}{3}(R^3(j+1) - R^3(j))$ for sphere.

For slab and spherical geometry and the P_0 and P_1 scattering orders of cylindrical geometry the scattering positions are

$$PS(G,g,z,\ell) = \sum_{j\varepsilon z} \phi(j,g',\ell')\phi^*(j,g,\ell')V(j) \qquad (3)$$

where

G = IHT + g'+1,

IHT is the total cross-section position,

$\ell = \ell'$ assumes values of 1 and 2.

For cylindrical geometry and scattering order higher than P_1

$$PS(G,g,z,\ell) = \sum_{\ell'=LL(\ell-1)}^{LL(\ell)} \sum_{j\in z} \phi(j,g',\ell')\phi^*(j,g,\ell')V(j) \qquad (4)$$

initially the code defines LL(2)=2 then $LL(\ell) = LL(\ell-1) + 1 + \frac{(2\ell-1)}{4}$

where

ℓ is the scattering order index and assumes values from 3 to ISCT

(order of scattering) ℓ' is the moment index.

V. SOURCE RESPONSE ALGORITHMS

A. The $[H_1\phi]$ and $[H_2\phi]$ Components of a Bilinear Response

The $[H_1\phi]$ function includes three terms, a total term, a scattering term, and a fission term.

1. Total

$$T_1(j,g,\ell') = -\Sigma_T(j,g)\phi(j,g,\ell')$$

where

j - spatial index,

g - group index,

ℓ' - moment index,

Σ_T - total cross section,

ϕ - forward moment flux.

2. Scattering for Slab and Spherical Geometrics

When $\ell' \leq$ ISCT, ISCT = order of scattering

$$T_2(j,g,\ell') = \sum_{g'} \Sigma_S\ (j,g' \rightarrow g,\ell')\phi(j,g',\ell') \tag{5}$$

where

Σ_S - scattering matrix.

3. Scattering for Cylindrical Geometry

For the P_0 and P_1 scattering orders Eq. (5) also applies for cylindrical geometry.

For scattering orders greater than P_1 Eq. (6) and Eq. (7) establish the correspondence between the cross-section scattering order (index ℓ) and the flux moment (index ℓ').

$$T\ (j,g,\ell') = \sum_{g'} \Sigma_S(j,g' \rightarrow g,\ell)\phi(j,g',\ell') \tag{6}$$

To define the values of ℓ and ℓ' in Eq. (6), initially the code defines ℓ=3 and the indexing control parameter LHI=4. Then as ℓ' assumes values from 3 to LMOM (number of moments) the values of ℓ' and LHI are compared. If $\ell' \leq$ LHI, the values of LHI and ℓ are unchanged. When $\ell' >$ LHI, $\ell=\ell+1$, and LHI is redefined by Eq. (7) as follows:

$$\text{LHI} = \text{LHI} + 1\ + (2\ell+1)/4 \tag{7}$$

when $\ell >$ ISCT

$$T_2(j,g,\ell') = 0\ . \tag{8}$$

4. Fission

For $\ell' = 1$

$$T_3(j,g,\ell') = \lambda\chi(g)\sum_{g'}\nu\Sigma_f(j,g')\phi(j,g',\ell') \tag{9}$$

where

$\lambda = \frac{1}{k}$

χ = fission spectrum .

For $\ell' > 1$

$$T_3(j,g,\ell') = 0 \quad . \tag{10}$$

5. The $[H_1\phi]$ Term

$$[H_1\phi](j,g,\ell') = T_1(j,g,\ell') + T_2(j,g,\ell') + T_3(j,g,\ell') \quad . \tag{11}$$

6. $[H_2\phi]$ is a fission function with one term.

For $\ell' = 1$

$$[H_2\phi](j,g,\ell') = \chi(g)\sum_{g'}\nu\Sigma_f(j,g',\ell')\phi(j,g',\ell') \quad . \tag{12}$$

For $[H_2\phi]$, $\nu\Sigma_f$ is a mixture of all fissionable materials in the assembly.

For $\ell' > 1$

$$[H_2\phi](j,g,\ell') = 0 \quad . \tag{13}$$

B. The $[H_1^*\phi^*]$ and $[H_2^*\phi^*]$ Components of a Bilinear Response

The $[H_1^*\phi^*](j,g,\ell')$ function has the same form as the $[H_1\phi]$ function.

1. Total

$$T_1(j,g,\ell') = -\Sigma_T(j,g)\phi^*(j,g,\ell') \tag{14}$$

2. Scattering

$$T_2(j,g,\ell') = \sum_{g'} \Sigma_s(j,g\rightarrow g',\ell)\phi^*(j,g',\ell') \tag{15}$$

The discussion of geometry and moments for the $[H_1\phi]$ function applies for the $[H_1^*\phi^*]$ function.

3. Fission

$$T_3(j,g,\ell') = \nu\Sigma_f(j,g)\sum_{g'}\chi(g')\phi^*(j,g',\ell') \tag{16}$$

4. The $[H_1^*\phi^*]$ Term

$$[H_1^*\phi^*]\ (j,g,\ell') = T_1(j,g,\ell') + T_2(j,g,\ell') + T_3(j,g,\ell') \tag{17}$$

5. The $[H_1^*\phi^*]$ function is very similar to the $[H_1\phi]$ function.

$$[H_1^*\phi^*](j,g,\ell') = \nu\Sigma_f(j,g)\sum_{g'}\chi(g')\phi^*(j,g',\ell') \tag{18}$$

C. The Bilinear Response

A bilinear response is defined as:

$$R \equiv \frac{\langle\phi^*H_1\phi\rangle}{\langle\phi^*H_2\phi\rangle} \tag{19}$$

where

$$\langle\phi^*H_1\phi\rangle = \sum_{\ell'}\sum_{g}\sum_{j}\phi^*(j,g,\ell')[H_1\phi](j,g,\ell')V(j)\ , \tag{20}$$

$$\langle\phi^*H_2\phi\rangle = \sum_{g}\sum_{j}\phi^*(j,g,1)[H_2\phi](j,g,1)V(j)\ , \tag{21}$$

$$\langle\phi H_1{}^*\phi^*\rangle = \sum_{\ell'}\sum_{g}\sum_{j}\phi(j,g,\ell')[H_1^*\phi^*](j,g,\ell')V(j)\ , \tag{22}$$

$$\langle\phi H_2{}^*\phi^*\rangle = \sum_{g}\sum_{j}\phi(j,g,1)[H_2^*\phi](j,g,1)V(j)\ . \tag{23}$$

D. The Bilinear Forward Source

$$S(j,g,\ell') = R\left[\frac{[H_1\phi](j,g,\ell')}{\langle\phi^*H_1\phi\rangle} - \frac{[H_2\phi](j,g,\ell')}{\langle\phi^*H_2\phi\rangle}\right] \tag{24}$$

E. The Bilinear Adjoint Source

$$S^*(j,g,\ell') = R\left[\frac{[H_1^*\phi^*](j,g,\ell')}{\langle\phi^*H_1\phi\rangle} - \frac{[H_2^*\phi^*](j,g,\ell')}{\langle\phi^*H_2\phi\rangle}\right] \tag{25}$$

F. The Worth in an Interval

Reactivity worth, w, is defined as:

$$w(\text{per mole}) = R\left[\frac{.6023}{N\ V}\right] \tag{26}$$

R - the bilinear response,

V - volume of the interval,

N - density of the material,

$$w(\text{per kilogram}) = \frac{1000}{A}\ [w(\text{per mole})] \tag{27}$$

A - the atomic mass.

G. The Linear Response

A linear response, R, is defined as:

$$R \equiv \frac{\langle H_1\phi\rangle}{\langle H_2\phi\rangle} \tag{28}$$

where

$$\langle H_1\phi\rangle = \sum_g \sum_j H_1(j,g)\phi(j,g,1)V(j) \tag{29}$$

$$\langle H_2\phi\rangle = \sum_g \sum_j H_2(j,g)\phi(j,g,1)V(j) \tag{30}$$

where

H_1 and H_2 are simply reaction cross sections or other response functions,

$\phi(j,g,1)$ - 0th moment flux,

g - group index,

j - spatial index.

H. The Linear Source

$$S^*(j,g) = R\left[\frac{H_1(j,g)}{\langle H_1\phi\rangle} - \frac{H_2(j,g)}{\langle H_2\phi\rangle}\right] \tag{31}$$

VI. GENERATION OF SENSITIVITY COEFFICIENTS

JULIET implements the sensitivity equations discussed in Section III of ORNL/TM-5563.[14] The equation below is solved to yield the sensitivity of a response to a cross section as defined by an operator. A common form of the operator is a single material--reaction type. However, the operator can take the form of a cross-section mixture. In the equation, the cross-section operator of interest is designated by the subscript X.

A. General Representation of Terms in Sensitivity Coefficient Definitions

$$T_1(g,z) = -\Sigma_X(g,z)\sum_{j\epsilon z} V(j)\sum_{k=1}^{NOA}\phi^*(j,g,k)\phi(j,g,k)w(k) \tag{32}$$

$$T_2(g,z) = \frac{1}{k}\sum_{j\epsilon z} V(j)[\nu(g,z)\Sigma_f(g,z)\phi(j,g,1)\sum_{g'=1}^{IGM}\phi^*(j,g',1)\chi(g',z) \tag{33}$$

$$T_3(g,z) = \sum_{\ell=1}^{LMOM} \sum_{j\epsilon z} V(j) \sum_{g'=1}^{IGM} \phi^*(j,g',\ell)\phi(j,g,\ell)\Sigma_X(g\rightarrow g',\ell) \tag{34}$$

$$T_4(g,z) = \Sigma_X(g,d)\phi(d,g,1)/\langle H_1\phi\rangle \tag{35}$$

$T_4(g,z) = 0$ unless Σ_X appears in the definition of H_1

$$T_5(g,z) = -\Sigma_X(g,d)\phi(d,g,1)/\langle H_2\phi\rangle \tag{36}$$

$T_5(g,z) = 0$ unless Σ_X appears in the definition of H_2

The d indicates the space increment where the direct effect $\neq 0$ (i.e., where H_1 and H_2 are defined).

$T_4(g,z) = T_5(g,z) = 0$ if d is not within zone z.

$$P(g,z) = \frac{1}{R}\left[T_1(g,z) + T_2(g,z) + T_3(g,z)\right] + T_4(g,z) + T_5(g,z) \tag{37}$$

where

g - group index,

g' - group index,

z - zone index,

j - spatial interval index,

k - angle index,

V(j) - volume of interval,

$\Sigma_X(g,z)$ - cross section operator,

$\phi^*(j,g,k)$ - adjoint angular flux,

$\phi(j,g,k)$ - forward angular flux,

w(k) - discrete ordinates weight,

$\nu(g,z)$ - neutrons per fission,

$\Sigma_f(g,z)$ - fission cross section,

$\phi(j,g,\ell)$ - forward moment flux,

$\phi^*(j,g,\ell)$ - adjoint moment flux,

$\chi(g',z)$ - fission spectrum,

$\Sigma_x(g'\rightarrow g,\ell)$ - scattering cross section.

All of the five terms in the equation do not appear in every sensitivity calculation. The terms included are a function of the response and the operator of interest.

B. K Sensitivity

1. Absorption Reactions, Nonfissionable, Nonscattering Reactions such as Capture

The equation reduces to $T_1(g,z)$ where $\Sigma_x(g,z)$ is the absorption cross section of the material of interest.

2. Fission Reactions

The fission reaction requires only $T_1(g,z)$ and $T_2(g,z)$. In T_1, $\Sigma_x(g,z)$ is the fission cross section of the material of interest.

3. ν Sensitivity

The ν reaction requires only $T_2(g,z)$.

4. Scattering Reactions

A scattering reaction such as elastic requires $T_1(g,z)$ and $T_3(g,z)$ where $\Sigma_x(g,z)$ in T_1 is the elastic scattering cross section. $\Sigma_x(g'\rightarrow g,\ell)$ in T_3 is the elastic group-to-group scattering matrix for moment ℓ of the material of interest.

5. Total Reaction of a Fissionable Material

The total reaction of a fissionable material requires the $T_1(g,z)$, $T_2(g,z)$ and $T_3(g,z)$ terms. $\Sigma_x(g,z)$ in T_1 is the total cross section and $\Sigma_x(g'\rightarrow g,\ell)$ is the total group-to-group scattering matrix.

6. Total Reaction of a Nonfissionable Material

The total reaction of non-fissionable materials is the same as (5) except the $T_2(g,z)$ term is 0.

The T_4 and T_5 terms do not enter into a k sensitivity since they are direct-effect expressions for reaction rate ratio responses. For k sensitivity, the R in Eq. (37) is to be interpreted as $R = \lambda\langle\phi^* H_2\phi\rangle$.

C. Reaction Rate Ratios

When the response is a reaction rate ratio such as ^{238}U capture/^{235}U fission, the ^{28}c/^{25}f, both indirect and direct effects must be considered. Direct effects occur only when the operator of interest is a material reaction type which is a constituent of the response definition. All operators have indirect effects.

1. Indirect Effect

The algorithm is identical to k sensitivity with Γ^* replacing ϕ^* in Eqs. (32), (33) and (34), and the R appearing in Eq. (37) is to be interpreted as:

$$R = \frac{1}{S}\left[\frac{\langle H_1\phi\rangle}{\langle H_2\phi\rangle}\right] \tag{38}$$

where $\dfrac{\langle H_1\phi\rangle}{\langle H_2\phi\rangle}$ is the response calculated by the source execution path and S is the source normalization from the ANISN generalized adjoint calculation.

2. H_1 Direct Effect

When the operator of interest is the material-reaction type which forms the numerator of the reaction rate ratio, the H_1 direct effect is calculated and summed with the indirect effect to complete the profile. The H_1 direct effect is calculated by the $T_4(g,z)$ term in Eq. (37). For the example, $\Sigma_x(g,z)$ in T_4 is the ^{238}U capture cross section. $\langle H_1\phi\rangle$ is available from the source execution path. The T_4 term and $\langle H_1\phi\rangle$ must be calculated over the same space; frequently this is the central interval. T_4 is zero in any zone that does not include the space increment used in the $\langle\phi H_1\rangle$ calculation.

3. H_2 Direct Effect

When the operator of interest is the material-reaction type which forms the denominator of the reaction rate ratio, an H_2 direct effect is calculated and summed with the indirect effect to complete the profile. The H_2 direct effect is calculated by the $T_5(g,z)$ term in Eq. (37). For the example, $\Sigma_x(g,z)$ in T_5 is the ^{235}U fission cross section. $\langle H_2\phi\rangle$ is available from the source execution path. The T_5 term and $\langle H_2\phi\rangle$ must be calculated over the same space; frequently this is the central interval. T_5 is zero in any zone that does not include the space increment used in the $\langle H_2\phi\rangle$ calculation.

D. Worth Sensitivities

The general definition of a worth response is $R = \dfrac{\langle\phi^* H_1\phi\rangle}{\langle\phi^* H_2\phi\rangle}$ for a material defined by H_1. The H_1 operator includes the total cross section, the total group-to-group scattering matrix and $\nu\Sigma_f$ if the material is fissionable. The H_2 operator is a macroscopic mixture of $\nu\Sigma_f$ over all

space for all fissionable materials in the assembly. These operators are reviewed here in an attempt to clarify worth direct effects.

1. H_1 Direct Effect

Assume the material worth is being calculated for ^{238}U. Because H_1 includes Σ_T and $\nu\Sigma_f$, an H_1 direct effect will be included in the worth profiles for the ^{238}U total, ν, and fission reactions.

$$H_1D(g,d) = \frac{P(g,d)\lambda\langle\phi^*H_2\phi\rangle}{\langle\phi^*H_1\phi\rangle} \tag{39}$$

where P(g,d) is a profile calculated with the k sensitivity equation but with the spatial dependence of the H_1 operator.

2. H_2 Direct Effect

The worth profile of any fissionable material in the system will include a direct effect contribution for the Σ_f and ν reactions.

$$H_2D(g,z) = \lambda P(g,z) \tag{40}$$

where P(g,z) is the k sensitivity for the ν reaction for the fissionable material of interest. Here spatial dependence is simplified because k sensitivity and the H_2 operator are defined over all space.

3. Forward Flux Indirect Effect

This component is an indirect effect calculated with the same equation as k sensitivity. In the equation ϕ^* is replaced with Γ^* and

$$R = \left[\frac{\langle\phi^*H_1\phi\rangle}{\lambda\langle\phi^*H_2\phi\rangle}\right]\frac{1}{S} \tag{41}$$

where S is the source normalization from the ANISN Γ^* run.

4. Adjoint Flux Indirect Effect

This component is also an indirect effect calculated with the same equation as k sensitivity. In the equation ϕ^* is replaced with Γ and ϕ is replaced with ϕ^*. Again

$$R = \left[\frac{\langle \phi^* H_1 \phi \rangle}{\lambda \langle \phi^* H_2 \phi \rangle}\right] \frac{1}{S} \tag{42}$$

where S is the source normalization from the ANISN Γ run.

VII. JULIET INPUT PREPARATION

JULIET performs two major functions, source generation and the calculation of sensitivity coefficients. A single computer run may be set up to accomplish both functions or they may be done independently. Normally a source calculation must precede a sensitivity calculation since source generates normalization parameters used in the sensitivity calculation.

A. Execution Paths

JULIET is divided into four execution paths. Path selection is accomplished by the user to solve the problem of interest. The paths are:

1. Operator Definition, Selected by the Word, MIX

This path must always be executed because operators are required for any JULIET function. Operators are defined from cross sections. They may have the form of a single material reaction cross-section type, a mixture of a single reaction from several materials or other combinations of materials and reaction cross-section types. A common operator

is a mixture or material which includes Σ_c, χ, Σ_f, Σ_a, $\nu\Sigma_f$, Σ_T and the total group-to-group scattering matrix. This is referred to as an automatic operator in JULIET. It is used to form both the H_1 and H_2 bilinear operators in a SOURCE calculation. When an automatic operator is referenced in a sensitivity calculation, sensitivity coefficients are calculated for the capture, fission, $\bar{\nu}$, χ, and total reactions.

2. Flux Preparation, Selected by the Word, FLUX

The path calculates moment fluxes from angular fluxes and also prepares the so-called $\phi^*\phi$ file used by the sensitivity calculation. Actually, the file may also be $\Gamma^*\phi$ or $\Gamma\phi^*$. The execution of this path is prerequisite to a SOURCE-RESPONSE calculation. The execution of the path may be omitted when going directly to the calculation of sensitivity coefficients and appropriate $\phi^*\phi$ files already exist.

3. Source Generation, Selected by the Word, SOURCE

This path is executed to calculate sources, responses and normalization parameters. The equations solved are outlined in Section IV. Do not execute this path in studies using two-dimensional sensitivity analysis.

4. Sensitivity Coefficient Generation, Selected by the Word, SENSE

This path implements the sensitivity coefficient generation algorithms outlined in Section V.

B. Input Blocks

Since JULIET input is a function of the execution paths selected, the input is divided into five distinct blocks. All of the blocks do not have to appear in a run.

1. Block 1 (always provided)

The content of Block 1 is a function of the execution paths selected. If FLUX is a member of the execution path, Block 1 input is:

15$$ Integer Parameters [36]

1. Any integer
2. ITH <100 only downscatter cross sections; >100 upscatter
3. ISCT - maximum order of scatter found in any zone
4. ISN - order of angular quadrature
5. IGE - 1 - slab; 2 - cylinder; 3 - sphere
6. Any integer
7. Any integer
8. IZM - number of zones
9. IM - number of mesh intervals
10. Any integer
11. IGM - number of energy groups
12. IHT - position of σ_{total} in $\phi^*\phi$ table
13. IHS - position of σ_{gg} (self-scatter) in $\phi^*\phi$ table
14. IHM - length of $\phi^*\phi$ table
15. .
. Any integer
. .
36.

T

T

1** Fission spectrum [IGM]

4** Radii by interval boundary [IM + 1]

5** Velocities [IGM], the array may be omitted

6** Angular quadrature weights [MM]

7** Angular quadrature cosines [MM]

8$$ Zone numbers by interval [IM]

T

Note that Block 1 input is ANISN input with deletions and minor modifications. The 8$$ card describes the spatial dependence in the sensitivity calculation except for reaction rate ratio direct effects. The 8$$ card does account for the spatial dependence of worth direct effects and the card used in the ANISN calculation usually must be modified. All entries on the 15$$ card are not used in JULIET, but the format is unchanged to permit the convenience of reproducing the card from existing ANISN input.

If FLUX is not a member of the execution path, Block 1 input simplifies to:

15$$ 0 ITH ISCT 4Z IZM 2Z IGM IHT IHS IHM FO

T

T

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where

ITH <100/>100, no upscatter/upscatter,

ISCT maximum order of scatter,

IZM number of zones,

IGM number of energy groups,

IHT position of σ_{total} in cross-section table,

IHS position of σ_{gg} (self-scatter) in cross-section table,

IHM length of cross-section table.

2. Block 2 (always provided) Operator Definition

This input defines the operators to be used in subsequent source and sensitivity calculations. All Block 2 input is in a fixed field format. Operators are defined as a function of cross sections and this input references the MATXS file.

MIX (columns 1-3) selects execution path.

Operator Definition Cards. Columns (1-5) (I5) Operator ID. This may be an arbitrary number assigned by the user. However, if applicable, an ENDF/B material identification number is suggested for this input.
Columns (11-16) (A6) MATXS particle identifier, NEUT is normal input.
Columns (21-26) (A6) MATXS type identifier, NSCAT is normal input.
Columns (31-36) (A6) MATXS material identifier.
Columns (41-46) (A6) MATXS reaction type identifier/blank/ALLINL/ELSCAT or other reaction type name.
Columns (51-60) (E10.4) Density.
Columns (61-65) (I5) Order of P_n (P_0-0).
Columns (66-70) (I5) If < 0, eliminates χ.
When all operators are defined, insert 1 blank card.

Mixing. Operators are frequently defined as cross-section mixtures. A set of two or more operator definition cards with identical operator identifiers define a mixture which may be referenced in source and sensitivity calculations.

Comments on the Operator ID (Columns 1-5). Sensitivity coefficients are placed in a proposed CCCC file SENPRO. Part of the identification of a set of coefficients in SENPRO is the ENDF/B material identification. The operator ID is passed to SENPRO and used as the ENDF/B material

identification number. If the operator is a mixture or something else that cannot be properly identified with an ENDF/B MAT number, the user must take appropriate action to insure proper identification and use of the data. For some applications, JULIET sabotages the SENPRO ENDF/B material identification scheme. Two or more equal operator ID numbers define a mixture. This can cause difficulty when several operators are defined for the same material but with different reaction types. Future code development will eliminate this problem. In the interim the ENDF/B material identification scheme must sometimes be abandoned and arbitrary unique operator IDs assigned. The SENPRO service module provides a quick and easy method to redefine the number used as an ENDF/B material identification. This service may also aid the user with an operator that cannot be correctly identified in ENDF/B terminology.

Comments on MATXS Reaction Type Identifier (Columns 41-46). Please note this is a six-character string, a word not an integer. The MATXS files currently in use were obtained by translating either ANISN files or AMPX master files. In either case, the ENDF/B reaction type numbers (MT) influence the procedure. The translators establish the following relationship:

ENDF/B (MT)	MATXS (Columns 41-46 entry)
1	TOTAL
2	ELSCAT
3	NONELS
4	INSTOT
16	N2N
17	N3N
18	FIS
19	FCFIS
20	SCFIS
21	TCFIS
51	INEL01
⋮	⋮
90	INEL40
91	CTNUUM
102	CAPT
452	NUBAR
1452	NUFIS

For other ENDF/B MT numbers the translator forms a MATXS six-character string as follows: If the MT = 1234, the MATXS identifier will be MT1234.

If columns (41-46) are left blank, an automatic operator is generated.

If columns (41-46) are ALLINL, sensitivity coefficients will be generated for all inelastic levels and the continuum.

Comments on Columns (66-70). If the operator is an automatic mixture, this entry prevents a mixing operation on the fission spectrum.

3. Block 3 (Optional)

FLUX Preparation

FLUX (Columns 1-4) selects execution path.

60$$ Integer Parameters [11]

KCI - 0/1, prepare $\int\phi V$ for central interval/no effect. This parameter controls spatial dependence of the direct effect for reaction rate ratio calculations. Central interval direct effect is the normal calculation. If a 1 is entered, then the direct effect spatial dependence is defined by the 8$$ card in Block 1.

IRF - identification number for forward flux.

IRA - identification number for adjoint flux.

FO - eight parameters reserved.

T

For both IRF and IRA, enter negative values when the adjoint flux component of a worth sensitivity is being calculated. This informs the code that the forward and adjoint fluxes are to be interchanged. When IRF=IRA=0, the adjoint flux used is identified by the FMANG identification number (second entry FMANG 1$$ card) and the forward flux is ϕ.

4. Block 4 (Optional)

SOURCE Generation

SOURCE (Columns 1-6) selects execution path.

70$$ Integer Parameter [1]

NRESP - number of responses.

71** Floating point parameters [2]

k - If k = 0 is entered, the value is retrieved from the repository.

F0.0

T

Repeat the following title, 72$$, 73$$, 74$$, 75**, T sequence of cards for each response

HOLLERITH TITLE of response (20 A4)

72$$ Integer parameters [2+IM] where IM is the number of mesh intervals.

1. ILBL - operator type identifier.

   0 - linear operator

   1 - bilinear operator

2. ISCT - scattering order (P_0=0).

3. H_1 operator identifier for each mesh interval. See Block 2 input for operator definition.

⋮

IM+2

73$$ Integer Parameters [2+IM]

1. 0

2. 0

3. H_2 operator identifier for each mesh interval.

⋮

IM+2

74$$ Integer Parameters [10]

1. LPRT - source print option.

   0 - no print

   1 - print

2. LSAVE - source save option.

   0 - no save

   1 - save

3. IDA - adjoint source identification number.

4. IDF - forward source identification number.

5.
⋮ FO, reserved for future options.
10.

75** Omit if response is not a reactivity worth [2]

A - Atomic mass of material of interest.

B - Density of material of interest.

T

5. Block 5 (Optional)

Sensitivity Coefficient Calculation

SENSE (Columns 1-5) selects execution path.

80$$ Integer Parameters [2]

NRESP - number of responses.

ILNG - last neutron group.

T

81** Floating point parameters [ILNG+1]

Neutron group structure.

82** Floating point parameters [NGG=1] where NGG is the number of γ groups.

γ group structure.

T

Repeat the following sequence of cards ending with 91$$ T for each response

HOLLERITH TITLE FOR ASSEMBLY (20 A4)

HOLLERITH TITLE FOR RESPONSE (20 A4)

When the response is a reaction rate for which direct effects will be calculated, extra care must be taken with the response description.

Columns (1-8) material identifier for the numerator, example U-238.

Columns (9-16) reaction rate identifier for the numerator, example CAPT.

Columns (17-24) material identifier for the denominator.

Columns (25-32) reaction rate identifier for the denominator.

83$$ Integer Parameters [13]

NE - number of operators to be processed.

IDR - response identifier for data retrieval from repository.

IDS - response identifier placed on SENPRO.

NTRN - reaction rate ratio identifier placed on SENPRO.

KERT - unit number of $\phi^*\phi$ file, default = 9, default used when 0 is entered.

FO - reserved for future options.

T

86** Floating point parameters [6]

R - calculated value of response.

R1 - $\langle H_1\phi \rangle$, used only when direct effects are to be calculated; otherwise enter 0.

R2 - $\langle H_2\phi \rangle$, used only when direct effects are to be calculated; otherwise enter 0.

EK - k; if not applicable, enter 0.

EVR - measured value of response; if not applicable, enter 1.0.

FUT - enter 0; reserved for future option.

T

When R, R1, R2 and EK are all entered as 0, these parameters are retrieved from the repository.

******Repeat following sequence for NE operators

HOLLERITH TITLE for material-reaction (20 A4)

87$$ Integer Parameters [10]

1. LMAX1 - Order of P_n, enter 0 for P_0.
2. IFISS - Fission option.
   - 0 - no fission
   - 3 - total sensitivity of fissionable material
   - 13 - sensitivity of fission cross section
   - 23 - sensitivity of $\overline{\nu}$
3. IOP - Direct effect option.
   - 0 - no direct effect
   - 1 - material-reaction type in response numerator
   - 2 - material-reaction type in response denominator
4. NZP - number of entries on 91$$ card.
5. JOPA(1) - 0/1 do not save/save indirect effect.
6. JOPA(2) - 0/1 do not save/save direct effect.
7. JOPA(3) - 0/1 do not save/save indirect + direct effect.
8. INC - 0/1 do not include/include results in summation over all operators.
9. LCRW - 0.

10. LPRT - 0/1 normal output/limited output. Normal output lists a sensitivity matrix which includes sensitivities by group and group-to-group transfers. Limited output lists only total sensitivities by zone.

T

88$$ Integer Parameters [NZONE]

Operator identifiers by zone.

89** Floating point parameters [NZONE]

Zone densities.

90$$ FO - reserved for future options.

91$$ Integer Parameters [NZP]

DO - loop limiters for zone summations.

Example: 91$$ 1 1 2 2 1 2 will produce three sets of coefficients: zone 1, zone 2, and a summation over zones 1 and 2.

T

******

VIII. RESOURCE UTILIZATION

The amount of computer core required is highly problem-dependent. The parameters affecting core size requirements are listed in the discussion of the container array. The most important parameters are the number of groups and the number of spatial mesh intervals. The number of moments and the scattering order have little impact on core requirements but are important factors in the amount of usage of external storage devices such as disks and tapes. Computer CPU usage by JULIET is trivial relative to cross-section preparation and neutronics calculations.

A. Container Array

Most data storage is in a single container array. The length of this array varies for each execution path. It is necessary to calculate the container array length for each execution path activated in a run. In the main program the length must be set to the maximum value calculated plus a common term IC. Parameters of interest in determining container array length:

IGM - number of groups.

IM - number of space intervals.

NOA - number of angles.

NZ - number of zones.

ITL - ANISN cross-section table length.

IDP - precision parameter.

IDP = 2 for double-word precision.

IDP = 1 for single-word precision.

MKNT - number of materials in the bilinear H_1 operator.

MLSA - length of the largest compressed scattering matrix in the problem.

ISCT - order of scattering.

MS - total number of reactions available for sensitivity analysis.

NH1 - number of materials in the linear H_1 operator.

NH2 - number of materials in the linear H_2 operator.

COMMON TERM

IC - 132 + 4*IGM + 3*IM + NZ

1. Operator Definition

ICO = MS*(2*ISCT + 14) + 2*IGM^2 + IGM*(6 + 2*ISCT) + MAXO(7500, IGM^2,75*IGM)

2. Flux Preparation

I1 = 2*(IM+1)*NOA + IGM * (IM + NZ)

I2 = IGM * (ITL + 2*NZ + ITL)

I3 = IGM * (ITL + 2*NZ + 2*IM)

ICF = MAXO(I1, I2, I3)

3. Source Response

Bilinear

I4 = IGM*(IM*IDP + MKNT + 1) + MKNT + MLSA + MS*(ISCT + 2)

I5 = IM*IGM*(2*IDP + 1)

IC1 = MAXO(I4, I5)

Linear

IC2 = 2*IGM*(NH1 + NH2) + MS + IM + IGM

ICR = 2*IM + 4 + MAXO(IC1, IC2)

4. Sensitivities

ICS = 2*MSOP + MS*(ISCT + 3) + 3*(ITL*IGM) + 2*IGM*(NZ + ISCT)
+ ISCT*NZ; MSOP is the total number of operator definition cards required (see p. 22).

Container Array Size

KS = IC + MAXO(ICO, ICF, ICR, ICS)

B. Overlay Structure

JULIET uses a simple overlay structure which could be made more detailed if required. Basically each execution path is contained in an overlay segment. The sensitivity path uses three overlay segments. The overlay structure is shown in Fig. 1.

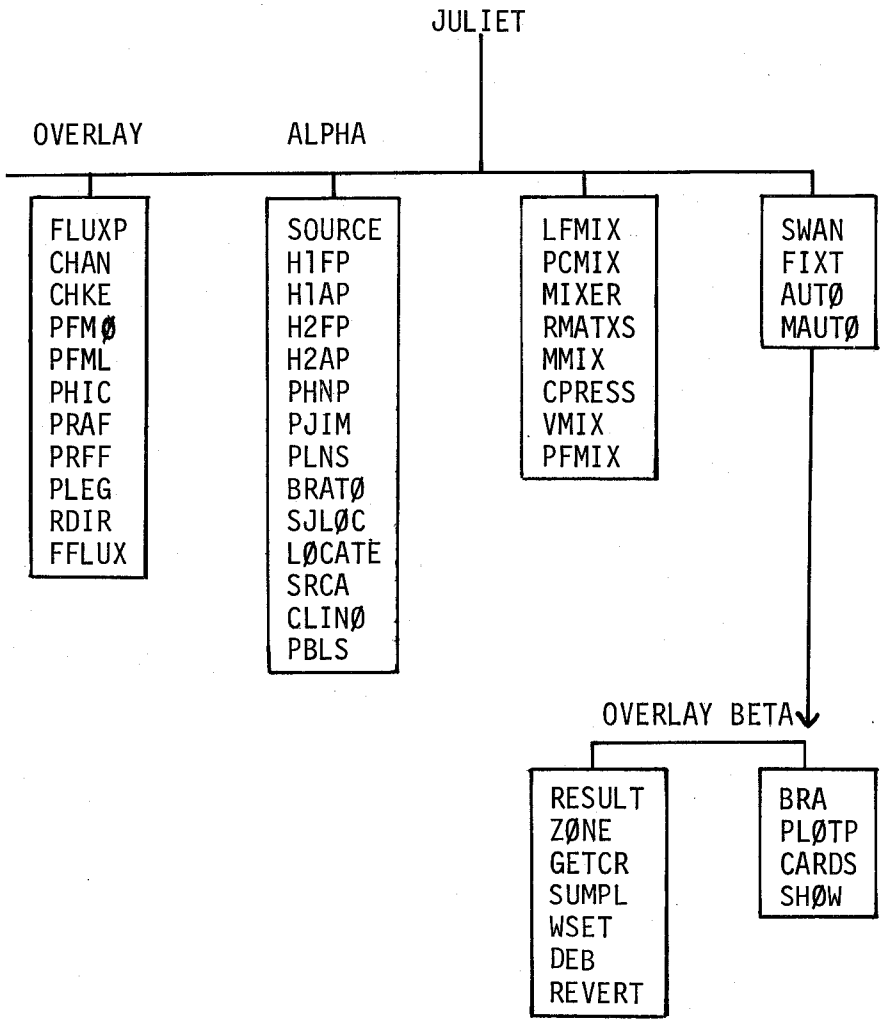

Fig. 1. Overlay Structure

C. I/O Units

Unit	Use	Record Length	Number of Records
1	PMANG Record	623	1
2	Repository	a	
5	Input		
6	Output		
8	MATXS Interface	b	
9	$\phi^*\phi$ File	ITL*IGM	1+NZ*ISCT
10	DA, Angular	(NOA+1)(IM)	2*IGM
11	DA, Moment	(IGM*IM)	2*LMOM1
12	DA, Bilinear Sources	IM	IGM*LMON1
13	DA, $\phi^*\phi$ Preparation	ITL*IGM	NZ*LMOM1
14	Scattering Blocks	c	NSR*ISCT
15	ID Cross Sections	IGM	NID
23	SENPRO Interface	IGM	NP
	In Source Execution Path		
31	Scratch (Unformatted)	2*IM*IGM	LMOM1
32	Scratch (Unformatted)	2*IM*IGM	LMOM1
33	Scratch (Unformatted)	2*IM*IGM	LMOM1
34	Scratch (Unformatted)	2*IM*IGM	LMOM1
35	Scratch (Unformatted)	2*IM*IGM	2*LMOM1
	In Sensitivity Execution Path		
31	Scratch (Unformatted)	ITL*IGM	ISCT
32	Scratch (Unformatted)	ITL*IGM	ISCT
33	Scratch (Unformatted)	ITL*IGM	ISCT
34	Scratch (Unformatted)	ITL*IGM	ISCT

Unit	Use	Record Length	Number of Records
35	Scratch (Unformatted)	ITL*IGM	ISCT
41	Scratch (Formatted)	80	NR
42	Scratch (Formatted)	80	NR

a. Problem-Dependent,

Angular flux record length = (NOA+1)(IM+1),

Number of records = IGM,

Source record length = IM*LMOM1,

Number of records = IGM.

There will be fluxes and sources for each response in the study.

b. Use a tape; if it is desirable to set up disk space, study the problem and the MATXS format and estimate space requirements.

c. For upscatter problems, the length of a scattering block is IGM^2.

For downscatter only problems, length = $\frac{IGM^2}{2} + IGM$.

NOA - number of angles. NSR - number of scattering reactions.

NZ - number of zones. NID - number of 1D reactions.

LMOM1 - number of moments + 1. IM - number of space points.

IGM - number of groups. ISCT - scattering order + 1.

ITL - cross-section table length. NP - total number of profiles.

DD Card Preparation for Direct Access (DA) Units

DD cards for direct access units require the entry of a block length and the number of blocks. These should be calculated with care since inadequate space will kill the run. Large block lengths use core storage; small block lengths increase I/O's. The procedure is illustrated by example.

Rule 1

Length < 32000 bytes.

Rule 2

Length must be an even multiple of 16.

Example

Determine record length and number of records for unit 13 when ITL = 131, IGM = 126, NZ = 3, LMOM1 = 4.

L = 131 * 126 = 16506 words

L = 66024 bytes

Rule 1 is violated since 66024 > 32000.

Therefore,

L1 = L/N where N is large enough for L1 < 32000.

Let N = 6, then L1 = 66024/6 = 11004.

Now for rule 2, 11004 is not an even multiple of 16 so set L1 = 11008. L1 = 11008 satisfies both rules 1 and 2. If N could have been 1, then the number of records would = NZ*LMOM1 = 3*4 = 12. Since N = 6, number of records = 12*6 = 72. Increase number of records by $\approx$ 10% and on the DD card for unit 13 enter 11008 for the block size and 82 for the number of blocks.

```
//GO.FT13F001 DD UNIT=SYSDA,
//    SPACE=(11008, (082),,CONTIG,ROUND),
//    DCB=(RECFM=FT,BUFNO=1)
```

IX. JULIET ERROR STOPS

Several error stops are built into JULIET which abort the calculation when a condition is detected that will invalidate the results. In addition to numbered and unnumbered stop statements, the code also includes two error detecting subroutines (ERRA and CRASH). The unnumbered STOP statements always follow a printed statement indicating the nature of the difficulty.

A. The Unnumbered STOP Statements

Location: Subroutine RMATXS, format statement 93

Message: RMATXS is dimensioned for 1500 materials, this problem has, IIIIIIII

Action: The fixed dimension of HMATNM(1500) in RMATXS must be increased or the problem size reduced. The latter is recommended.

Location: Subroutine RMATXS, format statement 23

Message: Dimensioning problem in RMATXS with variables associated with N2DB, take action in RMATXS, MIXER, PCMIX, N2DB = IIIII, MSCAT = JJJJJ.

Action: A material has been read from the MATXS file with a higher scattering order than anticipated by the program writer. If the scattering order for the problem is less than P_{21}, check MATXS for errors; if a scattering order greater than P_{20} is desired, program changes will be required in the routines cited in the message.

Location: Subroutine RMATXS, format statement 76

Message: See RMATXS, increase dimensions of variables associated with N1DR from 100 to IIIII.

Action: Check MATXS for an error; if none, take the action indicated in the message.

Location: Subroutine RMATXS, format statement 78

Message: Dimension of D exceeded in RMATXS; available space IIIIIIII, required space JJJJJJJJ.

Action: Increase the container array as indicated in the message or reduce problem size.

B. The Numbered STOP Statements

Statement: STOP 11

Location: Subroutine LOCATE

Action: An undefined cross-section operator was requested in either a 72$$ or 73$$ card. Insure that operator definition input (see Section VI, Block 2) is compatible with SOURCE input (see Section VI, Block 4).

Statement: STOP 67, STOP 74, STOP 75, STOP 76, STOP 78

Location: Subroutine SOURCE

Action: Increase container array size; for guidance see Section VII, A.(3).

Statement: STOP 111

Location: Subroutine ERRA

Action: See following discussion of ERRA.

C. Subroutine ERRA

Certain types of errors trigger a call to subroutine ERRA which prints a message containing an error STOP number and the subroutine name from which the call to ERRA originated. ERRA is misleading in that, when reference is made to subroutine MAIN, it should read subroutine SOURCE. Subroutine ERRA terminates with a STOP 111 statement.

Message: Error stop 2 in subroutine MAIN

Called from: Subroutine SOURCE

Action: The scattering order requested for the H_1 operator of a bilinear function exceeds the maximum scattering order allowed for the problem. Check the third entry on the 15$$ card (see Section VI, B, Block 1) and the second entry of a 72$$ card (see Section VI, B, Block 4). The entry on a 72$$ card cannot exceed the entry on the 15$$ card.

Message: Error stop 4 in subroutine MAIN

Called from: Subroutine SOURCE

Action: A non-zero scattering order was requested for the H_2 operator of a bilinear function. Correct the third entry of any 73$$ cards (see Section VI, B, Block 4) found in error.

Message: Error stop 6 in subroutine MAIN

Called from: Subroutine SOURCE

Action: A non-zero scattering order was requested for the numerator of a linear response. Locate and correct the 72$$ cards in error.

Message:	Error stop 8 in subroutine MAIN
Called from:	Subroutine SOURCE
Action:	A non-zero scattering order was requested for the denominator of a linear response. Locate and correct the 73$$ cards in error.

Message:	Error stop 1 in subroutine PLEG
Called from:	Subroutine PLEG
Action:	Check 15$$ card for input errors relating to the geometry and quadrature order.

Message:	Error stop 1 in subroutine RDIR
Called from:	Subroutine RDIR
Action:	Check input weights and cosines (see Section VI, B., Block 1).

Message:	Error stop 2 in subroutine RDIR
Called from:	Subroutine RDIR
Action:	Check input weights and cosines (see Section VI, B., Block 1).

Message:	Error stop 3 in subroutine RDIR
Called from:	Subroutine RDIR
Action:	Check all input relating to the S_n quadrature.

D. Subroutine CRASH

This routine is called several times throughout the code to insure that the size of the container array is adequate. When an insufficient size is detected, a self-explanatory message is printed stating:

***CRASH IN HHHHHHHH, Required IIIIIIII, Available JJJJJJJJ

where

H...H is the subroutine name,

I...I is the required container array size,

J...J is the available container array size.

X. THE MATXS CROSS-SECTION FILE

```
C*********************************************************************
C                     REVISED 08/24/76
C
CF                    MATXS
CE                    COMPREHENSIVE CROSS SECTION FILE
C
CN                          THIS FILES CONTAINS MACROSCOPIC AND
CN                          MICROSCOPIC CROSS SECTIONS, YIELDS AND
CN                          F-FACTORS FOR ALL PARTICLES, MATERIALS
CN                          AND REACTION TYPES
C
C                           R J BARRETT, R E MACFARLANE
C
C*********************************************************************


C---------------------------------------------------------------------
CS                    FILE STRUCTURE
CS
CS                    RECORD TYPE
CS                    ============================== ===============
CS                    FILE IDENTIFICATION            ALWAYS
CS                    FILE CONTROL                   ALWAYS
CS                    SET HOLLERITH IDENTIFICATION   ALWAYS
CS                    FILE DATA                      ALWAYS
CS
CS    ************(REPEAT FOR ALL PARTICLES)
CS    *               GROUP STRUCTURES               ALWAYS
CS    *************
CS
CS    *************(REPEAT FOR ALL DATA TYPES)
CS    *               DATA TYPE CONTROL ALWAYS
CS    *
CS    * **********(REPEAT FOR ALL MATERIALS
CS    * *             MATERIAL CONTROL               ALWAYS
CS    * *             VECTOR CONTROL                 N1DB.GT.0
CS    * *
CS    * * *******(REPEAT FOR ALL VECTOR PARTIAL
CS    * * *                BLOCKS)
CS    * * *              VECTOR PARTIAL BLOCK         N1DB.GT.0
CS    * * *******
CS    * *
CS    * *             SCATTERING MATRIX CONTROL      N2DB.GT.0
CS    * *
CS    * * *******(REPEAT FOR ALL SCATTERING
CS    * * *                SUB BLOCKS)
CS    * * *             SCATTERING SUB-BLOCK         N2DB.GT.0
CS    *************
C
C---------------------------------------------------------------------


C---------------------------------------------------------------------
CR                    FILE IDENTIFICATION
C
CL    HANME,(HUSE(I),I=1,2),IVERS
C
CW    1+3*MULT
C
CB    FORMAT(4H 0V ,A6,1H*,12A6,1H*,I6)
C
CD    HNAME           HOLLERITH FILE NAME - MATXS - (A6)
CD    HUSE            HOLLERITH USER IDENTIFIATION (A6)
CD    IVERS           FIELD VERSION NUMBER
CD    MULT            DOUBLE PRECISION PARAMETER
CD                          1 - A6 WORD IS SINGLE WORD
CD                          2 - A6 WORD IS DOUBLE PRECISION WORD
C
C---------------------------------------------------------------------
```

```
C--------------------------------------------------------------------
CR                    FILE CONTROL                                  -
C                                                                   -
CL     NPART,NTYPE,NHOLL                                            -
C                                                                   -
CW     3                                                            -
C                                                                   -
CB     FORMAT(4H 1D ,3I6)                                           -
C                                                                   -
CD     NPART           NUMBER OF PARTICLES FOR WHICH GROUP          -
CD                     STRUCTURES ARE GIVEN                         -
CD     NTYPE           NUMBER OF DATA TYPES PRESENT IN SET          -
CD     NHOLL           NUMBER OF WORDS IN SET HOLLERITH             -
CD                     IDENTIFICATION RECORD                        -
C                                                                   -
C--------------------------------------------------------------------


C--------------------------------------------------------------------
CR                    SET HOLLERITH IDENTIFICATION                  -
C                                                                   -
CL     (HSETID(I),I=1,NHOLL)                                        -
C                                                                   -
CW     NHOLL*MULT                                                   -
C                                                                   -
CB     FORMAT(4H 2D ,11A6/(12A6))                                   -
C                                                                   -
CD     HSETID          HOLLERITH IDENTIFICATION OF SET (A6)         -
CD                      (TO BE EDITED OUT 72 CHARACTERS PER LINE)   -
C                                                                   -
C--------------------------------------------------------------------


C--------------------------------------------------------------------
CR                    FILE DATA                                     -
C                                                                   -
CL     (HPRT(J),J=1,NPART),(HTYPE(K),K=1,NTYPE),(NMAT(K),K=1,NTYPE),-
CL    1(NINP(K),K=1,NTYPE),(NING(K),K=1,NTYPE),(NOUTP(K),K=1,NTYPE),-
CL    2(NOJTG(K),K=1,NTYPE),(LOCT(K),K=1,NTYPE),(NGRP(J),J=1,NPART) -
C                                                                   -
CW     (NPART+NTYPE)*MULT+6*NTYPE+NPART                             -
C                                                                   -
CB     FORMAT(4H 3D ,11A6/(12A6))      HPRT,HTYPE                   -
CB     FORMAT(12I6)                    NMAT,NINP,NING,NOUTP,NOUTG,  -
CB                                     LOCT,NGRP                    -
C                                                                   -
CD     HPRT(J)         HOLLERITH IDENTIFICATION FOR PARTICLE J      -
CD                              NEUT NEUTRON                        -
CD                              GAMA PHOTON                         -
CD                              BETA ELECTRON                       -
CD                              .    .                              -
CD                              .    .                              -
CD                              .    .                              -
CD     HTYPE(K)        HOLLERITH IDENTIFICATION FOR DATA TYPE K     -
CD                              NSCAT NEUTRON SCATTERING            -
CD                              NGAMA NEUTRON INDUCED GAMMA PRODUCTION -
CD                              NGCUP NEUTRON-GAMMA COUPLED SET     -
CD                              GSCAT GAMMA SCATTERING              -
CD                              NNFF  NEUTRON F-FACTORS             -
CD                              .    .                              -
CD                              .    .                              -
CD                              .    .                              -
CD     NMAT(K)         NUMBER OF MATERIALS IN SET FOR DATA TYPE K   -
CD     NINP(K)         NUMBER OF INCIDENT PARTICLES ASSOCIATED WITH -
CD                     DATA TYPE K                                  -
CD     NING(K)         NUMBER OF INCIDENT GROUPS ASSOCIATED WITH    -
CD                     DATA TYPE K                                  -
CD     NOUTP(K)        NUMBER OF OUTGOING PARTICLES ASSOCIATED WITH -
CD                     DATA TYPE K                                  -
CD     NOUTG(K)        NUMBER OF OUTGOING GROUPS ASSOCIATED WITH    -
CD                     DATA TYPE K                                  -
CD     LOCT(K)         NUMBER OF RECORDS TO BE SHIPPED TO READ DATA FOR -
CD                     DATA TYPE K LOCT(1)=0                        -
CD     NGRP(J)         NUMBER OF ENERGY GROUPS FOR PARTICLE J       -
C                                                                   -
C--------------------------------------------------------------------


C--------------------------------------------------------------------
CR                    GROUP STRUCTURE                               -
C                                                                   -
CL     (GPB(I),I=1,NGRP(J)),EMIN                                    -
C                                                                   -
CW     NGRP(J)+1                                                    -
C                                                                   -
CB     FORMAT(4H 4D ,1P5E12.5/(6E12.5))                             -
C                                                                   -
CD     GPB(I)          MAXIMUM ENERGY BOUND FOR GROUP I FOR PARTICLE J -
CD     EMIN            MINIMUM ENERGY BOUND FOR PARTICLE J          -
C                                                                   -
C--------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR                    DATA TYPE CONTROL                                -
C                                                                      -
CL     (HMATNM(I),I=1,NMAT),(TEMP(I),I=1,NMAT),(SIGZ(I),I=1,NMAT),     -
CL    1(LOCA(I),I=1,NMAT),(IINP(J),J=1,NINP),(IOUTP(J),J=1,NOUTP),     -
CL    2NSBLK                                                           -
C                                                                      -
CC     NMAT =NMAT(K)                                                   -
CC     NINP =NINP(K)                                                   -
CC     NOUTP=NOUTP(K)                                                  -
C                                                                      -
CW     (3*MULT)*NMAT+NINP+NOUTP+1                                      -
C                                                                      -
CB     FORMAT(4H 5D ,11A6/(12A6))          HMATNM                      -
CB     FORMAT(1P6E12.5)                    TEMP,SIGZ                   -
CB     FORMAT(12I6)                        LOCA,IINP,IOUTP,NSBLK       -
C                                                                      -
CD     HMATNM(I)       HOLLERITH IDENTIFICATION FOR MATERIAL I         -
CD     TEMP(I)         AMBIENT TEMPERATURE(DEGREES KELVIN)             -
CD     SIGZ(I)         MATERIAL DILUTION FACTOR                        -
CD     LOCA(I)         NUMBER OF RECORDS TO BE SKIPPED TO READ DATA FOR -
CD                     MATERIAL I LOCA(1)=0                            -
CD     IINP(J)         NUMBER OF THE PARTICLE TYPE CORRESPONDING       -
CD                     TO INCIDENT PARTICLE I FOR DATA TYPE K          -
CD     IOUTP(J)        NUMBER OF THE PARTICLE TYPE CORRESPONDING       -
CD                     TO OUTGOING PARTICLE I FOR DATA TYPE K          -
CD     NSBLK           SUB-BLOCKING PARAMETER                          -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR                    MATERIAL CONTROL                                 -
C                                                                      -
CL     HMAT,AMASS,IMAC,N1DR,N1DB,N2DB                                  -
C                                                                      -
CW     MULT+5                                                          -
C                                                                      -
CB     FORMAT(4H 6D ,A6,1H*,E12.5,4I6)                                 -
C                                                                      -
CD     HMAT            HOLLERITH MATERIAL IDENTIFIER                   -
CD     AMASS           GRAM ATOMIC MASS                                -
CD     IMAC            1/2 MEANS MICROSCOPIC/MACROSCOPIC CROSS SECTIONS -
CD     N1DR            NUMBER OF VECTOR PARTIALS                       -
CD     N1DB            NUMBER OF VECTOR PARTIAL BLOCKS                 -
CD     N2DB            NUMBER OF SCATTERING BLOCKS                     -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR                    VECTOR CONTROL                                   -
C                                                                      -
CL     (HVSP(I),I=1,N1DR),(IBLK(I),I=1,N1DR),(NFG(I),I=1,N1DR),        -
CL    1(NLG(I),I=1,N1DR)                                               -
C                                                                      -
CW     (3*MULT)*N1DR                                                   -
C                                                                      -
CB     FORMAT(4H 7D ,11I6/(12I6))                                      -
C                                                                      -
CD     HVPS(I)         HOLLERITH IDENTIFIER OF PARTIAL(I)              -
CD                             SNGAM NEUTRON CAPTURE                   -
CD                             SFIS FISSION                            -
CD                             SNHE HELIUM PRODUCTION                  -
CD                             .       .                               -
CD                             .       .                               -
CD                             .       .                               -
CD     IBLK(I)         NUMBER OF BLOCK IN WHICH PARTIAL(I) IS LOCATED   -
CD     NFG(I)          NUMBER OF FIRST NON-ZERO GROUP FOR PARTIAL(I)    -
CD     NLG(I)          NUMBER OF LAST NON-ZERO GROUP FOR PARTIAL(I)     -
C                                                                      -
C-----------------------------------------------------------------------


C-----------------------------------------------------------------------
CR                    VECTOR PARTIAL BLOCK                             -
C                                                                      -
CL     (VPS(I),I=1,KMAX)                                               -
C                                                                      -
CC     KMAX=SUM OVER PARTIALS IN BLOCK J OF NON-ZERO GROUPS            -
C                                                                      -
CW     KMAX                                                            -
C                                                                      -
CB     FORMAT(4H 8D ,1P5E12.5/(6E12.5))                                -
C                                                                      -
CD     VPS(I)          VECTOR DATA FOR ALL NON-ZERO GROUPS FOR ALL     -
CD                     PARTIALS WITH IBLK(I)=J                         -
C                                                                      -
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR                    SCATTERING MATRIX CONTROL                        -
C                                                                      -
CL     (HMTX(N),N=1,N2DB),(LONE(N),N=1,N2DB),(LORD(N),N=1,N2DB),       -
CL    1((JBAND(L,N),L=1,NOUTG(K)),N=1,N2DB)                            -
CL    2((IJJ(L,N),L=1,NOJTG(K)),N=1,N2DB)                              -
C                                                                      -
CW     (MULT+2+2*NOUTG(K))*N2DB                                        -
C                                                                      -
CB     FORMAT(4H 9D ,11A6/(12A6))        HMTX                         -
CB     FORMAT(12I6)                      LONE,LORD,JBAND,IJJ          -
C                                                                      -
CD     HMTX(N)          HOLLERITH IDENTIFICATION FC BLOCK N            -
CD     LONE(N)          LOWEST LEGENDRE ORDER PRESENT IN BLOCK N       -
CD     LORD(N)          NUMBER OF SCATTERING ORDERS PRESENT IN BLOCK N -
CD     JBAND(L,N)       SCATTERING BANDWIDTH FOR GROUP L,SCATTERING    -
CD                      BLOCK N                                        -
CD     IJJ(L,N)         LOWEST ENERGY GROUP OF BAND JBAND              -
C                                                                      -
C-----------------------------------------------------------------------
```

```
C-----------------------------------------------------------------------
CR                    SCATTERING SUB-BLOCK                             -
C                                                                      -
CL     ((SCAT(K,L),K=1,KMAX),L=1,LORD(N))                              -
C                                                                      -
CC     KMAX=SUM OVER I OF ALL JBAND(I,N) IN THE I RANGE OF SUB-BLOCK M -
C                                                                      -
CW     KMAX*LORD(N)                                                    -
C                                                                      -
CD     SCAT(K,L) MATRIX DATA FOR GROUP TO GROUP TRANSFER OF PARTICLES  -
C                                                                      -
C-----------------------------------------------------------------------
```

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