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SENSIT: A Cross-Section and Design Sensitivity and Uncertainty Analysis Code

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by

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ABSTRACT

SENSIT computes the sensitivity and uncertainty of a calculated integral response (such as a dose rate) due to input cross sections and their uncertainties. Sensitivity profiles are computed for neutron and gamma-ray reaction cross sections (of standard multigroup cross-section sets) and for secondary energy distributions (SED's) of multigroup scattering matrices. In the design sensitivity mode, SENSIT computes changes in an integral response due to design changes and gives the appropriate sensitivity coefficients. Cross-section uncertainty analyses are performed for three types of input data uncertainties: (a) cross-section covariance matrices for pairs of multigroup reaction cross sections, (b) spectral shape uncertainty parameters for secondary energy distributions (integral SED uncertainties), and (c) covariance matrices for energy-dependent response functions. For all three types of data uncertainties, SENSIT computes the resulting variance and expected standard deviation in an integral response of interest, based on generalized perturbation theory. SENSIT uses angular-flux files from one-dimensional discrete-ordinates codes like ONETRAN, ANISN and DTF and reads multigroup cross-section sets in three different formats. This report gives detailed input specifications; precise definitions of all input and output arrays; a discussion of the underlying theory; and details of program flow, data management, and storage requirements. Eight sample problems are described in detail for which complete input files and selected output prints are listed.

I. INTRODUCTION

Sensitivity analysis in radiation transport theory attempts to determine quantitatively how sensitive a calculated integral response is to the input data for the transport calculation. Such input data may concern either cross-section data, geometry specifications (design data), methods approximations, or any other

input required to perform a transport calculation. In an uncertainty analysis, the sensitivity information is used, together with additional data about the uncertainty of the input data, to calculate or estimate the uncertainty of a calculated integral response which results from these input data uncertainties. In a cross-section uncertainty analysis the data uncertainties may be quantified in cross-section covariance matrices and in spectral shape uncertainty parameters for secondary energy distributions (SED's), while the resulting response uncertainty is best quantified by a variance or relative standard deviation. In a design sensitivity analysis, usually a specific design change (e.g., a material replacement or a geometry modification) and its effect on a calculated integral response is of concern. Therefore, in such cases a resulting response change is calculated based on generalized perturbation theory.

The SENSIT code is in some respects more comprehensive than earlier sensitivity codes presently in use[1]. Specifically, SENSIT includes the calculation of sensitivity profiles for secondary energy distributions (SED's) and performs also an SED uncertainty analysis. In addition, SENSIT also allows design sensitivity analyses and detector response uncertainty analyses to be performed in addition to the standard cross-section sensitivity and uncertainty analysis.

II. SENSIT INPUT SPECIFICATIONS

The following pages describe the input data to SENSIT in the order in which they must be entered into the code. In addition to the title card, which is always first, all input data may be categorized as control integers on cards 2 and 3, and problem dependent data starting with card 4. Many of the problem dependent data are required only conditionally, depending on the value of certain control integers, as indicated. Therefore, mainly depending upon values for ITYP, the sequence of problem-dependent input data may be different from case to case.

Card 1: Format (8A10)

80-column title card for job description

Card 2: Format (12I6), control parameters

Integer Variable No.	Name	Description and Options
1	ITYP	Type of sensitivity/uncertainty analysis: 0 - standard cross-section sensitivity analysis 1 - design sensitivity analysis 2 - vector cross-section sensitivity and uncertainity analysis, 3 - SED sensitivity and uncertainty analysis.
2	IGE	Geometrical model: 1 - slab or plane geometry, 2 - one-dimensional cylindrical geometry, 3 - spherical geometry, 4 - two-angle slab geometry.
3	ISN	Order of S_N angular quadrature; must be even integer.
4	IM	Total number of spatial mesh intervals.
5	IGM	Total number of energy groups.
6	NCOUPL	Number of neutron groups in case of coupled neutron/gamma-ray calculations, Zero if pure neutron or pure gamma-ray calculation is performed.
7	LMAX	P_ℓ-order of cross-sections.
8	ITAPE	Type of angular fluxes to be read from TAPE1 (PHI) and TAPE2 (PHISTAR) (see. Sec. V.C): 0 - reads flux tapes generated by DTF or ANISN, 1 - reads flux tapes in CCCC-format; e.g., as generated by ONEDANT or ONETRAN.

Integer Variable (Card 2 continued)

No.	Name	Description and Options
9	IXSTAPE	Source of multigroup cross-section input (see Sec. V.A,B): 0 - expects cross sections from cards (i.e., in input stream of problem-dependent data), if ITYP = 0,1,3, 1 - expects cross sections from TAPE4, if ITYP = 0,1,3, 2 - expects vector cross sections and covariance data from TAPE10, only if ITYP = 2.
10	NPERXS	Number of successive cases to be run for the same PHI/PHISTAR, and the same perturbed zone identifications: - if ITYP = 0,1,3: number of perturbed cross-section sets to be read from TAPE4, or from cards - if ITYP = 2: number of vector cross-section pairs with covariance matrices to be read from TAPE10.
11	IDESIGN	Type of design sensitivity analysis (zero if ITYP = 0,2,3): 0 - for ITYP = 1 when 2 cross-section sets (perturbed and unperturbed) must be read per case, 1 - for ITYP = 1 when only 1 cross-section set (Σ) is read per case, and the special design perturbation of a 1% density increase is assumed ($\Delta\Sigma = 0.01\ \Sigma$) in all perturbed zones.

Card 3: Format (12I6), control parameters

Integer Variable

No.	Name	Description and options
1	KSRS	Number of source zones.
2	KDET	Number of detector zones.
3	KPER	Number of perturbed zones.

Integer Variable No.	Name	(Card 3 continued) Description and options
4	KXS	Format of input cross sections if ITYP = 0,1,3, cf. Sec.V.A.: 0 - if ITYP = 2 (KXS is not needed), 1 - LASL format: 6E12.5, 2 - ORNL format: limited fixed field FIDO format as read by ANISN (see Sec. V.A.1e).
5	IHT	Position (row) of total cross section in multigroup cross-section tables (typically 3), 0 - if ITYP = 2.
6	IHA	Position (row) of absorption cross section in multigroup cross-section tables (typically 1), 0 - if ITYP = 2.
7	DETCOV	0 - if no covariance matrix for the detector response function is provided, 1 - read covariance matrix for R(g) and perform relevant uncertainty analysis.
8	NSED	0 - for ITYP = 0,1,2, and for ITYP = 3 if no SED uncertainties are provided, 1 - read integral SED uncertainties if ITYP = 3.
9	IOUTPUT	0 - print sensitivity and uncertainty output only for the sum over all perturbed zones (in case KPER >> 1), 1 - print all sensitivity and uncertainty output for each individual perturbed zone and for the sum over all perturbed zones.
10	NSUMCOV	0 - if ITYP = 0,1,3, N - number of partial sums desired of individual response variances computed for ITYP = 2.

Integer Variable No.	Name	(Card 3 continued) Description and options
11	ITEST	Flag to output specific test prints (which may be very voluminous): 0 - no test printout, 1 - provide test printout including cross sections but no angular fluxes, 2 - provide test printout with angular fluxes but no cross sections. 3 - provide test printout with vector cross sections and covariance matrices if ITYP = 2.
12	IPRINT	Flag to provide test printouts of pointers, traces, and dumps as edited from the dynamic data management module BPOINTR: 0 - no test printout, 1 - print dumps only, 2 - print traces only, 3 - print dumps and traces.

Card 4 and all successive cards: Problem-dependent input data

Input Array Name	Number of Entries	Input Format	Required only if	Description and conditions
$E_n(g)$	IGM+1 (if NCOUPL=0) NCOUPL+1 (if NCOUPL≠0)	6E12.5	always	Energy group boundaries for neutron groups in eV, starting with highest energy (i.e., group 1). Zero is not allowed as group boundary.
$E_\gamma(g)$	IGM+1 -NCOUPL	6E12.5	NCOUPL≠0	Gamma-ray energy group boundaries in eV, starting with highest gamma-ray energy (i.e., group NCOUPL+1). Zero is not allowed as group boundary.

Input Array Name	Number of Entries	Input Format	Required only if	Description and conditions
W(m)	MM*	6E12.5	always	S_N quadrature weights consistent with those used in flux calculations for PHI and PHISTAR (level weights excluding starting weight).
MUE(m)	MM*	6E12.5	always	S_N quadrature direction cosines (level cosines excluding starting directions).
Z(i)	IM+1	6E12.5	always	Spatial mesh boundaries for the entire system in cm.
ISFIR(k), ISLAS(k)	2	2I6	always	Interval number of first and last interval of k-th source zone. 1 card with two numbers must be entered for each of the KSRS source zones!
IDFIR(k), IDLAS(k)	2	2I6	always	KDET cards describing all detector zones (like above)
IPFIR(k), IPLAS(k)	2	2I6	always	KPER cards describing all perturbed zones (like above).
RHO(g)	IGM	6E12.5	always	Energy distribution of detector response function R(g,i) by group, starting with g = 1 (see Sec. V.D).
RHO(j)	IDET	6E12.5	always	Spatial distribution of detector response function R(g,j), per detector

*)MM = ISN for slab and spherical geometry (IGE=1 or 3)
MM = ISN*(ISN+2)/4 for cylindrical geometry (IGE=2)
MM = ISN*(ISN+2) for two-angle slab geometry (IGE=4)
} see Sec. V.C.

Input Array Name	Number of Entries	Input Format	Required only if	Description and conditions
				interval j = 1,..., IDET, starting with first interval of first detector zone (see Sec. V.D).
COVR(g, gp)	IGM*IGM	6E12.5	ITYP=0 and DETCOV=1	Relative covariance matrix for detector response function starting with 1 title card.
QUE(g)	IGM	6E12.5	always	Energy distribution of source distribution functions Q(g,j) by group, starting with g = 1 (see Sec. V. D).
QUE(j)	ISRS	6E12.5	always	Spatial distribution of source distribution function Q(g,j), per source interval j = 1,...,ISRS, starting with first interval of first source zone (see Sec. V. D).
ID, DEN1, DEN2	3	(I6,6X, 2E12.5)	ITYP=2	Identification number and 2 number densities (in atoms/barn cm) for pair of vector cross sections read from tape 10. 1 card must be entered for each of the NPERXS vector cross-section pairs!
SUMSTRT, SUMEND	2	2I6	ITYP=2 and NSUMCOV≠0	SUMSTRT identifies the first (SUMEND the last) vector cross-section pair from the string of NPERXS cases, for which the response uncertainties are added and edited as partial sums of variances. 1 card must be entered for each of the NSUMCOV partial sums desired!

Input Array Name	Number of Entries	Input Format	Required only if	Description and conditions
GMED(g)	IGM1[+]	12I6	ITYP=3 and NSED=1	Array of energy-group numbers which identifies the median energy group for each SED associated with the initial energy group g. Use zero if no SED is identified for a given initial energy group g.
FSED(g)	IGM1[+]	6E12.5	ITYP=3 and NSED=1	Integral SED uncertainty associated with initial energy group g, corresponding to GMED(g).
ID, NUMDEN, XSNAME	3	I6,6X, E12.5, 2X,A10	IXSTAPE=1 and ITYP=0 or ITYP=3	ID identifies the cross-section set for the specific material for which a standard cross-section sensitivity analysis or an SED sensitivity/uncertainty analysis is to be performed. ID is the sequence number of the string of material cross sections on TAPE4, e.g., for the third XS-set on TAPE4: ID=3. NUMDEN is the number density for the material. XSNAME is an optional 10-column name designation which will reappear in the output. Note: If an SED sensitivity/uncertainty analysis is desired for more than 1 material per SENSIT run

+) IGM1 = Number of neutron groups in the problem:
IGM1 = IGM if pure neutron calculation is performed (NCOUPL = 0),
IGM1 = NCOUPL if coupled neutron/gamma-ray calculation is performed.

Input Array Name	Number of Entries	Input Format	Required only if	Description and conditions
				(NPERXS > 1), then the last three arrays GMED(g), FSED(g), and (ID, NUMDEN, XSNAME) must be provided for each material successively to make a total of NPERXS sets of these 3 arrays.
XS(g, gp,ℓ)	depends on control parameters		IXSTAPE = 0	Perturbed cross-section set with title card and number density card (see Sec. V. A).
XSBAR(g, gp,ℓ)	depends on control parameters		IXSTAPE =0 and ITYP=1 and IDESIGN =0	Reference or unperturbed cross-section set with title card and number density card (see Sec. V. A).

III. UNDERLYING THEORY

The basic theory upon which the present sensitivity and uncertainty analysis methods are based has developed over the past several years. We refer to only a few selected references here which can provide the user an overview of the field, Refs. (2) through (6). More mathematical detail is given in Ref. (7), with special emphasis on discrete-ordinates formulations. The description of the underlying theory in this section will be restricted to as much detail as is required to understand input and output of the SENSIT code, while a general knowledge of the field is assumed.

A. Standard Cross-Section Sensitivity Analysis (ITYP = 0)

Conventional sensitivity profiles P_Σ may be derived from the expression for the forward difference approximation, Eq. (36) in Ref. 7, or Eq. (17) in Ref. 3, or Eq. (26) in Ref. 4. The analytical definition of a cross-section sensitivity function $F_\Sigma(E)$ expresses the sensitivity of a calculated integral response I to a particular cross section Σ_x at energy E and may be expressed as

$$F_{\Sigma_x}(E) = (1/I) \int d\underline{r} \int d\underline{\Omega} \left\{ - \phi(\underline{r},\underline{\Omega},E)\, \Sigma_{x,T}(\underline{r},E)\, \phi^*(\underline{r},\underline{\Omega},E) + \int d\underline{\Omega}' \int dE'\, \phi(\underline{r},\underline{\Omega},E)\, \Sigma_{x,S}(\underline{r},\underline{\Omega}\to\underline{\Omega}',E\to E')\, \phi^*(\underline{r},\underline{\Omega}',E') \right\} . \quad (1)$$

In a multigroup formulation one usually prefers to identify and work with a sensitivity profile P^g_Σ, which is related to the above sensitivity function through the scaling factor Δu^g by $P^g_\Sigma = \bar{F}_\Sigma(E_g)/\Delta u^g$ and refers to a group-averaged sensitivity. Δu^g is the lethargy width of energy group g. The exact numerical definition of a multigroup cross-section sensitivity profile for the macroscopic cross section Σ^g_x is:

$$P^g_{\Sigma_x} = \left\{ - \Sigma^g_{x,T} \cdot \chi^g + \sum_{\ell=0}^{LMAX} \sum_{g'=g}^{GMAX} \Sigma^{g\to g'}_{s,\ell} \cdot \psi^{gg'}_\ell \right\} \Big/ I_\phi \cdot \Delta u^g \quad , \quad (2)$$

where $\Sigma^{g}_{x,T}$ = total macroscopic cross section for reaction type x,

$\Sigma^{g\to g'}_{s,\ell}$ = ℓ'th Legendre coefficient of the scattering matrix element for energy transfer from group g to group g', as derived from the differential scattering cross section for reaction type x,

$$\chi^{g} = \sum_{i=1}^{IPERT} V_i \cdot \sum_{m=1}^{MM} \phi_m^{g}(i) \cdot \phi_m^{*g}(i) \cdot w_m \quad ,$$

= numerical integral of the product of forward and adjoint angular fluxes over all angles and all spatial intervals described by i = 1,...,IPERT.

$$\psi_\ell^{gg'} = \sum_{i=1}^{IPERT} V_i X_\ell^{g}(i) \cdot Y_\ell^{g'}(i) \quad ,$$

= spatial integral of the product of Legendre coefficients of forward and adjoint angular fluxes.

$$X_\ell^{g}(i) = \sum_{m=1}^{MM} \phi_m^{g}(i) \cdot P_\ell(\mu_m) \cdot w_m$$

$$Y_\ell^{g'}(i) = \sum_{m=1}^{MM} \phi_m^{*g'}(i) \cdot P_\ell(\mu_m) \cdot w_m$$

$\phi_m^{g}(i), \phi_m^{*g}(i)$ = discrete-ordinates representations of forward and adjoint angular fluxes for group g, spatial mesh point i and discrete direction m.

$P_\ell(\mu_m)$ = Legendre polynomial of order ℓ at direction cosine μ_m.

$\{\mu_m, w_m\}$ = discrete-ordinates quadrature direction cosines μ_m and associated quadrature weights w_m.

V_i = volume of spatial mesh interval i.

Δu^g = lethargy width of energy group g,
= $\ell n\ (E^g/E^{g+1})$, where E^g and E^{g+1} are upper and lower energy group boundaries.

I_ϕ = integral response as calculated from forward fluxes only,

$$= \sum_{i=1}^{IDET} \sum_{g=1}^{IGM} \sum_{m=1}^{MM} V_i R_i^g \cdot \phi_m^g(i) \cdot w_m$$

R_i^g = spatially and group-dependent detector response function.

The basic Eq. (2), as well as its corresponding Eq. (1), consist of two terms on the right-hand side. The first term, which is always negative, is called the "loss term"[3,7] and involves always the total (collision) cross section for a certain reaction type. The second term involves only the differential scattering cross section and is always positive; it is called the "gain term"[3,7]. Loss term and gain term, respectively, indicate a loss or a gain in (positive) sensitivity in the sense that the total cross section always indicates a neutron interaction which removes the neutron from the considered phase-space volume $\{\Delta\underline{r}_i, \Delta\underline{\Omega}_m, \Delta E_g\}$ represented by $\{i,m,g\}$, while scattering interactions can transfer neutrons from other phase-space regions into the specific phase-space volume under consideration.

In order to avoid ambiguities in the interpretation of sensitivity profiles, careful consideration must be given to cases when the reaction cross section Σ_x is a composite cross section. Ideally, Σ_x should always be chosen as a partial reaction cross section of one exclusive type, like (n,α), (n,2n), (n,n')-elastic, etc. However, in practice, complete cross-section sets, including full scattering matrices, are seldom available for all desired partials. In such cases, composite cross sections must be used, such as total absorption, total inelastic or even total scattering cross sections, which complicates the interpretation of the resulting sensitivity profiles. If, for example, the (n,2n) cross section is treated as a negative portion of the total absorption cross section, which is the case in some standard transport cross-section sets, then it is possible that the loss term for the absorption cross section is positive for those groups where the (n,2n)-reaction dominates.

In order to facilitate the interpretation of sensitivity results, SENSIT prints loss and gain terms in addition to the net sensitivity profiles. In the following we give the discrete-ordinates equations which are the exact equivalents to the algorithms coded in SENSIT to produce the standard sensitivity profile output. A verbal synopsis of Eqs. (3) through (13) is printed with the SENSIT output if ITYP=0 or 3.

1. Pure Loss Terms. For the neutron sensitivity profiles 4 loss terms are printed but only 3 for the gamma-ray profiles:

$$\text{AXS} = P^g_{\Sigma_{abs},\text{Loss}} = -\Sigma^g_{abs}\cdot\chi^g/I_\phi\cdot\Delta u^g \quad , \tag{3}$$

where Σ^g_{abs} is the absorption cross section in group g as taken from position IHA in the input cross-section tables (see Sec.V.A).

$$\text{NU-FISS} = P_{\nu\Sigma_{fiss},\text{Loss}} = -\nu\Sigma^g_f\cdot\chi^g/I_\phi\cdot\Delta u^g \quad , \tag{4}$$

where $\nu\Sigma^g_f$ is the standard group-averaged product of fission cross section and number of fission neutrons per incident neutron. This "cross section" is taken from position IHA+1 of the input cross-section tables. One may note here, that if no absorption or fission cross-section profiles are desired, the data in cross-section table positions IHA and IHA+1 may be replaced with any other multigroup cross section to produce the loss-terms of sensitivity profiles for such substitute cross sections.

$$\text{SXS} = P^g_{\Sigma_{s,loss}} = -\Sigma^g_{s,loss}\,\chi^g/I_\phi\cdot\Delta u^g \quad , \tag{5}$$

where $\Sigma^g_{s,loss}$ is the total scattering cross section for all group transfers within group g and out of group g:

$$\Sigma^{g}_{s,loss} = \sum_{g' = g}^{GMAX} \Sigma^{g \to g'}_{s,o} \quad . \tag{6}$$

Equation (6) is evaluated in SENSIT by summing the P_o component of the scattering matrix along the appropriate diagonal, where GMAX denotes either the total number of neutron groups or the total number of gamma-ray groups for neutron or gamma-ray profiles, respectively.

$$TXS = P^{g}_{\Sigma_{T,loss}} = -\Sigma^{g}_{T} \; \chi^{g}/I_{\phi} \cdot \Delta u^{g} \quad , \tag{7}$$

where Σ^{g}_{T} is the total interaction cross section for group g as taken from position IHT in the input cross-section tables.

2. Pure Gain Terms. SENSIT prints 3 gain terms for the neutron profiles, but only one for gamma rays. The two additional gain terms for neutrons refer to (n,γ)-reactions and neutron secondary energy distributions as explained below.

$$\text{N-GAIN or G-GAIN} = P^{g}_{\Sigma_{s,gain}}$$

$$= \left\{ \sum_{\ell = 0}^{LMAX} \sum_{g' = g}^{GMAX} \Sigma^{g \to g'}_{s,\ell} \; \psi^{gg'}_{\ell} \right\} \Big/ I_{\phi} \cdot \Delta u^{g} \quad . \tag{8}$$

The inner summation in Eq. (8) indicates that all sensitivity gains are counted which relate to scattering transfers within and out of group g into all other groups g'. For the neutron profile (N-GAIN) the upper limit of the group summation, GMAX, is the total number of neutron groups, while for the gamma-ray profile (G-GAIN), GMAX is chosen as the total number of gamma-ray groups.

$$\text{N-GAIN(SED)} = \tilde{P}^{g}_{\Sigma_{s,gain}} = \left\{ \sum_{\ell=0}^{LMAX} \sum_{g'=1}^{g} \Sigma^{g'\to g}_{s,\ell}\, \psi^{g'g}_{\ell} \right\} \Big/ I_{\phi}\cdot\Delta u^{g} \quad . \tag{9}$$

This partial profile is only printed for neutron groups and differs from N-GAIN of Eq. (8) by re-arranging g and g' and the group summation. N-GAIN(SED) therefore counts all sensitivity gains due to scattering transfers from all (higher) energy groups g' into group g. Hence, this profile may be considered as an adjoint to N-GAIN; its physical interpretation relates to the importance of neutron secondary energy distributions, as described in Section D.

$$\text{NG-GAIN} = P^{g}_{\Sigma_{(n,\gamma),gain}}$$

$$= \left\{ \sum_{\ell=0}^{LMAX} \sum_{g'=NCOUPL+1}^{IGM} \Sigma^{g\to g'}_{(n,\gamma),\ell}\, \psi_{\ell}{}^{gg'} \right\} \Big/ I_{\phi}\cdot\Delta u^{g} \quad , \tag{10}$$

where $\Sigma^{g\to g'}_{(n,\gamma),\ell}$ is the ℓ'th Legendre coefficient of the gamma-ray production cross section for neutron group g as taken from the input scattering matrix. The group summation in Eq. (10) indicates that all sensitivity gains are counted, which are due to transfers from neutron group g into all gamma-ray groups g'.

3. Net Sensitivity Profiles. SENSIT prints for both, the neutron as well as the gamma-ray profiles, two net (or total) sensitivity profiles which are obtained by summing the appropriate loss and gain terms according to Eq. (2).

$$\text{SEN} = P^{g}_{\Sigma_{s,net}} = P^{g}_{\Sigma_{s,loss}} + P^{g}_{\Sigma_{s,gain}} \quad , \tag{11}$$

where simply the partial profiles defined in Eqs. (5) and (8) are added for each group.

$$\text{SENT} = P^{g}_{\Sigma_{T,\text{net}}} = P^{g}_{\Sigma_{T,\text{loss}}} + P^{g}_{\Sigma_{s,\text{gain}}} \quad , \tag{12}$$

where the partial profiles of Eqs. (7) and (8) are added.

It may be noted here that Eqs. (11) and (12) differ only with respect to which loss term is chosen. The loss term of Eq. (12) may include the effects of many more reaction types than that of Eq. (11), depending on the contents of position IHT in the input cross-section tables. In contrast, however, the net sensitivity profile of Eq. (11) may be considered self-consistent because it utilizes only the information contained in the input transfer matrix, independent of the values for Σ^{g}_{T} in cross-section table position IHT.

4. Integral Sensitivities. All sensitivity profiles printed by SENSIT are also integrated over neutron energies and gamma-ray energies separately, i.e.

$$\text{Integral} = \sum_{g} \text{SEN}^{g} \cdot \Delta u^{g} \quad , \tag{13}$$

where the group summation extends form g = 1 through g = NCOUPL for neutron profiles and from g = NCOUPL+1 through g = IGM for gamma-ray profiles. As a test for the consistency of the calculation one might note that the integrals over Eqs. (8) and (9) must be identical and equal to the total neutron-scattering gain term. If any n-gamma gain terms (NG-GAIN) are calculated, they will be offset again in the net total neutron profile (SENT), because Σ_T includes a component due to (n,γ)-reactions which is counted in TXS as a neutron loss mechanism.

5. Source and Detector Sensitivity Profiles. All SENSIT runs (for any value of ITYP) print sensitivity profiles for the source and detector distribution functions Q(E) and R(E) even before any cross sections are read. These sensitivity profiles are based on the dualism[4] that the integral response I may be calculated independently either from the forward flux alone:

$$I_{\phi} = \int d\underline{r} \int d\underline{\Omega} \int dE \; R(\underline{r},E) \; \phi(\underline{r},\underline{\Omega},E)$$

$$= \sum_{i=1}^{IDET} \sum_{m=1}^{MM} \sum_{g=1}^{IGM} V_i \cdot R_i^g \cdot \phi_m^g(i) \cdot w_m \quad , \tag{14}$$

or from the adjoint flux alone:

$$I_{\phi^*} = \int d\underline{r} \int d\underline{\Omega} \int dE \; Q(\underline{r},E) \; \phi^*(\underline{r},\underline{\Omega},E)$$

$$= \sum_{i=1}^{ISRS} \sum_{m=1}^{MM} \sum_{g=1}^{IGM} V_i \cdot Q_i^g \cdot \phi_m^{*g}(i) \cdot w_m \quad , \tag{15}$$

where R_i^g and Q_i^g are the spatially and group dependent detector response function and neutron source distribution, respectively. If it is desired to determine how sensitive the integral response I is to the energy distribution of either R_i^g or Q_i^g, Eqs. (14) and (15) can be used to define a detector and source sensitivity profile, which may then be interpreted in exact analogy to the standard cross-section sensitivity profiles:

$$P_R^g = \sum_{i=1}^{IDET} \sum_{m=1}^{MM} V_i R_i^g \phi_m^g(i) \; w_m / I_\phi \cdot \Delta u^g \quad , \tag{16}$$

$$P_Q^g = \sum_{i=1}^{ISRS} \sum_{m=1}^{MM} V_i Q_i^g \phi_m^{*g}(i) w_m / I_{\phi^*} \cdot \Delta u^g \quad . \tag{17}$$

For internal consistency, the detector sensitivity profile P_R^g is normalized to I_ϕ from Eq. (14), while the source sensitivity profile P_Q^g is normalized to I_{ϕ^*} from Eq. (15). Ideally, of course, $I_\phi = I_{\phi^*}$. The integrals over Eqs. (16) and (17), according to Eq. (13), must be 1.0 if the spatial integrations are carried out over <u>all</u> source and detector zones. However, if the control parameter IOUTPUT

is set to 1, then SENSIT prints P_R^g and P_Q^g and their integrals for each individual source and detector zone as well. These zone-wise integral sensitivities allow a quantitative interpretation of the relative importance of the various source and detector zones to the total integral response I.

B. Design Sensitivity Analysis (ITYP = 1)

The objective in a design-sensitivity analysis is to estimate the change of an integral response I due to a given design change without repeating the transport calculation for the altered design. Methods, based on generalized perturbation theory, have been developed which allow such estimates to be made with second-order accuracy in respect to the associated flux changes[4,7]. These perturbation methods require only the forward and adjoint flux solutions to a reference case and the specification of a perturbation to this reference design, which is equivalent to a postulated design change. All such design changes can be described then by a perturbation, ΔL, in the linear Boltzmann operator L.

Due to the dualism of forward and adjoint formulations for radiation transport calculations, two different but equivalent expressions can be derived for the estimated integral response in the perturbed system[4,7]. These expressions are both second-order with respect to flux changes but first-order with respect to the perturbation and are denoted as the adjoint difference (AD) and the forward difference (FD) formulation. Using the convenient operator notation of Refs. 4 and 7, we obtain for the integral response in the perturbed system the two expressions

$$I_{AD}^{(2)} = < R,\phi > - < \phi^*,\Delta L\phi > \equiv I_{\phi}^{(1)} - \Delta I_{AD}^{(2)} \quad , \tag{18}$$

$$I_{FD}^{(2)} = < Q,\phi^* > - < \phi,\Delta L^*\phi^* > \equiv I_{\phi^*}^{(1)} - \Delta I_{FD}^{(2)} \quad , \tag{19}$$

where <, > indicates integrations over all independent variables, and ϕ, ϕ^* are the forward and adjoint angular fluxes for the reference design. It may be noted that the first-order terms on the right sides of Eqs. (18) and (19) are computationally identical to I_{ϕ} and I_{ϕ^*} as defined in Eqs. (14) and (15). In addition, if the operators ΔL and ΔL^* are written down explicitly[7], it is

noted that the second-order term in Eq. (19) is equivalent to the negative of the numerator of Eq. (2) when the cross sections Σ_x are replaced by cross-section changes $\Delta\Sigma$, and when an additional integration over all energies E, namely, a summation over all groups g, is performed:

$$\Delta I_{FD}^{(2)} = \sum_{g=1}^{IGM} \left\{ \Delta\Sigma_T^g \cdot \chi^g - \sum_{\ell=0}^{LMAX} \sum_{g'=g}^{IGM} \Delta\Sigma_{s,\ell}^{g\to g'} \cdot \psi_\ell^{gg'} \right\} \quad . \tag{20}$$

The analogous expression for the seond-order term in Eq. (18) becomes

$$\Delta I_{AD}^{(2)} = \sum_{g=1}^{IGM} \left\{ \Delta\Sigma_T^g \cdot \chi^g - \sum_{\ell=0}^{LMAX} \sum_{g'=1}^{g} \Delta\Sigma_{s,\ell}^{g'\to g} \cdot \psi_\ell^{g'g} \right\} \quad . \tag{21}$$

The perturbation, as expressed by macroscopic cross-section changes in Eqs. (20) and (21) is calculated in SENSIT from two sets of input cross-section tables, the unperturbed or reference cross-section set $\{\bar{\Sigma}\}$ and the perturbed cross-section set $\{\Sigma\}$:

$$\Delta\Sigma_T^g = \Sigma_T^g - \bar{\Sigma}_T^g \quad , \tag{22}$$

$$\Delta\Sigma_{s,\ell}^{g\to g'} = \Sigma_{s,\ell}^{g\to g'} - \bar{\Sigma}_{s,\ell}^{g\to g'} \tag{23}$$

$$\Delta\Sigma_{s,\ell}^{g'\to g} = \Sigma_{s,\ell}^{g'\to g} - \bar{\Sigma}_{s,\ell}^{g'\to g} \quad . \tag{24}$$

A design sensitivity coefficient X may be defined for both (AD and FD) formulations according to

$$X_{AD} = I_{AD}^{(2)}/I_\phi^{(1)} = 1 - \Delta I_{AD}^{(2)}/I_\phi^{(1)} \quad , \tag{25}$$

$$X_{FD} = I_{FD}^{(2)}/I_{\phi^*}^{(1)} = 1 - \Delta I_{FD}^{(2)}/I_{\phi^*}^{(1)} \quad , \tag{26}$$

from which the estimated fractional change of the integral response I due to the introduction of the perturbation can be easily determined.

It has been demonstrated in Refs. 4 and 7 that the AD-formulation is more appropriate for cases where the perturbation is geometrically closer to the detector than to the source, while the FD-fomulation is better suited for cases where the perturbation is geometrically closer to the source than to the detector. However, if both reference fluxes, ϕ and ϕ^*, are completely converged, then both formulations will give identical results.

SENSIT prints all design sensitivity information, as defined in Eqs. (18) through (26), separately for neutrons and gamma rays; also, if IOUTPUT = 1, it prints the same information for each perturbed zone as well as integrated over all perturbed zones. If the control parameter ITYP is set to 1, the SENSIT output will also contain a synopsis defining the variable names used to edit the design sensitivity information.

If the control parameter IDESIGN is set equal to 1, then the special case of a design perturbation is assumed, which is equivalent to a 1% increase in all cross sections in all perturbed zones, i.e., Eqs. (22) through (24) are replaced by $\Delta\Sigma = 0.01\Sigma$. Such a perturbation may also be interpreted as if the material density in the perturbed zones were increased by 1%. In this mode only one cross-section set $\{\Sigma\}$ needs to be read into SENSIT per case.

C. Vector Cross-Section Sensitivity and Uncertainty Analysis (ITYP = 2)

The term "vector cross-section" has been chosen to identify a multigroup cross-section set which consists of a linear string of numbers with one group-averaged reaction cross section per group, but no scattering matrix. Such a cross-section set can be described by a vector, or one-dimensional array, with IGM elements, in contrast to the two-dimensional cross-section tables, which include transfer matrices. All reaction cross sections which do not need to describe the production of secondary neutrons or gamma rays, such as (n,α), (n,abs.), Σ_T, etc., are completely described by a vector cross section. Obviously, by definition, such vector cross-sections can only generate a loss term in a sensitivity analysis. However, existing correlations between two individual vector cross sections are easily described by a simple two-dimensional correlation

matrix. As a consequence, therefore, it is also straightforward to describe correlated cross-section uncertainties of pairs of vector cross sections by a two-dimensional covariance matrix[5]. For ITYP = 2, SENSIT performs a complete sensitivity and response uncertainty analysis for given sets of vector cross-section pairs $\{\Sigma_1^g\}$ and $\{\Sigma_2^g\}$ with an associated covariance matrix $\mathrm{Cov}(\Sigma_1^g,\Sigma_2^{g'})$ attached to each pair. These pairs of vector cross sections with their covariance matrix are read from TAPE10 by identification numbers as specified in the input stream. In coupled (n,γ)-calculations, this analysis is treating only the neutron groups.

As a first step SENSIT calculates the sensitivity profiles P_1^g and P_2^g for each individual vector cross section according to an equation equivalent to Eq. (3), i.e., a pure loss term. Then the covariance matrix $\mathrm{Cov}(\Sigma_1^g,\Sigma_2^{g'})$ is used to compute the resulting integral response uncertainty due to the correlated cross-section uncertainties of this pair of vector cross sections according to[5]

$$\mathrm{Var}(I_\phi) = \sum_{g=1}^{IGM1} \sum_{g'=1}^{IGM1} P_1^g \cdot P_2^{g'} \cdot \mathrm{Cov}\ \Sigma_1^g,\Sigma_2^{g'} \quad . \tag{27}$$

The upper limit of the double sum, IGM1, is the number of neutron groups (IGM1 = NCOUPL in a coupled (n,γ)-problem). Both, the variance $\mathrm{Var}(I_\phi)$ as well as the relative standard deviation

$$\frac{\delta I}{I} = \sqrt{\mathrm{Var}(I_\phi)} \quad , \tag{28}$$

are printed by SENSIT for each vector cross-section pair. Since all cross-section uncertainties pertaining to one material may be described by a sum of several vector cross-section covariance matrices, SENSIT also prints specified sums of response variances

$$\mathrm{Var}(I_\phi)_{MAT} = \sum_{n=1}^{NSUMCOV} \mathrm{Var}_n(I_\phi) \quad , \tag{29}$$

and the resulting standard deviation $(\delta I/I)_{MAT}$, assuming that NSUMCOV vector cross-section pairs describe the cross sections for one material sufficiently.

D. SED Sensitivity and Uncertainty Analysis (ITYP = 3)

It has only recently been recognized[8] that sensitivity profiles for secondary energy and angular distributions are obtained as adjoints of the standard sensitivity profiles, i.e., from the differential form of the adjoint difference (AD) formulation. For ITYP = 3, SENSIT computes and prints the double-differential and single-differential sensitivity profiles for secondary energy distributions (SED's) and performs also an SED uncertainty analysis based on the hot/cold concept of integral SED uncertainties[9]. A sensitivity or uncertainty analysis for secondary angular distributions is not implemented in this version of SENSIT. Also, the SED sensitivity and uncertainty analysis is not performed for secondary gamma rays in the case of a coupled (n,γ)-calculation.

As shown in Ref. (8), a double-differential SED sensitivity profile is described by the differential form of the gain term in the AD-formulation; cf. Eq. (21) and Eq. (9):

$$P_{SED}^{g',g} \equiv \text{PSED(g-in,g-out)} = \left\{ \sum_{\ell=0}^{LMAX} \Sigma_{s,\ell}^{g' \to g} \cdot \psi_{\ell}^{g'} \right\} \Big/ I_{\phi} \cdot \Delta u^{g'} \cdot \Delta u^{g} \quad . \tag{30}$$

This double-differential SED sensitivity profile quantifies the sensitivity of the integral response I_{ϕ} to the scattering matrix element $\Sigma_s^{g' \to g}$. Therefore, $P_{SED}^{g',g}$ is a pure gain term for the sensitivity gain due to the transfer of neutrons from the incident energy group g' to the final energy group g. $P_{SED}^{g',g}$ is double differential because it is scaled to the product of both lethargy widths, $\Delta u^{g'}$ and Δu^{g}, of the incident and the final energy groups.

From Eq. (30), two single-differential SED sensitivity profiles may be obtained, depending upon which of the two group indices an integration is performed:

$$P_{SED}^{g} \equiv PSED(g\text{-out}) = \sum_{g'=1}^{g} P_{SED}^{g',g} \cdot \Delta u^{g'} \quad , \tag{31}$$

and

$$P_{SED}^{g'} \equiv PSED(g\text{-in}) = \sum_{g=g'}^{g} P_{SED}^{g',g} \cdot \Delta u^{g} \quad . \tag{32}$$

Equation (31) describes the sensitivity of I_{ϕ} to the sum of all scattering transfer cross sections which transfer neutrons from any incident energy group g' into the specific final energy group g. $P_{SED}^{g} \equiv PSED(g\text{-out})$ is identical to N-GAIN(SED), as defined earlier in Eq. (9). In complete analogy, Eq. (32) adds up all sensitivit gains due to neutron transfers originating in group g' and transferring into any final energy group $g \geq g'$. $P_{SED}^{g'} \equiv PSED(g\text{-in})$, when given as a function of g' is, therefore, identical to the standard sensitivity gain term N-GAIN(g), as defined in Eq. (8), where the nomenclature for g and g' is reversed.

In order to perform an SED uncertainty analysis based on the hot/cold concept introducted in Ref. 9, it is required to specify the median energy group of the SED for each incident neutron energy group, GMED(g'), as well as the associated integral SED uncertainty (spectral shape uncertainty parameter), $F_{SED}(g')$, for each SED with incident energy group g'. GMED(g') and $F_{SED}(g')$ are expected input arrays in SENSIT if ITYP = 3 and NSED = 1. Hot and cold integral SED sensitivity coefficients, $S_{HOT}(g')$ and $S_{COLD}(g')$, are then computed by SENSIT according to[9].

$$S_{HOT}(g') = \Delta u^{g'} \cdot \sum_{g=g'}^{GMED(g')} P_{SED}^{g',g} \cdot \Delta u^{g} \quad , \tag{33}$$

$$S_{COLD}(g') = \Delta u^{g'} \cdot \sum_{g=GMED+1}^{IGM1} P_{SED}^{g',g} \cdot \Delta u^{g} \quad . \tag{34}$$

From these two components of an integral SED sensitivity, SENSIT obtains the net integral SED sensitivity cofficient

$$S(g') = S_{HOT}(g') - S_{COLD}(g') \quad , \tag{35}$$

which quantifies how much more sensitive the integral response I_ϕ is to the hot component of the SED at incident energy group g' than to its cold component. The simplest possible response uncertainty estimate due to estimated SED uncertainties is then obtained from[9]

$$\left(\frac{\delta I}{I}\right)_{SED} = \sum_{g'=1}^{IGM1} \left|S(g')\right| \cdot F_{SED}(g') \quad . \tag{36}$$

Values for all SED sensitivity profiles, as defined in Eqs. (30) through (32), all integral SED sensitivity coefficients, Eqs. (33) through (35), and the estimated response uncertainty due to all integral SED uncertainties according to Eq. (36), are printed by SENSIT for each set of material cross sections and associated integral SED uncertainties.

IV. COMPUTATIONAL OUTLINE

Basically the SENSIT code reads angular-flux data and differential cross-section data and then performs the arithmetic calculations defined in the previous section. Therefore, no intrinsically complex computational algorithms are of concern, but an efficient management of large arrays of data is of prime importance. The code therefore employs variable dimensioned arrays throughout and uses for economical storage allocations a separate data management package (BPOINTR) subroutines. This software package has been developed by Argonne National Laboratory and is also a part of most ANL originated codes such as MC^2-2 (ANL-8144) or FX2-TH (ANL-78-97). Our version of BPOINTR is described

in Ref. 10; a later, more comprehensive version of this data management package has recently been issued and its documentation is in print[11].

A. Overall Program Flow

The entire SENSIT code consists of four functionally different parts:

1. The main program which operates as a driver routine to allocate core space through BPOINTR subroutine calls.
2. Computational subroutines which evaluate the expressions defined in the previous section.
3. Data management subroutines from the BPOINTR package and standard FORTRAN functions from systems libraries.
4. Text editing routines which output the computed results.

In the following we describe the functions of all relevant subroutines in as much detail as may be required to understand the flow of computations performed in SENSIT.

B. Data Management and Storage Requirements

SENSIT uses one-, two-, and three-dimensional arrays to manage the large amount of numerical data involved in its execution. Core storage is reserved for a particular dimensioned array only during the time the corresponding data are required to be in-core; at other times, the space is made available for the storage of other data. In order to alleviate bookkeeping chores associated with such dynamic storage allocation techniques, Argonne National Laboratory developed a collection of subroutines, called the BPOINTR package[10,11], which is incorporated in SENSIT. The user needs to know nothing about the BPOINTR routines themselves, only that they require two large blocks of workspace called "containers" for data storage during execution of a job. The container sizes are set in the main program by four FORTRAN statements as explained below, and the choice of sizes is problem dependent. The first container, the FCM (fast-core memory) or SCM (small-core memory) container, is in the CDC-7600's fast memory. The second, the ECM (extended-core memory) or LCM (large-core memory) container, is in the slower memory banks of the CDC-7600. On IBM machines, both containers are in fast memory[10,11].

In SENSIT, the main program is the control routine which defines the two container arrays and makes appropriate calls to BPOINTR subroutines to control the dynamic allocation of space within these containers. Calls to calculational sub-

routines transmit pointers corresponding to array locations through the calling sequences. Detailed program documentation for the BPOINTR package, including flow charts, common block information and subroutine descriptions, is available in Ref. 11. A shorter, functional write-up is provided in Ref. 10, which gives calling sequences for the BPOINTR routines.

The SCM container is a blank common block BLK and is assigned in the main program by the two FORTRAN statements

```
COMMON BLK(24000)
MAXSIZ = 24000  .                                                    (37)
```

The container size of 24 000 words is chosen so that the SENSIT code uses all of the available small (fast) core memory on the CDC-7600 at execution, after the code itself is stored there. Only the relatively small data arrays and arrays which are being used repeatedly during execution are allocated to this SCM container. On the CDC-7600 the full SCM is always available for any job, therefore, no operational advantage is achieved by reducing this pre-programmed container size to a smaller SCM allocation.

The LCM container is a named common block, ARRAY2, and is assigned in the main program by the two FORTRAN statements

```
COMMON /ARRAY2/ BLKECS(80000)  ,
CALL BULK(80000)  .                                                  (38)
```

The container size (in this case 80 000 words) is completely problem dependent and should be chosen before execution according to the specific problem or machine size. An advantage at execution (quicker access to the machine, shorter job turn-around time, less computer costs if the charging algorithm counts the required LCM size) is realized when BLKECS is chosen as small as possible. To achieve this, the LCM container size in the two statements, given in (38), at the beginning of the main program must be changed simultaneously. The optimal size of BLKECS is probably best obtained by trial and error.

All large data arrays (two- and three-dimensional arrays) are stored in the LCM container BLKECS at the time when they are needed for execution in one of the computational subroutines. At one specific time there are never all LCM arrays stored in BLKECS, because the BPOINTR package allows to take out unneeded arrays and re-use that space to put in new arrays. Therefore, it is very difficult to predict the minimum size required for BLKECS just on the basis of input array sizes. However, if even the maximum available LCM on a specific computer may not be large enough to accomodate the minimum required BLKECS for a specific problem, the knowledge of which arrays are stored in LCM can help to indicate how or on which input arrays the problem might be trimmed down to fit the maximum available core space.

The major input arrays assigned to BLKECS are the angular flux arrays for ϕ and ϕ^* in the detector, source and perturbed zones, and the cross section arrays, as listed in Table I. The lengths of these arrays are also given in Table I as a function of input control parameters. This table allows the user to identify the largest arrays, which must be stored for a specific problem. If a problem must be trimmed in size to fit into LCM, it is then recommended to attempt to first cut down on the largest arrays. For example, if the cross-section arrays are dominating the LCM container space, a reduction in array size is easily achieved by choosing a lower order of cross section anisotropy; i.e., a smaller LMAX. Or, if the angular flux arrays are overwhelming the LCM container, one can simply reduce IPER, ISRS or IDET by including only a part of all perturbed, source, or detector zones in one SENSIT run. In this case the full problem is solved by a series of smaller size SENSIT runs.

C. Summary of Subroutine Functions

Basically, all subroutines are called from the main program with a few exceptions where subroutines are called from other subroutines. Comment cards are inserted generously at the subroutine calls as well as in between executable statements in the main program and in all subroutines. Here we summarize only the general functions carried out by each computational subroutine. We use the nomenclature defined in previous sections.

Since data management, as opposed to computational complexity, is of prime concern in SENSIT, as explained above, most subroutine calls refer to the dynamic

TABLE I

ARRAYS ALLOCATED TO THE LCM CONTAINER ARRAY BLKECS

Array Name	Length of array (words)	Subroutine in which array is first used	Array only used if
PHI	(IM+1)*MM	SUB2A	always
PHID	IGM*IDET*MM	SUB2A	always
COVR	IGM*IGM	SUB2A	DETCOV = 1
FISTAR	(IM+1)*MM	SUB2B	always
FISTAS	IGM*ISRS*MM	SUB2B	always
FISS	IGM*ISRS*MM	SUB2B	always
PHIP	IGM*IPER*MM	SUB3	always
FISP	IGM*IPER*MM	SUB3	always
FISTAP	IGM*IPER*MM	SUB3	always
XS	(IGM+IHT)* *IGM*(LMAX+1)	SUB5	ITYP = 0,1,3
XSBAR	(IGM+IHT)* *IGM*(LMAX+1)	SUB5	ITYP = 0,1,3
DSL	IGM*IGM* *NMOM (+)	SUB6	ITYP = 0,1,3
DSLFD	IGM*IGM* *NMOM (+)	SUB6	ITYP = 0,1,3
PSI	IGM*IGM *NMOM	SUB4	ITYP = 0,1,3
PSED	IGM1*IGM1	SUB11	ITYP = 3
COV	IGM1*IGM1	SUB5V	ITYP = 2

(+)NMOM = LMAX+1 for IGE = 1,3
= $(LMAX+2)^2/4$ for IGE = 2
= $(LMAX+1)^2$ for IGE = 4

storage allocation scheme provided by the BPOINTR package. Since these routines are described in detail elsewhere[10,11], we just summarize here the subroutine names which belong and refer to the BPOINTR package.

1. BPOINTR Package. Subroutines from the BPOINTR package which perform all dynamic storage allocation functions within SENSIT are:

POINTR	IPTERR	PRTI1E	ALLOC1
PUTPNT	PUTM	PRTI2E	ALLOC2
BULK	REDEF	PRTI2	IPT2
FREE	REDEFM	PRTR1E	ILAST
WIPOUT	PURGE	PRTR2	MEMGET
GETPNT	STATUS	PRTR2E	MEMGET1
IGET	PRTI1	FREE1	SQUEEZE
			SQUEEZEX

These subroutines are attached to SENSIT after the computational subroutines.

2. Subroutine SUB1. This routine reads, from input cards, the neutron and gamma-ray group structures $E_n(g)$ and $E_\gamma(g)$, the S_N quadrature weights w(m) and level cosines MUE(m), all geometry information such as spatial mesh boundaries z(i), and the interval numbers which identify source, detector and perturbed zones in the problem. SUB1 calculates the lethargy widths per group, Δu^g, and spatial mesh cell volumes V_i. The numbering sequence of the spatial mesh cells is reordered for the source, detector, and perturbed zones as described in Sec. V.C. This renumbering is achieved by three calls to subroutine MAP as described later. A somewhat elaborate editing algorithm is also built into SUB1 which prints the geometry information in one summary table that allows for easy debugging of input errors.

3. Subroutine SNCON. This routine is borrowed from the ONETRAN discrete-ordinates transport code[12] and generates point directions and point weights for the input S_N quadrature set $\{w_m,\mu_m\}$. It also computes the Legendre polynomials $P_\ell(\mu_m)$ and the more general spherical harmonic functions required for cylindrical and two-angle slab geometries.

4. Subroutine SUB2A. The main function of this routine is to calculate I_ϕ or $I^{(1)}_\phi$, the integral response for the unperturbed reference case, computed only from forward fluxes from Eq. (14). For this purpose the energy and spatial distribution functions for the detector response, RHO(g) and RHO(j), are read from input cards. The forward angular flux in the detector zones is read from TAPE1. As a by-product of the calculation of I_ϕ according to Eq. (14), the detector sensitivity profile P^g_R, Eq. (16), is also obtained and edited. If DETCOV = 1 and a covariance matrix COVR(g,g') is provided in the input, then subroutine SUB9 is called to perform a detector response uncertainty analysis.

5. Subroutine SUB2B. This routine performs functions analogous to SUB2A, except for the adjoint fluxes. First the energy and spatial distribution functions for the source distribution, QUE(g) and QUE(j), are read from input cards. Then, the adjoint angular flux in the source zones is read from TAPE2 and its group and directional order reversed to confirm to the same ordering as used for the forward flux. The integral response I_{ϕ^*}, obtained from the adjoint flux distribution alone, is calculated via Eq. (15), together with the source sensitivity profile P^g_Q via Eq. (17).

6. Subroutine SUB3. The main function of this routine is to read forward and adjoint angular fluxes from TAPE1 and TAPE2 for all perturbed zones. The adjoint angular fluxes are also reordered with respect to their group and angular variables to confirm with the ordering principle of the forward fluxes.

7. Subroutine MAP. MAP is a special utility routine which is called from subroutine SUB1 to renumber spatial mesh cells for given zones . Specifically, MAP generates an integer map for all spatial mesh boundaries, such that those mesh boundaries within specified (disjoint) zones are numbered consecutively, while those outside these zones are set to zero (Sec. V. C).

8. Subroutine SUB4. Using the forward and adjoint angular fluxes, $\phi^g_m(i)$ and $\phi^{*g}_m(i)$, for spatial intervals within perturbed zones, SUB4 calculates the arrays χ^g and $\psi^{gg'}_\ell$ required for the evaluation of sensitivity loss and gain terms, respectively. Two intermediate arrays, $X^g_\ell(i)$ and $Y^{g'}_\ell(i)$, are used to finally compute $\psi^{gg'}_\ell$ as defined in Sec. II. A.

9. Subroutine SUB4V. For vector cross-section sensitivity analyses (ITYP = 2) only sensitivity loss terms are computed. Therefore only the array χ^g is needed, but not $\psi_\ell^{gg'}$. Hence, if ITYP = 2, subroutine SUB4V is called instead of SUB4 to calculate χ^g as a spatial integral over all perturbed zones.

10. Subroutine SUB5. The general function of this routine is to read into SENSIT the needed differential cross sections, either from input cards or from TAPE4. SUB5 is only called for ITYP = 0, 1, 3, but not for ITYP = 2 because the vector cross-section sensitivity analysis requires a special cross-section tape, TAPE10, which is differently formatted than TAPE4. SUB5 is written in 3 different sections to read cross sections (a) in LASL format from cards, (b) in LASL format from TAPE4, and (c) in limited FIDO (ORNL) format from cards. For detailed format specifications we refer to Sec. V.A. SUB5 reads a complete cross-section table for each material, which includes LMAX Legendre components with IGM energy groups and a table length of IGM+IHT. After the (assumed) microscopic cross sections are read, SUB5 converts them immediately to macroscopic cross-sections using the input number densities.

11. Subroutine SUB5V. For the case of a vector cross-section sensitivity and uncertainty analysis (if ITYP = 2) SUB5V is called instead of SUB5 to read cross sections into SENSIT. SUB5V first reads, from input cards, the identification number and two number densities for the pair of vector cross sections to be read from TAPE10. Then subroutine COVARD is called from SUB5V, which actually reads the microscopic cross-section pair, Σ_1^g and Σ_2^g, together with the relative covariance matrix $\mathrm{Cov}(\Sigma_1^g,\Sigma_2^{g'})$. This information is printed if ITEST = 3. Finally, SUB5V generates macroscopic cross sections using the number densities read from input cards.

12. Subroutine SUB6. This routine extracts from the full cross-section tables the vector cross-sections Σ_{abs}^g, $\nu\Sigma_f^g$, $\Sigma_{s,loss}^g$, Σ_T^g, and the down-scattering matrix $\Sigma_{s,\ell}^{g\to g'}$. For design sensitivity analyses (ITYP = 1) these cross-section data are prepared for both the perturbed (Σ) as well as the unperturbed ($\bar{\Sigma}$) cross sections in order to then calculate the net cross-section perturbations, according to Eqs. (22) through (24). In addition, the total macroscopic scattering cross section per group is calculated directly from the scattering matrix, according to Eq. (6), by summing $\Sigma_{s,o}^{g\to g'}$ along diagonals. In coupled neutron/

gamma-ray calculations (if NCOUPL > 0) the total gamma-ray production cross section per neutron group is also evaluated. If ITEST = 1 is chosen, SUB6 will print all of the above calculated cross sections for all groups.

13. Subroutines TEXT and TEXTA. These two routines have the exclusive function to print definitions of variable names which are used when the computational results are edited. TEXT prints a list of definitions pertaining to the standard cross-section sensitivity analysis when ITYP is chosen as 0 or 3. TEXTA prints another list of definitions used for design sensitivity output (if ITYP=1).

14. Subroutine SUB8. This routine calculates and edits the final results of the sensitivity analyses for the standard (ITYP = 0) and design sensitivity (ITYP = 1) cases. SUB8 uses the previously prepared cross-section arrays from SUB6 and the arrays χ^g and $\psi_\ell^{gg'}$ from SUB4 to evaluate Eqs. (3) through (5), Eqs. (8) through (15), Eqs. (18) through (21) and Eqs. (25) and (26). If IOUTPUT = 1, all sensitivity results are printed for each individual perturbed zone and for the sum over all perturbed zones, while for IOUTPUT = 0 a considerably shorter printout is provided by editing only the sensitivity results integrated over all perturbed zones.

15. Subroutine SUB8V. In the case of a vector cross-section sensitivity and uncertainty analysis (ITYP = 2) all editing is provided by SUB8V instead of SUB8. First the sensitivity profiles, P_1^g and P_2^g, for the pair of vector cross sections read from TAPE10 via SUB5V are evaluated and edited. Then the uncertainty analysis, according to Eqs. (27) and (28), for this cross-section pair is performed using the relative covariance matrix $\mathrm{Cov}(\Sigma_1^g, \Sigma_2^{g'})$, which has also been read from TAPE10 via subroutine SUB5V.

16. Subroutine SUB9. Should a covariance matrix be provided for the detector response function R(g), i.e., if DETCOV = 1, then SUB9 is called to read these data and perform the relevant uncertainty analysis. Response variances are also calculated for the special cases of assumed full correlation (+1) and the completely uncorrelated case.

17. Subroutine SUB9V. This routine is called only if ITYP = 2 and NSUMCOV > 0, i.e., when partial sums are required of individual response vari-

ances. SUB9V first reads the integers SUMSTRT and SUMEND which define the variances to be summed. Assuming no correlations between the individual vector cross-section errors specified in any or all of the NCOV covariance matrices, SUB9 then computes the total variance and relative standard deviation.

18. Subroutine COVARD. For vector cross-section uncertainty analyses (ITYP = 2), the routine COVARD is called to read into SENSIT, from TAPE10, the pair of vector cross sections with their respective covariance matrix for each specified identification number. The input ID number is correlated with ENDF/B specifications through a call to subroutine SETID. It is important to note that all arrays in subroutine COVARD are fixed-dimensioned, i.e., their field length is not dynamically allocated as is the case for all other arrays in SENSIT. In the present version of SENSIT, the 2 arrays describing the covariance matrices are restricted to a maximum size of 50 x 50 each. This is not a serious restriction of the code and may be changed at any time. The choice of 50 x 50 was rather arbitrary, considering our specially prepared TAPE10 which uses only 30 neutron groups.

19. Subroutine SETID. This routine is called only from COVARD and has the sole function to translate the input ID numbers for vector cross-section pairs into ENDF/B nomenclature. It is these latter identifiers which are required to read data from TAPE10.

V. DETAILS OF PROGRAM OPTIONS

In this section we describe special details which are helpful in preparing input to SENSIT or may prove valuable if modifications of the FORTRAN coding are considered.

A. Cross-Section Input Options

If ITYP = 0, 1, 3, complete transport cross-section tables are read into SENSIT by subroutine SUB5; if ITYP = 2, a specially formatted vector cross-section file is read from TAPE10 as described later.

1. Transport Cross-Section Tables. Three options are built into subroutine SUB5 to read standard neutron (or coupled neutron/gamma-ray) cross-section sets: first, LASL format cross sections from cards; second, LASL format cross sections from TAPE4; and third, limited FIDO (ORNL) format cross sections from cards. The general structure of all transport cross-section tables is as described in the transport code literature; e.g, the ONETRAN[12] or ANISN manual[13]. Each nuclide is described by a cross-section table of IGM columns and length ITL = IGM + IHT. The position of a certain cross section in each of the IGM columns is specified relative to the total cross-section (pos. IHT). The following ordering is assumed in the column for group g:

general XS-position	XS type	XS-position in typical standard XS set
'	'	
'	'	
'	'	
IHT-4	$\sigma_{n,2n}$	–
IHT-3	$\sigma_{transport}$	–
IHT-2 = IHA	σ_{abs}	1
IHT-1	$\nu\sigma_f$	2
IHT	σ_T	3
IHS = IHT + 1	$\sigma_s^{g\to g}$	4
IHS + 1	$\sigma_s^{g-1\to g}$	5
'	'	'
'	'	'
'	'	'
IHT+IGM = ITL	$\sigma_s^{g-IGM+1\to g}$	IGM + 3

The requirements that IHS = IHT + 1 and ITL = IHT + IGM restricts these cross-section tables to include only downscattering but no upscattering. The test printout in sample problem 1 contains an example of a coupled 6-group cross-section set with 3 neutron and 3 (identical) gamma-ray groups. Since this printout is generated line-by-line, the sequence of data along lines corresponds to the ordering along columns as discussed above.

If anisotropic scattering is considered, then the complete cross-section set for an isotope or reaction is expected to consist of LMAX+1 cross-section tables representing Legendre exapansion coefficients. Note, however, that two different conventions are presently being used for such expansions. Omitting the energy dependence and abbreviating $\mu_o = \underline{\Omega}\cdot\underline{\Omega}'$ we have:

a. LASL (ONETRAN, etc.) convention:

$$\Sigma_s(\mu_o) = \sum_{\ell=0}^{LMAX} \frac{2\ell+1}{4\pi} \cdot \Sigma_{s,\ell}^{LASL} \cdot P_\ell(\mu_o) \quad , \tag{39}$$

so that

$$\Sigma_{s,\ell}^{LASL} = 2\pi \int_{-1}^{+1} \Sigma_s(\mu_o)\, P_\ell(\mu_o)\, d\mu_o \quad . \tag{40}$$

b. ORNL (ANISN, etc.) convention:

$$\Sigma_s(\mu_0) = \sum_{\ell=0}^{LMAX} \frac{1}{4\pi} \cdot \Sigma_{s,\ell}^{ORNL} \cdot P_\ell(\mu_0) \quad , \tag{41}$$

so that

$$\Sigma_{s,\ell}^{ORNL} = 2\pi\,(2\ell+1) \int_{-1}^{+1} \Sigma_s(\mu)\, P_\ell(\mu_0)\, d\mu_0 \quad . \tag{42}$$

Due to these different conventions the higher-order components of the scattering tables differ by a factor of $(2\ell + 1)$:

$$\Sigma_{s,\ell}^{ORNL} = (2\ell + 1)\, \Sigma_{s,\ell}^{LASL} , \tag{43}$$

which is compensated for in SENSIT subroutines SUB8 and SUB11 according to KXS = 1 or 2.

The actual formats in which the cross sections are read into SENSIT differ also according to KXS = 1 or 2, and IXSTAPE = 0 or 1:

c. LASL-Formatted Transport Cross Sections From Cards (KXS = 1 and IXSTAPE = 0: The standard LASL cross-section format expects a string of data which corresponds to reading the above-mentioned cross-section table columnwise in ascending group order. The format for the numerical data is a 6E12.5 data field which expects 6 numbers per card. The only difference between cross sections read from cards or from tape lies in the title cards and the number density specifications. If KXS = 1 and IXSTAPE = 0, the format for one complete cross-section set is:

Input Array Name	Number of Entries	Input Format	Required only if	Description
TITLE	1 card	20A4	always	XS title card for this material
NUMDEN, JCOVAR	2 words	12X,E12.6, 11X,I1	always	NUMDEN.= number density of cross section. JCOVAR = indicator if the last P_ℓ-XS set is followed by a covariance matrix, 0/1 = no/yes.
PLTITL	1 card	20A4	always	title card for P_0-component.
XS(g,g',0)	IGM*ITL	6E12.5	always	microscopic cross-section set for P_0-component.
PLTITL	1 card	20A4	LMAX > 0	title card for P_ℓ-component
XS(g,g',ℓ)	IGM*ITL	6E12.5	LMAX > 0	microscopic cross-section set for P_ℓ-component.

Input Array Name	Number of Entries	Input Format	Required only if	Description
				Note: For each P_L-component a set of {PLTITL,XS} must be input, until L = LMAX is reached.
CTITL	1 card	8A10	JCOVAR = 1	title card for covariance matrix.
COV(g,g')	IGM*IGM	6E12.5	JCOVAR = 1 and ITYP = 0	covariance matrix for cross-section set XS(g,g',ℓ)

If a design sensitivity is required (ITYP = 1) with an independent reference cross-section $\bar{\Sigma}$ (IDESIGN = 0), then a second complete cross-section set XSBAR(g,g',ℓ), starting with a material title card, is expected.

If JCOVAR on the number density card is 1 and a relative covariance matrix is entered, then SENSIT performs a cross-section uncertainty analysis analogous to the vector cross-section uncertainty analysis, where Eqs. (27) and (28) are evaluated for the net sensitivity profile as defined in Eq. (11), i.e., $P_1 = P_2 =$ SEN.

d. LASL-Formatted Transport Cross Sections From TAPE4 (KXS = 1 and IXSTAPE = 1):

In this case the cross-section data are read from a card-image tape according to their material sequence number. It is assumed that, for ITYP = 0 or 3, a tape has been prepared which contains complete cross-section sets for an arbitrary number, say MAXMAT, of materials. Then each cross-section set per material is identified by its sequence number between 1 and MAXMAT, which is then the material's ID number. The card input then must specify only this ID-number and the associated number density in order for SENSIT to read the desired cross-section set from TAPE4, as described in the detailed input specifications: 1 card with (ID, NUMDEN, XSNAME) is required for each of the NPERXS cases.

TAPE4 must then be formatted as follows:

1. record: title card (20A4) for material 1, P_0 component
2. record: P_0-XS data for ID = 1, IGMxITL words in (6E12.5)-format

3. record: title card for ID = 1, P_1 component

4. record: P_1-XS data for ID = 1,

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,

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n-th. rec.: title card for ID = 2, P_0 component

(n+1)st. rec.: P_0-XS data for ID = 2

(n+2)nd. rec.: title card for ID = 2, P_1 component

,

,

,

m-th. rec.: P_{LMAX}-XS data for last material (ID = MAXMAT).

e. FIDO (ORNL)-Formatted Cross Sections From Cards (KXS = 2 and IXSTAPE = 0):

This option has been incorporated for convenience in cases when ANISN angular fluxes are used. We transferred the cross-section input algorithm from our (rather old) version of ANISN into SUB5 of SENSIT, which allows SENSIT to read the same cross sections as ANISN when KXS is set to 2. However, we caution the use of this option because there are a great many different versions of ANISN and FIDO routines in existence and compatibility among these different versions is not guaranteed. Moreover, we are unable to precisely date our version of ANISN from which this cross-section input algorithm was taken.

A total of LMAX+1 P_ℓ cross-section tables, based on definitions given in Eqs. (41) and (42), define a complete material cross-section set, where again each P_ℓ-table is preceded by a title card. The actual cross-section data are expected in a fixed-field FIDO format which allows blank fields and the repeat option. For a detailed description of the FIDO format we refer to Ref. 13, but stress again the limitations of our version, as mentioned above. To eliminate any remaining ambiguity, we recommend the editing of any cross sections used with ANISN and then reformatting them into the simpler LASL-formatted TAPE4 as described in the previous paragraph.

2. Vector Cross-Section and Covariance Matrix Input. If ITYP = 2, SENSIT reads pairs of vector cross-sections with their associated covariance matrix from TAPE10 which, therefore, must be specially prepared as described below.

3. Multigroup Processing of ENDF/B Covariance Data to Generate TAPE10.*

The NJOY code[14] was used for processing the ENDF/B-V covariance data into the 30-energy group multigroup structure used in a separate study[15] for TAPE10. The module in NJOY that specifically does this processing is the ERRORR module. The multigroup output of the ERRORR module is in an ENDF-like format; a sample of this output is given in Table II.

The data in Table II are given in standard ENDF/B BCD records or "cards" consisting of 80 columns divided into 10 fields. The first 6 fields are 11 digits wide and are used for either floating point numbers or integers. The 7th, 8th, 9th, and 10th field are 4, 2, 3, and 5 digits wide, respectively, and are used for integers only. In these latter 4 fields, that is, fields 7, 8, 9, and 10, the digits in the field of 4 (field No. 7) represent the MAT or "material number" of the isotope or element processed; the next 2 digits (field No. 9) are the MT or "section number" that usually indicates the nuclear reaction processed; and the final 5 digits (field No. 10) are just the card sequence number. Sections are delimited by zeros in the MT fields, files by zeros in the MF fields, and materials by zeros in the MAT fields. The first card shown in Table II, with zeros in all of the last four fields, is the delimiter for the preceding material.

The next card shown in Table II is the first card for the material with MAT-1326, which is natural iron. Note that on this card the number 2.6×10^4 appears in the first field and 55.365 is in the second field. These are the "ZA" (1 000 x Z + A) and "AWR" (atomic weight ratio, i.e., atomic weight of the material divided by weight of the neutron) numbers as taken by the NJOY code directly from the ENDF/B file. The fact that 1 000 x Z is 26 000 and A=0 just means that the data is for the element Fe rather than for an isotope.

Also note that MF=1 and MT=451 on cards 1 to 8. This MF-MT combination is normally used in the ENDF/B formats for descriptive Hollerith information, but it is used here for the boundaries of the multigroup set used for the processed data to follow. On card No. 2, note the number 30 in field 3 and the number 31 in field 5, which indicates, respectively, the number of energy groups and the

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