International Atomic Energy Agency

INDC(BZL)-21/G

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

PROCEDURE FOR CALCULATING SENSITIVITY PROFILES BY TRANSPORT THEORY - THE FORSS SYSTEM

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(Translated by the IAEA)

October 1986

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

Translated from Portuguese

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Reproduced by the IAEA in Austria
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86-05694

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ABSTRACT

The main modules for the FORSS system needed for generating sensitivity profiles are presented in this paper. The interfaces created for linking the modules are described. Preliminary results are shown to be consistent with those found in the literature.

1. INTRODUCTION

Sensitivity theory has been the object of considerable development work since the 1970s [1-4]. Within the context of various study groups, the FORSS system was drawn up by that of the Oak Ridge National Laboratory. This system is composed of various programs, some of which were already known and were modified for the purpose. Its principal objective is to study the relations between cross-sections, integral parameters in reactors and associated uncertainties.

The work described here constitutes the implementation of certain available modules for the FORSS system and the creation of an interface for writing a library of multigroup cross-sections in MATXS format [2] needed for the JULIET module [6].

Part 2 of the paper contains a theoretical description of the sensitivity profile calculated with the FORSS system. In part 3 the calculation procedure starting from the ENDF/B basic data library up to the production of the sensitivity profile is described. The preliminary calculations which have been performed are presented in part 4, and the conclusions and recommendations are contained in part 5. Appendixes A, B, C, D and E provide users with necessary information and descriptions of the entries for the various modules.

2. METHODOLOGY APPLIED BY THE FORSS SYSTEM

2.1. Sensitivity profiles

Sensitivity profiles are parameters of great importance in sensitivity theory [7]. They represent the variation in a given integral parameter due to the variation in a given cross-section. Where R is an integral parameter and Σ is a cross-section, the sensitivity profile P is written as:

$$\frac{\frac{dR}{R}}{\frac{d\Sigma}{\Sigma}} = P_{\Sigma} \tag{1}$$

To obtain it, the FORSS system calculates the Boltzmann equations:

$$(A - \lambda B) \quad \phi = L \, \phi = 0 \tag{2}$$

$$(A^* - \lambda B^*) \quad \phi^* = L^* \quad \phi^* = 0 \tag{3}$$

where:

A = leakage and scattering operator

A* = operator adjoint to A

B = fission operator

B* = operator adjoint to B

λ = system eigenvalue

ϕ = forward flux

ϕ^* = adjoint flux.

Considering an integral parameter R defined as a bilinear ratio

$$R = \frac{\int \phi^* (\xi) \, H_1 [\Sigma (\xi)] \, \phi (\xi) \, d\xi}{\int \phi^* (\xi) \, H_2 [\Sigma (\xi)] \, \phi (\xi) \, d\xi} \tag{4}$$

where H_1 and H_2 are operators which depend on the cross-section, ξ and $d\xi$ are position and volume element vectors in phase space. Equation (1) will be found by differentiating Eqs (2), (3) and (4) with respect to $\Sigma(\rho)$, using a functional derivative notation[3]. The parameter ρ represents a point in phase space ξ. Thus:

$$\frac{\frac{dR}{R}}{\frac{d\Sigma(\rho)}{\Sigma(\rho)}} = P_{\Sigma(\rho)} = I_1 + I_2 + I_3 + I_4 \tag{5}$$

with:

$$I_1 = \Sigma(\rho) \frac{\int \phi^*(\xi) \frac{dH_1[\Sigma(\xi)]}{d\Sigma(\rho)} \phi(\xi)\, d\xi}{\int \phi^*(\xi) H_1[\Sigma(\xi)] \phi(\xi)\, d\xi} \quad (6)$$

$$I_2 = -\Sigma(\rho) \frac{\int \phi^*(\xi) \frac{dH_2[\Sigma(\xi)]}{d\Sigma(\rho)} \phi(\xi)\, d\xi}{\int \phi^*(\xi) H_2[\Sigma(\xi)] \phi(\xi)\, d\xi} \quad (7)$$

$$I_3 = -\frac{\Sigma(\rho)}{R} \int \Gamma^*(\xi) \frac{dL[\Sigma(\xi)]}{d\Sigma(\rho)} \phi(\xi)\, d\xi \quad (8)$$

$$I_4 = -\frac{\Sigma(\rho)}{R} \int \Gamma(\xi) \frac{dL^*[\Sigma(\xi)]}{d\Sigma(\rho)} \phi^*(\xi)\, d\xi \quad (9)$$

where $\Gamma(\xi)$ and $\Gamma^*(\xi)$ are the generalized forward and adjoint fluxes respectively, which are the solutions of:

$$(A - \lambda B)\Gamma = \frac{\partial R}{\partial \phi^*} = R\left(\frac{H_1\phi}{\int \phi^* H_1 \phi\, d\xi} - \frac{H_2\phi}{\int \phi^* H_2 \phi\, d\xi}\right) \quad (10)$$

and:

$$(A^* - \lambda B^*)\Gamma^* = \frac{\partial R}{\partial \phi} = R\left(\frac{H_1^* \phi^*}{\int \phi^* H_1 \phi\, d\xi} - \frac{H_2^* \phi^*}{\int \phi^* H_2 \phi\, d\xi}\right) . \quad (11)$$

In Eq. (5), I_3 and I_4 represent the "indirect effect" contained in the integral parameter R due to differentiation of the forward flux and the adjoint flux with respect to $\Sigma(\rho)$. I_1 and I_2 represent the "direct effect" of differentiating R with respect to the cross-section which appears explicitly in the definition of the integral parameter. For example, when the sensitivity profile of the ratio between the fission rate of ^{238}U and the fission rate of ^{235}U is being studied in relation to fission of ^{238}U, in addition to the indirect effect, the direct effect I_1 will be found. If the previous profile were in relation to fission of ^{235}U, the direct effect I_2 would be found. With this example we have a linear relationship between operators, namely in Eq. (4) the adjoint flux $\phi^*(\xi)$ is made to be equal to one, $H_1 = \Sigma_f^{28}$ and $H_2 = \Sigma_f^{25}$.

3. CALCULATION PROCEDURE

3.1. Generation of composition-dependent cross-section libraries

In calculations of integral parameters it is necessary to have cross-sections in a given number of energy groups for a series of materials making up a specific standard problem. To obtain these libraries by means of the NJOY system [8] (transport theory), use must be made of five modules of the system: RECONR, BROADR, UNRESR, GROUPR and DTFR.

The RECONR module reconstructs the cross-sections in terms of points on the basis of resonance parameters and interpolation schemes available in the evaluated nuclear data file (ENDF/B). Processing for the desired temperature is carried out by BROADR, and the UNRESR module adds the contribution from unresolved resonances. The multigroup cross-sections and multigroup flux are calculated by the GROUPR module. The DFTR module reformats the output from GROUPR for subsequent use of the multigroup library in transport codes such as ANISN [9] or DTF-IV.

In the library generated in this form (DTF-IV or ANISN format), the cross-sections occupy well-defined positions in the table; for example, if the total cross-section occupies position 5 in the table and there is no upscattering, in position 4 there will be found the product $\nu\sigma_f$, in position 3 σ_a and in position 6 σ_{gg}.

The JULIET module [6] requires a cross-section library in MATXS format. In this format the cross-sections are identified by names; for example, the total cross-section is called TOTAL, the multigroup fission spectrum CHI, and so on. To obtain this library an interface, AMX, was created which converts a library characterized by positions into one specified by names.

The diagram in Fig. 1 summarizes the steps necessary for generating sensitivity profiles.

When using the NJOY system for obtaining a multigroup cross-section library, the GROUPR module requires a weighting function that characterizes the energy spectrum of the medium to be studied. This spectrum must be provided by the user since the system does not perform spectrum calculations. As the GODIVA benchmark was selected for comparison studies and it is composed solely of uranium, the ^{235}U fission spectrum, which is very similar to the spectrum of the medium, was used as a weighting function.

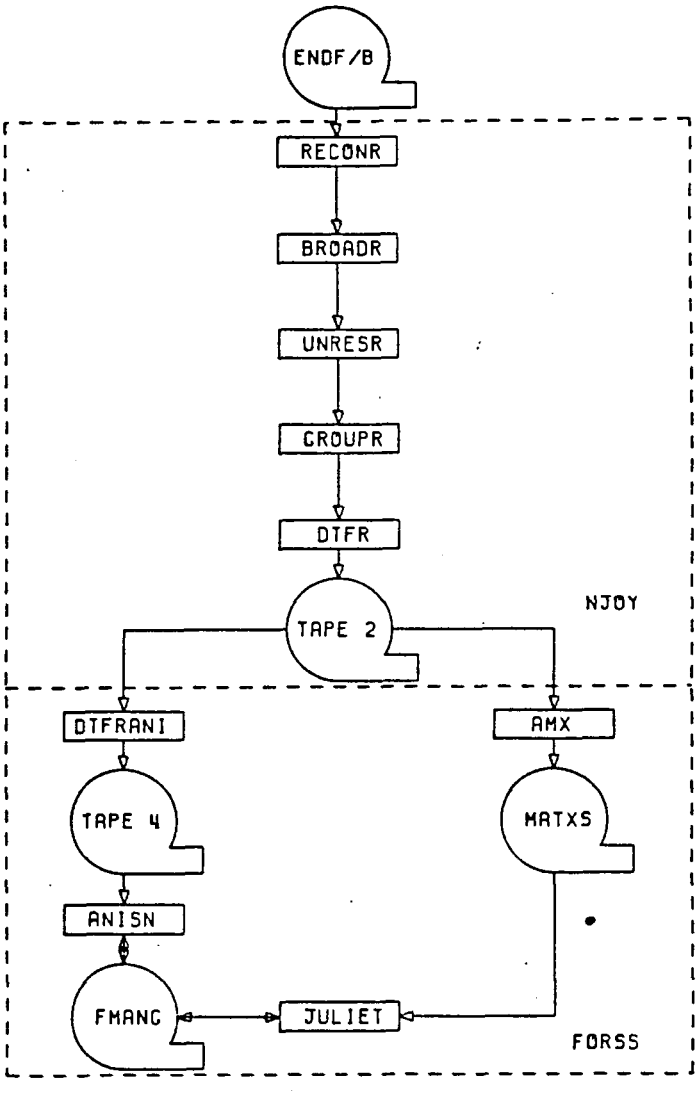

Fig. 1. Block diagram of the calculation procedure.

3.2. The modules for calculations

The FORSS system performs the calculations described earlier by means of the above equations using of modular programs.

The forward flux and the adjoint flux described by Eqs (2) and (3) are calculated by the FANISN model. This is the ANISN program [9] with some modifications to include calculation of the generalized fluxes in accordance with Eqs (10) and (11). The terms I_1, I_2, I_3 and I_4 belonging to Eq. 5, $\partial R/\partial \phi^*$ and $\partial R/\partial \phi$, terms called generalized sources, are calculated by the JULIET module, which was derived from the SWANLAKE program [10].

In the study of an integral parameter, whether k effective, the ratio between reaction rates, reactivity worth, etc., there is a hierarchy of events and of modules to be used. For example, if the profile to be obtained were a ratio between reaction rates, the following events should occur:

a) Preparation of a multigroup cross-section library in ANISN format;

b) Calculation of the forward flux by the FANISN module;

c) Calculation of the adjoint flux, also by the FANISN module;

d) Re-formatting of the cross-section library used by FANISN in MATXS format. This work is done by the AMX module developed by us;

e) Finding, with the JULIET module, the generalized sources used in Eqs (10) and (11);

f) Calculation of the generalized fluxes of Eqs (10) and (11) by the FANISN module;

g) Calculation of the sensitivity profile of Eq. (5) by the JULIET module.

The result of the calculations performed under (b), (c), (e) and (f) above are placed in a logical unit known in the FORSS system as FMANG [5]. It is this unit which makes the exchange of information between the FANISN and JULIET modules.

As mentioned earlier, the FANISN module is used in exactly the same way as the ANISN program, except that the first input card to be included contains the parameters needed for the FMANG sub-routine described in the previous paragraph. The title of this card is "1$$", and it is described in Appendix D.

The JULIET module calculates sources, responses (reaction rates and reactivity worth), normalization parameters and sensitivity profiles. It was constructed in such a way as to carry out tasks in accordance with words given in its input. There are four keywords which define sub-modules:

- The operators are defined by the word MIX. These operators will be used during execution and may be a single material-reaction pair or a mixture of materials including various reactions;
- Various integrals involving the forward, adjoint or generalized fluxes are used for calculating the sensitivity profiles. The sub-module which prepares them is selected by the word FLUX;
- The linear and bilinear sources and normalization and calculation parameters for responses are obtained by the sub-module selected by the word SOURCE;
- The sensitivity profiles are calculated with the relevant sub-module being selected by the word SENSE.

The final result of combining such sub-modules is the sensitivity profiles written in SENPRO format [5], in logical unit No. 23. For investigating these numbers, it is found necessary to use a service module. In addition to its other functions, which are described in Appendix E, this converts an unformatted file into a formatted one.

4. PRELIMINARY CALCULATIONS

Some calculations have been performed for purposes of validating the implementation of the FANISN and JULIET modules.

Using the procedure described above, a cross-section library with 26 energy groups was obtained for the GODIVA benchmark. The AMX program was used to re-format this library for execution of the JULIET module. Although the energy boundaries used in our calculations do not coincide exactly with the boundaries contained in the file of sensitivity profiles supplied by the Oak Ridge National Laboratory, the results can be compared if this is done only with the total profile. The total profile is defined as the sum of the individual partial profiles for all the energy groups. Table 3 shows the values of the integral parameters obtained.

It will be seen from Tables 1 and 2 that there is a good agreement between the values calculated. The main differences are found in the sensitivity profile of the 28F/25F ratio in relation to the ^{234}U fission cross-section and nubar. It will be seen from the values obtained in this table that the function [Translator's note: The function has been omitted in the original; perhaps it should be: $\Gamma^*(\xi)$.] calculated by Eq. (11) is correct in view of the fact that it is involved in the calculation of all the profiles and that the discrepancies are observed in particular profiles. In the calculation of the profiles in relation to nubar, the contributions of $\nu\sigma_f$ and χ appear explicitly [5]. Any difference in the basic data for these components leads to large variations in the calculated profiles. This fact is not verified in the k effective profile calculations since the parameters described appear in the form of a relation, which may cause errors to be cancelled out. The variations observed are attributed to small differences that have arisen in the generation of the multigroup library.

5. CONCLUSIONS AND RECOMMENDATIONS

In sensitivity studies applied to nuclear data, the FORSS system is considered as a code of high validity. The fact that the processing system is based on transport theory, together with modular programming, ensures its versatility and accuracy in calculation.

Table 1. Total sensitivity profile of k effective calculated with the FORSS system for the GODIVA benchmark.

MATERIAL	REACTION	TOTAL PROFILE (IEAv)	TOTAL PROFILE (ORNL)
^{234}U	CAPTURE	-6,0311-04	-6,0959-04
	FISSION	5,7933-03	5,6781-03
	NUBAR	8,4029-03	8,2857-03
^{235}U	CAPTURE	-3,6201-02	-3,6807-02
	FISSION	6,6190-01	6,5921-01
	NUBAR	9,8179-01	9,8197-01
^{238}U	CAPTURE	-1,3185-03	-1,3314-03
	FISSION	6,8575-03	6,7763-03
	NUBAR	9,8301-03	9,7592-03

Table 2. Total sensitivity profile of the ratio between fission of ^{238}U and of ^{235}U calculated with the FORSS system for the GODIVA benchmark.

MATERIAL	REACTION	TOTAL PROFILE (IEAv)	TOTAL PROFILE (ORNL)
^{234}U	CAPTURE	4,9456-04	5,2259-04
	FISSION	2,1463-05	5,7642-04
	NUBAR	2,1668-05	8,1253-04
^{235}U	CAPTURE	3,2280-02	3,4063-02
	FISSION	-8,7321-01	-8,1866-01
	NUBAR	4,1318-03	6,8381-02
^{238}U	CAPTURE	1,0616-03	1,1191-03
	FISSION	9,9805-01	9,9782-01
	NUBAR	1,3094-05	4,4756-04

Table 3. Calculated values of k effective and 28F/25F.

	IEAv(*)	ORNL(**)
k	0.9953	1.0033
28F/25F	0.1667	0.1663

* 26 groups P1
** 126 groups P3

In Ref. [4] a system for calculating sensitivity profiles with diffusion theory is described. The main differences between transport and diffusion for obtaining profiles are in the integrals involving forward and adjoint flux. The FORSS system uses angular fluxes, which do not exist when processing with diffusion. Another difference between the two systems is that the value of k effective included in the profile equations is, when calculated by diffusion, restricted by limitations imposed by diffusion theory.

Among the various modules for the system, the main ones are FANISN and JULIET, which can be used for a number of applications. The numbers of figures involved in these calculations are generally very large, which may frequently be confusing to the user. It is therefore recommended that, for any application, particular attention should be paid to the input and output files.

The computer time needed for obtaining a file containing sensitivity profiles is spent almost entirely in obtaining the forward, adjoint and generalized fluxes. Optimization of the input file of the FANISN module would therefore be desirable.

The aim is to extend these sensitivity studies by implementing the modules and by drawing up procedures in the future for processing covariance matrices.

6. REFERENCES

[1] WEISBIN, C.R., PEELLE, R.W., MARABLE, J.H., de SAUSSURE, G., COLLINS, J.P., KUJAWSKI, E., GREENSPAN, E., Sensitivity and uncertainty analysis of reactor performance parameters, Advances in Nuclear Science and Technology, Vol. 14, Plenum Press (1982).

[2] WEISBIN, C.R., OBLOW, E.M., MARABLE, J.H., PEELLE, R.W., LUCIUS, J.L., Application of sensitivity and uncertainty methodology to fast reactor integral experiment analysis, Nucl. Sci. Eng. 66 (1978) 307.

[3] OBLOW, E.M., Sensitivity theory from a differential viewpoint, Nucl. Sci. Eng. 59 (1976) 187.

[4] MENEZES, A., CLARO, L.H., ROSA, M.A.P., UNISENS: A System for Sensitivity Analysis of Integral Parameters with Diffusion Theory. Technical Note IAEv/NT-01/84 (1984) [in Portuguese].

[5] LUCIUS, J.L., WEISBIN, C.R., MARABLE, J.H., DRISCHLER, J.D., WRIGHT, R.Q., WHITE, J.E., A User Manual for the FORSS Sensitivity and

Uncertainty Analysis Code System, ORNL-5316, Oak Ridge National Laboratory (1981).

[6] LUCIUS, J.L., OBLOW, E.M., CUNNINGHAN III, G.W., A User's Guide for the JULIET Module of FORSS Sensitivity and Uncertainty Analysis Code System, ORNL/TM-6594 (1979).

[7] CLARO, L.H., MENEZES, A., Sensitivity Profiles Calculated with the UNISENS System. Technical Note IAEv/NT-01/85 (1985) [in Portuguese].

[8] MacFARLANE, R.E., MUIR, D.W., BOICOURT, R.M., The NJOY Nuclear Data Processing System, Vol. I: User's Manual, LA-9303-M (ENDF-324) (1982).

[9] ENGLE Jr., W.W., A User's Manual for ANISN, a One-Dimensional Discrete Ordinates Transport Code with Anisotropic Scattering, K-1693, Oak Ridge National Laboratory (1967).

[10] BARTINE, D.E., OBLOW, E.M., MYNATT, F.R., Swanlake - A Computer Code Utilizing ANISN Radiation Transport Calculation for Cross-Section Sensitivity Analysis, ORNL/TM-3809 (1973).

APPENDIX A

1. Name and title:

   DTFRANI-IEAv

2. Language and computer:

   FORTRAN-V; CDC CYBER 170/750

3. Nature of problem solved:

An interface has been created between the output from the DTFR module, the NJOY system and the ANISN program which provides a binary output in ANISN format.

4. Limitations and restrictions

In the DTFRANI program a vector XSEC with 2000 positions was dimensioned. The length of this vector is given by LTAB = IGM*IHM, that is, the number of energy groups times the length of the mixture table. When the vector length exceeds 2000, file 6 is created with the following error message: "DIMENSION OF XSEC SHOULD BE **********".

5. Files used:

   File 5 - input (output from the DTFR module)
   File 6 - output (if it is created, there is a dimensioning error)
   File 4 - output (input for ANISN, binary library)

6. Date of creation

   July 1985

Acknowledgement: The authors wish to thank Ezzat Selim Chalhoub for clarifications and assistance with the preparation of this interface.

APPENDIX B

1. Name and title:

AMX-IEAv

2. Language and computer:

FORTRAN-V; CDC CYBER 170/750

3. Nature of the problem solved:

The multigroup library created by the NJOY code using the DTFR module is processed by the AMX module, which transforms it into MATXS format.

The set of input cross-sections for the AMX must be in accordance with the following sequence:

Position in table	Name
1- SIGCAP	CAP
2- SIGFIS	FIS
3- SIGABS	ABS
4- NUFISS	NUFIS
5- SIGTOT	TOTAL
6- SIGSCA	SCAT

Limitations and restrictions:

Identical to DIFRANI with the following increases:

- Maximum number of groups: 30;
- Maximum number of materials: 10;
- Maximum number of data types: 1 (neutrons)

If the problem to be solved goes beyond these limitations, modifications will be needed in the dimensions of the vectors.

5. Files used:

Input files:

File 2 (output from the DTFR module)

File 5 (input data)

Output files:

File 6: (MATXS-BCD file)

File 8: (MATXS-binary file)

6. Date of creation:

July 1985

APPENDIX C

1. Name and title:

JULIET - ORNL - IEAv

2. Language and computer:

FORTRAN IV; CDC CYBER 170/750

3. Nature of the problem solved:

JULIET is a module of the FORSS system which calculates sources, responses (e.g. criticality, reaction rates, reactivity worths etc.), normalization parameters and sensitivity coefficients. This module withdraws information and deposits it in the FMANG respository, which is the data exchange medium between ANISN and JULIET. When ANISN is used as a neutronics code for studying sensitivity profiles, JULIET will receive angular fluxes and store generalized source data. For subsequent studies, ANISN is used for generating generalized fluxes. Sensitivity analysis requires partial access to cross-sections. The MATXS file contains the basic cross-section data for JULIET. A MATXS file is prepared with the AMX program (c.f. Appendix B). The final product from JULIET is the calculation of the sensitivity coefficients.

This module performs two main functions: it obtains the source and calculates the sensitivity coefficients. Normally, a source calculation should precede a sensitivity calculation, since the normalization parameter is used in these calculations.

This module is divided up into four execution paths. The paths selected are accomplished by the user to solve problems of interest.

3.1. Definition of the operator selected by the word MIX

This path should always be executed, because the operators are required for calculating any function of JULIET. The operators are defined on the basis of the cross-sections. These may take the form of a single material - reaction pair or of other combinations of materials and cross-sections. A common operator is a mixture or a material which includes Σ_c, χ, Σ_f, Σ_a, $\nu\,\Sigma_f$, Σ_t and the total group-to-group scattering matrix.
When an automatic operator is referenced, the sensitivity profiles for the capture cross-section, the fission cross-section, nubar and the total profile will be calculated.

3.2. Preparation of the flux selected by the word FLUX

This prepares the calculation paths for the moment fluxes on the basis of the angluar fluxes and the file $\phi^*\phi$ used for calculating the sensitivity profiles. Execution of this path is a prerequisite for calculating sources or responses.

3.3. Generation of the source selected by the word SOURCE

This path is executed for calculating linear and blilinear sources, responses and normalization parameters.

3.4. Generation of the sensitivity coefficients selected by the word SENSE

This path implements the algorithm for generating the sensitivity coefficients which contain the direct and indirect effects.

4. Files used:

Input files:

File 2 - FMANG

File 5 - data

File 8 - MATXS library

Output files:

File 6 - Output (BCD)

File 23 - Profiles in SENPRO (binary) format

Apart from the files defined earlier, others are used as working files in the execution of these modules.

5. Preparation of input data for the JULIET module:

The input data, which are a function of the execution paths selected, are divided into five distinct blocks. The reading format used is the FIDO format [5]. The numbers in brackets on each card show the number of values to be read. Unless otherwise specified, free format is used.

Block I (always provided)

1$$ - integer parameters (36)

1 - any integer

2 - IHT < 100 downscattering only

\- > 100 containing upscattering

3 - ICST maximum scatter order established for any zone

4 - ISN angular quadrature order

5 - IGE geometry

- 1 - slab
- 2 - cylindrical
- 3 - spherical

6 - any integer

7 - any integer

8 - IZM number of zones

9 - IM number of intervals

10 - any integer

11 - IGM number of energy groups

12 - IHT position of σ total in table

13 - IHS position of σ_{gg} in table

14 - IHM length of table

15 -

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36 - Positions 15-36: any integer

T

T

1** fission spectrum (IGM)

4** radii by interval boundary (IM + 1)

5** velocity (IGM)

6** angular quadrature weights

7** angular quadrature cosines

8$$ Number of zones per interval (IM)

T

N.B. Block I input consists of ANISN input with some deletions and minor alterations. The 8$$ card describes the spatial dependence in the sensitivity calculation, except for reaction rates where the source positions will be given by the 72$$ and 73$$ cards.

Not all entries on the 15$$ card are used by the JULIET code, but the format is unchanged for convenience of reproducing the card from existing ANISN input. If FLUX is not executed, the 15$$ card can be written as:

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

T

T

T

where:

ITH - < 100 does not contain upscattering
> 100 contains upscattering

ISCT - maximum order of scatter

1ZM - number of zones

IGM - number of energy groups

IHT - position of σ total in table

IHS - position of $\sigma_{g\bar{g}}$ total in table

IHM - size of table

Block II (always provided)

Definition of operators

This block defines the operators used in subsequent source and sensitivity calculations. The operators are defined as a function of cross-section, and it is recommended that the names contained in the MATXS file be used.

(Columns 1-3) card 1

MIX - execution path selected

(Columns 1-5) card 2

format I5 - number which defines the operator. If applicable, use the MAT defined in ENDF/B.

(Columns 11-16)

format A6 - name which identifies the particle. NEUT is normal input.

(Columns 21-26)

format A6 - name which identifies the data type, format MATXS. NSCAT is normal input.

(Columns 31-36)

format A6 - name which identifies the material, format MATXS

(Columns 41-46)

format A6 - name which identifies the reaction type, format MATXS, /blank/, ALLINL, ELSCAT, or other reaction names

(Columns 51-60)

format E10.4 - densities

(Columns 61-65)

format I5 - order of P_n (P_o = 0)

(Columns 66-70)

format I5 - if < 0, eliminate χ (if the automatic operator is a mixture, this entry prevents a mixture operation on the fission spectrum).

When all the operators have been defined, a blank card should be inserted.

Block III (optional)

Preparation of flux

(Columns 1-4) card 1

FLUX - execution path selected

60$$ - integer parameter (11) card 2

KCI - 0/1, prepares $\int\phi v$ for central interval/does no effect. This parameter checks the spatial dependence of the direct effect for calculation of reaction rates. Central direct effect is the normal calculation. If a 1 is entered, the spatial dependence of the direct effect is then defined by the 8$$ card in Block I. If KCI < 0, no $\phi^*\phi$ file will be made.

IRF - number which identifies the forward flux

IRA - number which identifies the adjoint flux

LPATH - If < 0, no adjoint flux will be read from the repository

KERT - unit number of the $\phi^*\phi$ file. Default = 9

FO - reserved for future options

T

Note: A negative entry for IRF and IRA should be made to the module when the adjoint flux component of a worth sensitivity is being calculated. This informs the module that adjoint flux and forward flux are to be interchanged. When IRF = IRA = 0, the adjoint flux used is defined by FMANG, (identification number of the adjoint flux, second entry of the 1$$ card) and the forward flux is ϕ.

Block IV (optional)

Source generation

(Columns 1-6) card 1.

SOURCE - selects execution path

70$$ integer parameters (1) card 2

NRESP - number of responses

71** floating-point parameters (2)

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

FO.0

T

Repeat the following sequence of cards for each response:

Title, 72$$, 73$$, 74$$, 75**, T

Title of response: format 20A4

72$$ integer parameters (2 + IM), where IM is the number of mesh intervals

ILBL - operator type identifier

0 - linear operator

1 - bilinear operator

ICST - order of scatter (P_o = 0)

H_1 - operator identifier for each mesh interval. See Block II input for operator definition

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(2 + IM)

73$$ integer parameters (2 + IM)

0

0

H_2 - operator identifier for each mesh interval

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.

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(2 + IM)

74$$ integer parameters (10)

LPRT - source print option

0 - no print

1 - print

LSAVE - source save option in the repository

0 - no save

1 - save

IDA - adjoint source identification number

IDF - forward source identification number

FO - reserved for future options

75$$ Omit if the response is not a reactivity worth (2)

A - atomic mass of the material of interest

B - density of the material of interest

T

Block V (optional)

Calculation of sensitivity coefficient

(Columns 1-5) card 1

SENSE - selects execution path

80$$ - integer parameters (2) card 2

NRESP - number which identifies the response

ILNG - number which identifies the last group of neutrons

T

81** floating-point parameters (ILNG + 1)

"neutron group structure"

T

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

Title for assembly format 12A6

Title for response format 12A6

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

(Columns 1-6) Name which identifies the material of the numerator, e.g. U-238

(Columns 7-12) Name which identifies the reaction rate for the numerator, e.g. CAP

(Columns 13-18) Name which identifies the material for the denominator

(Columns 19-25) Name which identifies the reaction rate for the denominator

Note: These identifiers of materials and reaction rates should be identical to those put on the operator identification card. If the automatic operator has been designated, the reaction type is left blank on the operator definition card and the identifier should be identical to that assigned by the code.

83$$ integer parameters (13)

NE - number of operators to be processed

IRESP - identifier of the response for data retrieval from the repository

IDS - identifier of the response placed on SENPRO

NRTN - identifier of the reaction rate placed on SENPRO

KERT - unit number of file $\phi^*\phi$, default = 9. The default will be used when the entry is 0.

IPRO - unit number of SENPRO file (default = 23)

FO - reserved for future options

T

86** floating-point parameters (6)

R - calculated value of the response

R1 - $< H_1\phi >$, used only when direct effect is calculated

R2 - $< H_2\phi >$, used only when indirect effect is calculated

EK - k; if not applicable, enter as 0

EVR - measured value of the response; if not applicable, enter as 1

FUT - enter as 0; reserved for future options

T

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

Repeat the following sequence for NE operators:

Title for material-reaction (12A6)

87$$ integer parameters (10)

LMAX1 - order of P_n, enter as 0 for P_0

IFISS - fission option

0 - no fission

3 - total sensitivity of fissionable material

13 - sensitivity of fission cross-section

23 - sensitivity of nubar

IOP - option for direct effect

0 - no direct effect

1 - type of material-reaction in numerator response

2 - type of material-reaction in denominator response

NEP - number of entries on the 91$$ card

JOPA(1) - 0 don't save

1 save indirect effect

JOPA(2) - 0 no save

1 save indirect effect

JOPA(3) - 0 don't save

1 save indirect effect + direct effect

INC - 0 don't include

- 1 include results in summation over all operators

LCRW - 0 normal output

1 limited output

Normal output lists a sensitivity matrix which includes sensitivities by group and group-to-group transfers. Limited output lists only the contribution of the indirect effect in the profile.

88$$ integer parameters (NZONE)

"identifier of the operator by zone "

89** floating-point parameters (NZONE)

"zone densities"

Note: When the densities of the materials have been specified in Block II, on this card they should be equal to 1.0.

90$$ FO reserved for future options

91$$ integer parameters (NZP)

loop limiters for zone summations

T

Note: When the response processed does not contain the direct effect, e.g. k, then JOPA(1) = 1 and JOPA(2) = JOPA(3) = 0 is sufficient to save the sensitivity coefficients on a SENPRO file. This is also true when responses which have a direct effect are processed, but the material-reaction type to be processed does not appear in the definition of the response, i.e. the sensitivity of the direct effect is 0. In the above situation, it should not be concluded that, if JOPA(1) = JOPA(2) = 0 and JOPA(3) = 1, the calculated indirect effect will be saved. This will not occur, and the sensitivity coefficients will be lost.

APPENDIX D

The exchange of data needed between the FANISN and JULIET modules is performed by means of the FMANG file. Designated as logical unit 2, it is responsible for saving and providing fluxes, sources, integral parameters and normalization parameters.

The FANISN and JULIET modules incorporate a sub-routine called FMANG, which performs the work specified. For this, it is necessary to access the sub-routine before such modules are executed. The input data for the sub-routine are written on a free-format card and are preceded by "I$$". The following data are to be provided:

I$$ IASB, IRESP, ISIG, IAC, ITH, IQM, 0, 0, IR2, 0, T.

IASB = Identification number of assembly

IRESP = Identification number of response

ISIG = 0 - Data to be used do not exist in store
1 - Data to be used exist

IAC = Number of logical unit containing the cross-section file used by the FANISN module (default = 4)

ITH = 0 - normal calculation
1 - if the case being studied was the finding of adjoint flux

IQM = 0 - normal calculation
1 - calculation performed uses adjoint source

IR2 = Number of logical unit of store (default = 2)

Because FANISN and JULIET contain the FMANG sub-routine, the "1$$" card must precede the input cards in these modules.

APPENDIX E

1. Name and title:

   Service module SENPRO-ORNL

2. Language and computer:

   FORTRAN V; CDC, CYBER 170/750

3. Nature of the problem solved:

Sets of sensitivity coefficients are calculated by the JULIET module of the FORSS system and put into SENPRO format [5]. Each set is identified by a number for the assembly, one for the response, one for the material, one for the reaction type and, if applicable, one for the reaction rate response. These sets of coefficients are referred to as sensitivity profiles. The current numbers for the response and reaction rate are listed in the description of the MAT-MT control record of the SENPRO file. The numbers for indentification of the material and reaction type are respectively, MAT and MT, the numbers used in the ENDF/B file. When generation of the SENPRO file is complete for a study, it is recommended that it be examined carefully before use. The SENPRO service module is available for assisting with this examination. If problems are encountered with identification and normalization, these can rapidly be solved by the SENPRO service module. This comprises eleven execution paths for assisting in the event of failure to understand and to use the sensitivity coefficients. The execution paths carry out the following operations on the SENPRO file:

1. List the contents of a SENPRO file;
2. Operate on a SENPRO file by adding or deleting a set of sensitivity coefficients;
3. Merge two files and create a new one;
4. Alter the mode of a file from binary to BCD or vice versa;
5. List, in descending order of absolute magnitude of the total sensitivity, the title and the total sensitivity for each profile on the SENPRO file;
6. Renormalize the sensitivity coefficients;
7. Redefine any entry in the MAT-MT control record;
8. Put the sensitivity coefficients into a group structure provided by the user;
9. Selectively edit or copy a file;

10. Sum all the profiles of a file and produce a new profile;

11. Modify the group structure on a SENPRO file.

The user selects the desired execution path by entering one of the following words, beginning with column 1 of the first card: LIST, ADD, MERGE, DELETE, SEND, SIZE, NORM, FIX, GRID, EDIT, SUM, GROUP. The entry for each execution path is described below. The number in brackets shows the number of variables to be read in free format.

4. Preparation of input data for the SENPRO service module

LIST

1$$ integer parameter (1)

NBIN - unit number of the SENPRO file. If NBIN < 0, only the titles of the profiles will be listed.

T

ADD/DELETE

This execution path performs three functions. The profiles may be added to the file from card input. Profiles may also be deleted from the file. If no profile is added or deleted, the file is copied without any variation.

ADD

1$$ integer parameters (4)

NOLD - unit number of the existing SENPRO file

NEW - unit number of the new SENPRO file

NADD - number of profiles to be added (may be equal to 0)

NDL - number of profiles to be deleted (may be equal to 0)

T

ADD option

If NADD > 0, enter the 2$$ array

2$$ integer parameters (12)

IASB - Identifier of the assembly in accordance with BNL-19302 (ENDF 202)

IRESP - Identification number of response:

- 1 - k
- 2 - breeding ratio
- 3 - reactivity worth
- 4 - reaction rate
- 5 - others

MATID - Identification number of material

MT - Identification number of reaction type

NZONE - Number of zones

ISCT - Order of scatter for the total coefficient

NPART - Number of partial sets

NWRD - Number of words (A6) used for writing the response

NZDEN - Zone density option

0 - Zone densities are omitted

1 - Zone densities are present

MATRIX - Reserved

NTRN - Identification number of reaction rate

1 - 28C/49F

2 - 28F/49F

3 - 28C/25F

4 - 28F/25F

5 - 49F/25F

6 - 28C/28F

NRTD - Reserved

T

"Title for description of response" - format 11A6

"Title of response" format 11A6

"Sensitivity coefficients" - format 6E12.4

Repeat the sequence NADD times.

Note: The entry 2$$ is defined as the MAT-MT card of the SENPRO file.

DELETE optional

If NDL > 0, enter the "3$$" array

3$$ integer parameters (5*NDL)

IASB - Identification number of assembly

IRESP - Identification number of response

MATID - Identification number of material

MT - Identification number of reaction type

NTRN - Identification number of reaction rate

.

.

.

This sequence is repeated for each profile deleted

T

If NADD = 0 and NDL = 0, the old SENPRO file (NOLD) is copied without change to the new file (NEW).

MERGE

This execution path merges two existing SENPRO files and creates a new one containing all the profiles of the original files. The files to be merged should have the same group structure.

```
MERGE
1$$ integer parameter (3)
NL - unit number of the SENPRO file
N2 - unit number of the SENPRO file to be merged
N3 -  "     "         " new "     "        "
T
```

SENDIN

This execution path converts the SENPRO file in binary format into BCD format and vice-versa.

```
SEND
1$$ integer parameters (4)
NBE - select conversion mode
    = 0 from binary to BCD
    ≠ 0 from BCD to binary
NIN  - unit number of the existing SENPRO file (default = 23)
NOUT - unit number of the SENPRO file to be prepared by
       SENDIN (default = 24)
NO6 - print option
    ≤ 0 file is printed
    > 0 file is not printed
T
```

SIZE

The total sensitivity of each file profile is determined. The titles of the profiles are then listed in descending order as a function of the absolute magnitude of total sensitivity.

```
SIZE
1$$ integer parameter (1)
NBIN - unit number of the SENPRO file
T
```

NORM

This execution path makes it possible to modify the sensitivity coefficients of the SENPRO file. The following two options are available:

1. Renormalizes all the coefficients by a constant defined as R1/R2, see card "2**". This is useful for salvaging a set of incorrectly normalized coefficients.

2. Applies a group-dependent multiplication factor. It is useful for applying disadvantage factors. If a profile title card does not have total sensitivity (A) or has an incorrect sensitivity, 3** F1.0 will correct it.

NORM

1$$ integer parameters (2)

NOLD - unit number of the old SENPRO file

NEW - unit number of the new SENPRO file

2** floating-point parameters (2)

R1 - old normalization

R2 - new "

T

If R1 = R2 = 0, option 2 is executed

3** floating-point parameters (IGM)

"group-dependent multiplication factors"

T

FIX

This execution path makes it possible to redefine any of the twelve words contained in the MAT-MT control record.

FIX

1$$ integer parameters (3)

N1 - number of old logical unit

N2 - number of new logical unit

NFIX - number of redefinitions to be performed

T

2$$ - integer parameters (3*NFIX)

IP - position in the MAT-MT(IP) control record to be redefined

NVC - current value of the MAT-MT in the file. If NVC < -1000, the current value is not considered and MAT-MT(IP) = NDV

NDV - desired value of MAT-MT(IP)

.

.

.

.

T

Note: The sequence of three parameters is repeated until 3*FIX entries have been completed.

GRID

This execution path puts each profile of the file in a group structure designated by the user. The group structure can be input from cards or retrieved from another SENPRO file. The redistribution of sensitivity coefficients on the new grid is performed linearly in lethargy.

GRID

1$$ integer parameters (3)

N1 - unit number of the old SENPRO file

N2 - unit number of the new SENPRO file

NG - selection option

When NG > 0, NG is the number of groups in the new structure to be defined on input card "2**". When NG < 0, NG is the unit number of the SENPRO file containing the new group structure

T

2** group boundaries (NG + 1)

0 card 2** is included when NG > 0. Enter values from high energies to low energies in units of eV

T

EDIT/COPY

This execution path can be used for selective listing and copying of a SENPRO file. Each profile on the SENPRO file has five identification numbers: assembly, response, material, reaction type and reaction rate. These numbers are put in the following positions of the MAT-MT record of the SENPRO file:

Identifier	Position
Assembly	1
Response	2
Material	3
Reaction type	4
" rate	11

The five identifiers and their positions on the MAT-MT card are used to achieve general EDIT/COPY capability. An EDIT command consists of the identifiers ordered by assembly, response, material, reaction type and reaction rate response. Any identifier may be entered as 0. This indicates that any value found for the identifier qualifies for the EDIT/COPY

operation. To complete input requirements, a precise hierarchy must be established, which determines the order in which the identifiers in the EDIT command will be tested. This hierarchy is defined as a function of the position of the identifiers in the MAT-MT record. A default hierarchy of 1, 2, 3, 4, 11 is set by the coding. This default hierarchy may be replaced by data input on the 2$$ card.

As each profile is read from the SENPRO file, these five identifiers are compared with the corresponding ones in each EDIT command. The order in which the identifiers are compared is controlled by the hierarchy established. If all the identifiers different from 0 in an EDIT command and the corresponding identifier in the MAT-MT record of the profile are found to be equal, the profile will qualify for the EDIT/COPY operation.

EDIT

1$$ integer parameters (5)

|NI| - unit number of the existing SENPRO file; if NI < 0, the edited profile will be copied with the listing omitted.

NC - number of EDIT commands

NEW - copy option

> 0, the unit number of a SENPRO file to be written containing only those profiles edited

= 0, no file is written

NSS - unit number of a scratch device, default = 31

NHI - hierarchy definition option

> 0, prepare 2$$ card

= 0, use the default definition

T

2$$ integer parameters (5) (omitted if NHI = 0).

Input positions 1, 2, 3, 4 and 11 of the MAT-MT record in the order required for defining an appropriate hierarchy.

T

3$$ integer parameters (5*NC)

Assembly ID

Response ID

Material ID

Reaction type ID

Reaction rate ID

.

.

.

T

SUM

This execution path prepares a sensitivity profile by summing all the profiles contained in a SENPRO file. Practical application usually involves the execution of the EDIT/COPY, SUM and MERGE paths in sequence.

```
SUM
1$$     integer parameters (2)
N1    - old unit number
N2    - new   "     "
T
2$$ integer parameters (12)
Define the MAT-MT control record for the new profile
T
"title of the response for the new profile" (format 11A6)
"title of the profile" (format 8A6)
```

Note: The program will supply the 3A6 last words of a profile title.

GROUP

This execution path places, replaces or modifies the group structure on a SENPRO file.

```
GROUP
1$$ integer parameters (2)
NOLD - unit number of the existing SENPRO file
NEW  - unit number of the new SENPRO file
T
2$$ group boundaries or modifiers (number of groups + 1)
T
```

Comments:

If the first and last entries in the 2** array are equal, the contents of the 2** array will be used for modifying the group boundaries on the SENPRO file.

$$GB(i) = GB'(i) * GBM(i)$$

where:

GB'(i) - group boundaries on SENPRO

GBM(i) - modifiers read in 2** array.

The objective is to make it possible to alter the unit of the group boundaries on a SENPRO file.

For example, with card 2** equal to F1.0E+06 T, the units will be changed from MeV to eV.

If the first and last entries in the 2** array are not equal, the contents of the 2** array will replace the group boundaries on the SENPRO file.

The group boundaries entered may be in ascending or descending order. GROUP will ensure that the boundaries put on the SENPRO file will be in descending order.

GROUP assumes that the number of entries in the 2** array is equal to the number of boundaries of the SENPRO file. Since all the information on the number of boundaries is taken from the SENPRO file, any indication of an error in the number of entries read in the 2** array will be disastrous, and the input will have to be carefully checked.