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REACTOR CROSS-SECTION SENSITIVITY STUDIES USING TRANSPORT THEORY

E. M. Oblow

OAK RIDGE NATIONAL LABORATORY

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TABLE OF CONTENTS

ABSTRACT

An approach to making reactor sensitivity studies and reactor parameter uncertainty analysis using transport theory is developed. Sensitivity functions based on variational principles are reviewed and compared with an alternate approach using generalized perturbation theory. The computational implementation of the method using transport codes is also discussed. Finally, the use of cross-section error files in conjunction with sensitivity coefficients in estimating uncertainties in reactor parameters is described.

I. INTRODUCTION

This technical report is intended to be an introduction to reactor sensitivity theory as it has evolved from the ongoing program in shielding sensitivity analysis at ORNL. In this new effort we are attempting to determine what cross sections are most important in calculating reactor physics parameters for fast reactors and what effect uncertainties in the basic nuclear data have on the performance of such reactor systems. The theoretical developments follow closely methods based on diffusion theory already applied to reactor sensitivity studies by Stacey[1,2] using a variational approach and Gandini[3] using generalized perturbation theory. Both of these methods result in successful formalisms for predicting changes in arbitrary reactor parameters based on system perturbations. Our own efforts in shielding analysis[4-7] have stressed both analytic and predictive aspects of sensitivity theory and the use of transport calculations. This approach is embodied in the code SWANLAKE.[8] Such techniques are continued with the present effort in reactor analysis. Adopting this philosophy means that physical principles similar to those developed by Usachev[9] and Lewins[10] for interpreting generalized adjoint fluxes as importance functions for particular reactor parameters will be used as the basis for analytic aspects of our studies and a middle road between variational methods and generalized perturbation theory will be used for the predictive phase of the work.

The extension of transport theory calculational methods, specifically those employed in ANISN,[11] to the reactor field pose new problems, and at least an initial attempt at overcoming some of the more difficult ones is presented in this memorandum. In this phase of the effort, additional development work is indicated. The approach at present has been to theoretically justify use of methods which differ as little as possible from those which are already in current use in the shielding program and have a clear history of proven value.

One of the most important aspects of the program will be to attempt to estimate reasonable uncertainties in reactor parameters based on uncer-

tainties in microscopic cross-section data. Only a preliminary introduction to the use of cross-section error files and sensitivity coefficients are discussed here since two other papers will address this area in more detail.[12,13] The implementation of this phase of the work will certainly evolve as our experience with uncertainty estimation procedures increases. It is only the question of the character of the sensitivity coefficients, specifically the need for coefficients with linear operators, and their use in conjunction with predicting variances in reactor parameters that will be discussed in this work.

II. REACTOR SENSITIVITY THEORY

A. Definitions

The developments in this section are designed to introduce the defining equations for the sensitivity functions needed to implement a sensitivity study. In accordance with our past approach to this problem, we will try to develop bilinear functions suitable for analysis and prediction of the form:

$$R_L(\bar{\xi}) = \psi^*(\bar{\xi})\ L\phi(\bar{\xi}) \tag{1}$$

where $\psi^*(\bar{\xi})$ is an adjoint flux; L a general linear operator; $\phi(\bar{\xi})$ a flux; $\bar{\xi}$ a point in phase space defined by position $\bar{r}$, energy E, and solid angle $\bar{\Omega}$; and $R_L(\bar{\xi})$ the general sensitivity function for operator L whose applicability has been discussed in previous papers.[4,6]

For reactor applications, the governing balance equation for neutrons is the homogeneous Boltzmann equation, noted symbolically as:

$$A\phi - \lambda B\phi = 0 \tag{2}$$

where A is the Boltzmann operator for leakage and scattering processes; B is the fission source operator and λ is the eigenvalue related to the multiplication constant for the system by $\lambda = k^{-1}$. An alternate and also useful form of Eq. (2) is:

$$P\phi = (A - \lambda B)\phi = 0 \tag{3}$$

The homogeneous adjoint equation for this system is given similarly by:

$$(A^* - \lambda B^*)\phi^* = 0 \tag{4}$$

where A* and B* are the adjoint operators of A and B, respectively, and ϕ^* is the adjoint flux. The eigenvalue λ in the forward and adjoint equations is the same since the eigensolutions to Eq. (2) are biorthonormal to those in Eq. (4). The operator A* and B* satisfy the conventional defining relationship for an adjoint operator:

$$\langle \psi^*, A\psi \rangle = \langle \psi, A^*\psi^* \rangle \tag{5}$$

where ψ^* and ψ are arbitrary functions and the braces $\langle\rangle$ denote an integration over all phase space $\overline{\xi}$. Vanishing boundary terms for the leakage operator included in A are implied in using Eq. (5).

In deriving a useful sensitivity function, the result of a calculation (whose sensitivity is being studied) must be defined. For reactor work, the most general result will be a bilinear ratio of the form:

$$R(\phi, \phi^*) = \frac{\langle \phi^*, H_1\phi \rangle}{\langle \phi^*, H_2\phi \rangle} \tag{6}$$

where ϕ and ϕ^* solve Eqs. (2) and (4), respectively, and H_1 and H_2 are arbitrary operators. Included in this definition are the defining equations for reactivity worth, Doppler coefficient, etc. (see Appendix A for a summary of the specific forms of R). Also included are simple reaction rate ratios where R is not a function of ϕ^*. That is:

$$R(\phi) = \frac{\langle H_1\phi \rangle}{\langle H_2\phi \rangle} \tag{7}$$

It should be noted here that reactivity worth is a special case of Eq. (6) since the worth definition[2] involves the use of ϕ' (i.e., the perturbed flux resulting from a perturbation defined by the worth operator H_1).

This case is special in that it is necessary to estimate ϕ' with ϕ in order to have a simple analytic expression for R.

B. Perturbed System and Criticality Reset

In order to assess the sensitivity of R to cross-section data in the same manner as was used in the shielding work, it is necessary to be able to define analytically the differential rate of change of R with respect to cross-section changes. It is also necessary to have a method for making an estimate of a finite change in R, δR, which is a linear function of finite changes in the cross section. This is most easily done for reactor applications with use of a variational principle for estimating the result R in a perturbed system. The method of defining variational principles using Lagrange multipliers as suggested by Pomeraning[14] and Stacey[1] will be employed here. The major difference in our approach, however, will be in the definition of the equations for the perturbed system. Our approach in this regard will be consistent with that of Gandini[3] and the proponents of generalized perturbation theory. The basic reason for choosing this middle road is due to the nonlinear nature of Stacey's resulting variational principle, which is incompatible with our linearity requirements in uncertainty analysis (to be discussed later). We choose, however, to pursue Stacey's approach of deriving sensitivity functions based on variational methods because of the relative simplicity of the derivations and the fact that they include important effects which can be overlooked without careful application of the generalized perturbation approach.

Thus we define a perturbed system (resulting from cross-section changes) in line with the Gandini approach as follows:

$$A'\phi' - \lambda B'\phi' = 0 \tag{8}$$

where,

$$\begin{aligned} A' &= A + \delta A \\ B' &= B + \delta B \\ \phi' &= \phi + \delta\phi \end{aligned} \tag{9}$$

For comparison purposes, Stacey's perturbed equation is:

$$A'\phi' - \lambda'B'\phi' = 0, \tag{10}$$

The major difference between Eqs. (8) and (10) is the fact that Stacey uses the perturbed eigenvalue λ' and Gandini uses the unperturbed value λ. Implied in both of these approaches is the controversy of how to restore a system to critical after a perturbation has been introduced into it. The fact that the reactor system must be restored to critical is a physical fact and not subject to debate from either side. Stacey's approach is equivalent to assuming that criticality is restored in a purely mathematical way by adjusting ν, the average number of neutrons released per fission. That is, if we write the fission operator term as follows:

$$\lambda B = \lambda \nu D \tag{11}$$

The perturbed system can then be represented by:

$$\lambda'B' = \lambda'\nu D' = \lambda\nu'D' \tag{12}$$

or equivalently

$$\lambda'B' - \lambda B = \delta(\lambda B) = \lambda\delta(\nu D) \tag{13}$$

Thus, the restoration of λ' to its original value λ can be thought of in terms of a change in ν from ν to ν'. Any term which involves a $\delta\lambda = \lambda' - \lambda$ is a result of this method of restoring criticality and can be thought of as a $\delta\nu$. In this regard, Stacey's perturbed equation is just a specific case of the one we will use [i.e., Eq. (8)], and a ν change is possible from our point of view also. In Stacey's approach, however, this $\delta\nu$ form of the return-to-critical is built into all his perturbation equations and proves to be the source of terms nonlinear in the cross-section changes. From our point of view and that of Gandini, Eq. (8) is more physical. In this case A' and B' imply a physical change in the system operators which will maintain criticality. The exact mode of returning the system is left unspecified and can be dealt with outside of the mathematical formalism that follows because of the linear nature of the sensitivity functions which result. A return to critical, however, is

implied in the perturbed operators of Eq. (8), and this should not be forgotten.

C. Variational Principle

Proceeding then, with the derivation of the general sensitivity function we introduce Pomraning's variational principle for R, given by:

$$F_p(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = R(\phi,\phi^*) - \langle \Gamma^*,(A - \lambda B)\phi\rangle - \langle \Gamma,(A^* - \lambda B^*)\phi^*\rangle \tag{14}$$

It should be noted that Γ and Γ^* act as unspecified Lagrange multipliers which introduce, as auxilliary conditions, the equations that ϕ and ϕ^* must solve for F_p to be stationary. In this case, the unperturbed equations for ϕ and ϕ^* are used. The stationary properties of F_p are as follows:

$$F_p(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = R(\phi,\phi^*) \tag{15}$$

$$\delta F_p(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = 0 \tag{16}$$

That is, the functional is identically equal to R when the flux estimates used in evaluating the functional are solutions to the Boltzmann equation and its adjoint, and the first variation of F_p around this stationary point is equal to zero. The expression for the first variation F_p determines the equations which Γ and Γ^* must solve and can be written as follows:

$$\begin{aligned}\delta F_p(\phi\ \phi^*,\Gamma,\Gamma,\lambda) = {} & \delta\lambda \langle \Gamma^*,B\phi\rangle + \delta\lambda \langle \Gamma,B^*\phi^*\rangle \\ & - \left\langle \delta\phi,(A^* - \lambda B^*)\ \Gamma^* - \frac{dR(\phi,\phi^*)}{d\phi}\right\rangle \\ & - \left\langle \delta\phi^*,(A - \lambda B)\Gamma - \frac{dR\ \phi,\phi^*)}{d\phi^*}\right\rangle\end{aligned} \tag{17}$$

Here, the derivatives of R are functional derivatives defined by[14]

$$\frac{dR}{d\phi} = \lim_{\varepsilon\to 0}\left\{\frac{R[\phi(\bar{\eta}) + \varepsilon\delta(\bar{\xi} - \bar{\eta})] - R[\phi(\bar{\eta})]}{\varepsilon}\right\} \tag{18}$$

Some particular examples of these derivatives for several reactor parameters appear in Appendix B.

The conditions which must be met for F_p to be stationary are therefore:

$$(A - \lambda B)\Gamma = \frac{dR(\phi,\phi^*)}{d\phi^*} \tag{19}$$

$$(A^* - \lambda B^*)\Gamma^* = \frac{dR(\phi,\phi^*)}{d\phi} \tag{20}$$

$$\left\langle \Gamma, B^*\phi^* \right\rangle = 0 \tag{21}$$

$$\left\langle \Gamma^*, B\phi \right\rangle = 0 \tag{22}$$

Equations (19) and (20) are the governing equations for the generalized functions Γ and Γ^*, and Eqs. (21) and (22) are the conditions that require Γ^* and Γ to be orthogonal to the fundamental mode flux and adjoint solutions to the critical equations, Eqs. (2) and (4). These latter conditions will be discussed more fully in the next section.

D. Order of Errors

One further statement about the properties of F_p is needed before a sensitivity function can be derived. The statement involves the conditions that insure that the use of F_p to estimate R in a perturbed system involves only second-order errors in the functions $\phi,\phi^*,\Gamma,\Gamma^*$, and λ. Thus, writing the perturbed principle F_p' as:

$$F_p'(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = R(\phi,\phi^*,H_1',H_2') - \left\langle \Gamma^*, (A' - \lambda B')\phi \right\rangle - \left\langle \Gamma, (A^{*\prime} - \lambda B^{*\prime})\phi^* \right\rangle \tag{23}$$

Here explicit reference is made to a perturbation which results in a change in the operators H_1 and H_2 used in defining R, so that the discussion is completely general (note the perturbed principle F_p' is stationary about the perturbed result R').

Expanding the perturbed operators A', B', H_1', H_2', we get

$$F_P'(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = R(\phi,\phi^*,H_1,H_2) - \langle\Gamma^*,(A-\lambda B)\phi\rangle - \langle\Gamma,(A^*-\lambda B)\phi^*\rangle$$
$$+ R(\phi,\phi^*,H_1',H_2') - R(\phi,\phi^*,H_1,H_2) \tag{24}$$
$$- \langle\Gamma^*,(\delta A-\lambda\delta B)\phi\rangle - \langle\Gamma,(\delta A^*-\lambda\delta B^*)\phi^*\rangle$$

Since unperturbed fluxes were used, the second and third terms in this expression are identically zero and we get:

$$F_P'(\phi,\phi^*,\Gamma,\Gamma^*,\lambda) = R(\phi,\phi^*,H_1,H_2) + \left[R(\phi,\phi^*,H_1',H_2') - R(\phi,\phi^*,H_1,H_2)\right] \tag{25}$$
$$- \langle\Gamma^*,(\delta A-\lambda\delta B)\rangle - \langle\Gamma,(\delta A^*-\lambda\delta B^*)\phi^*\rangle$$

The first variation of Eq. (24) is given as:

$$\delta F_P' = \delta F_P - \langle\delta\Gamma^*,(\delta A-\lambda\delta B)\phi\rangle - \langle\delta\Gamma,(\delta A^*-\lambda\delta B^*)\phi^*\rangle$$
$$+ \delta\lambda\,\langle\Gamma^*,\delta B\phi\rangle + \delta\lambda\,\langle\Gamma,\delta B^*\phi\rangle \tag{26}$$
$$+\left\langle\delta\phi,(\delta A^*-\lambda\delta B^*)\Gamma^* - \frac{d}{d\phi}\left[R(\phi,\phi^*,H_1',H_2') - R(\phi,\phi^*,H_1,H_2)\right]\right\rangle$$
$$+\left\langle\delta\phi^*,(\delta A-\lambda\delta B)\Gamma - \frac{d}{d\phi^*}\left[R(\phi,\phi^*,H_1',H_2') - R(\phi,\phi^*,H_1,H_2)\right]\right\rangle$$

The δF_P term in the expression is identical to Eq. (17) and arises from variation of the first three terms in Eq. (24). All the other terms in Eq. (26) arise from variation of the remaining terms in Eq. (24).

If the unperturbed fluxes are now used in evaluating Eq. (26), we see that $\delta F_P=0$ identically, and all the remaining terms are of second order. Thus, an estimation of R', the perturbed result, can be made using F_P', with the unperturbed quantities $\phi,\phi^*,\Gamma,\Gamma^*$, and λ, since it is stationary to second order about R'. As a result, we can write:

$$\delta R = R' - R = F_P' - F_P + \text{second order errors}$$
$$= R(\phi,\phi^*,H_1',H_2') - R(\phi,\phi^*,H_1,H_2) \tag{27}$$
$$-\langle\Gamma^*,(\delta A-\lambda\delta B)\phi\rangle - \langle\Gamma,(\delta A^*-\lambda\delta B^*)\phi^*\rangle + \text{second order errors}$$

Noting that to first order:

$$R' - R \cong R(\phi,\phi^*,H_1,H_2) \left\{ \frac{\langle \phi^*,\delta H_1\phi\rangle}{\langle \phi^* H_1\phi\rangle} - \frac{\langle \phi^*,\delta H_2\phi\rangle}{\langle \phi^* H_2\phi\rangle} \right\} \tag{28}$$

and using an adjoint form of the fourth term in Eq. (27), we can finally write:

$$\begin{aligned} \delta R \cong\ & R(\phi,\phi^*,H_1,H_2) \left\{ \frac{\langle \phi^*,\delta H_1\phi\rangle}{\langle \phi^* H_1\phi\rangle} - \frac{\langle \phi^*\delta H_2\phi\rangle}{\langle \phi^* H_2\phi\rangle} \right\} \\ & - \langle \Gamma^*,(\delta A - \lambda\delta B)\phi\rangle - \langle \phi^*,(\delta A - \lambda\delta B)\Gamma\rangle \end{aligned} \tag{29}$$

Equation (29) is in a form which is now completely compatible with the form of the equations handled in shielding sensitivity studies. In particular for predictive applications, SWANLAKE was developed to handle integrations of bilinear functions of perturbed operators (i.e., forms like $\langle \phi^*,\delta L\phi\rangle$), and all terms in Eq. (29) are of this form apart from the simple normalizations of the form $\langle \phi^*,H\phi\rangle$ and $R(\phi,\phi^*,H_1,H_2)$. For the analytic aspect of sensitivity theory, the integrations implied by the braces $\langle\ \rangle$ and the actual perturbed operators can be dispensed with and differential sensitivity functions of the form given in Eq. (1) can be used for a sensitivity analysis of the entire subset of operators which make up H_1, H_2, A, and B. In this instance, the general operator L in Eq. (1) can be replaced by any subset of the operators H_1, H_2, A, and B in studying any part of Eq. (29) independently. A desirable feature of Eq. (29) from the analytic and predictive standpoint is that the reset of the system to critical implied in δA and δB can be studied independently. That is, a completely separate semsitivity analysis of the reset perturbation is possible utilizing the same basic approach used for cross-section sensitivity studies.

E. Criticality Reset

One additional point is worth considering briefly at this point before a discussion of numerical methods is begun, that being the explicit criticality reset which Stacey uses in his variational approach.

The form of criticality reset Stacey builds into his variational principle appears excplicitly in his derivations as terms of the form $\delta\lambda\langle\Gamma^*,B'\phi\rangle$ and $\langle\Gamma,B'^*,\phi^*\rangle$. Using Pomeraning's variational principle, we see that for the functional F_p to be stationary, Eqs. (21) and (22) must be satisfied. That is, the generalized functions Γ and Γ^* must be orthogonal to the fundamental mode fluxes ϕ^* and ϕ, respectively -- Γ and Γ^* cannot contain any fundamental mode contamination. The nature of the criticality reset terms under these conditions are then of the form $\delta\lambda\langle\Gamma^*,\delta B\phi\rangle$ and $\delta\lambda\langle\Gamma^*,\delta B\phi\rangle$ and are thus higher order terms than any of the terms retained in the process of deriving Eq. (29). Stacey realizes this, but argues in favor of retaining these terms since they are easily calculated. From our standpoint these terms are theoretically unjustifiable in a derivation which neglects all other higher order effects and computationally they change the proportional nature of the relationship existing between δR and any of the perturbation operators. This linear relationship is crucial for the uncertainty analysis phase of a sensitivity study, and we therefore must neglect such terms. To the same order as the other terms in Eq. (29), therefore, we can state that a criticality reset involving a change in ν as reflected in $\delta\lambda$ terms can be neglected.

III. COMPUTATIONAL IMPLEMENTATION WITH ANISN

To continue the philosophy of using computational tools which already exist in our current shielding sensitivity program, the calculation of all flux quantities will initially make use of the transport code ANISN. Further development work will be necessary to remove any limitations imposed by this choice. For the present, however, it is possible to implement reactor sensitivity studies using ANISN provided care is exercised and certain limitations are imposed on the options available in the code. A discussion of these and other solution criteria follow.

A. Generalized Flux Equations

The normal forward and adjoint flux calculations in a critical system pose no problems for a transport code, one simply solves Eqs. (2) and (4)

using the standard k-calculation option in ANISN. The generalized equations, however, are another matter, posing new problems which are best illustrated by looking at the generalized adjoint equation:

$$(A^* - \lambda B^*)\Gamma^* = S^* = \frac{dR(\phi,\phi^*)}{d\phi} \tag{30}$$

with the associated condition that:

$$\langle \Gamma^*, B\phi \rangle = 0 \tag{31}$$

Equation (30) is an inhomogeneous, fixed source equation having a general solution made up of homogeneous and particular parts. For the homogeneous equation, the solutions are the eigenmodes ϕ_i^* corresponding to the eigenvalues γ_i which solve

$$(A^* - \lambda_i B^*)\phi_i^* = 0 \tag{32}$$

These solutions are biorthonormal with respect to the forward eigenmodes which solve:

$$(A - \lambda_i B)\phi_i = 0 \tag{33}$$

such that:

$$\left\langle \phi_i, \lambda_j B^* \phi_j^* \right\rangle = \left\langle \phi_i, A^* \phi_j^* \right\rangle = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases} \tag{34}$$

For clarity of notation, we will let $\lambda \equiv \lambda_o$, $\phi^* \equiv \phi_o$, and $\phi = \phi_o$ to denote the fundamental mode (critical) eigenvalue and eigenmodes, respectively.

If the ϕ_i^* solutions form a complete set, then the source in Eq. (30) can be expanded in terms of the ϕ_i^*'s as follows:

$$S^* = \sum_{i=o}^{\infty} a_i \lambda_i B^* \phi_i^* \tag{35}$$

where the biorthonormality conditions gives:

$$a_i = \langle S^*, \phi_i^* \rangle \tag{36}$$

The general solution to Eq. (30) can be similarly written as:

$$\Gamma^* = b_o \phi^* + \sum_{i=1}^{\infty} b_i \phi_i^* \tag{37}$$

Here, in general, b_o is an arbitrary constant since ϕ^* solves the homogeneous adjoint equation [Eq. (4)]. For the particular case, we are considering the orthogonality condition imposed by Eq. (31) restricts the solution to be orthogonal to the fundamental mode, so that $b_o = 0$. The remaining coefficients, b_i, are gotten from the orthonormality properties of the ϕ_i and ϕ_i^* as follows:

$$b_i = \frac{a_i}{1 - \lambda/\lambda_i} \tag{38}$$

From this latter expression, it is clear that a unique solution for Γ^* is possible only if $b_o = 0$, since b_o otherwise could be arbitrary. Uniqueness thus also requires the condition that:

$$\langle S^*, \phi \rangle = 0 \tag{39}$$

since any fundamental mode existing in the source (i.e., $a_o \neq 0$) would result in a fundamental mode component in Γ^* (i.e., $b_o \neq 0$).

The character of the generalized source S^* and the generalized adjoint flux Γ^*, then are that they are both orthogonal to the fundamental mode flux, ϕ, and neither one can have any fundamental mode contamination for the solution to Eq. (30) to exist and be unique. The non-uniqueness would arise from the fact that b_o in Eq. (37) is arbitrary if any fundamental mode solution is present in S^* or Γ^*. Care that this orthogonality condition is met cannot be stressed strongly enough for solutions of the generalized perturbation equations. In addition, fundamental contamination is a major problem in using transport theory, as opposed to diffusion methods. These problems are illustrated in the discussions which follow.

B. Method of Successive Approximations

In actual numerical computations, Eq. (30) can be solved by the method of successive approximations which is implemented in an iterative fashion as follows:

$$\begin{aligned} A^*\Gamma^{*(0)} &= S^* \\ A^*\Gamma^{*(1)} &= \lambda B^*\Gamma^{*(0)} + S^* \\ &\vdots \\ A^*\Gamma^{*(N)} &= \lambda B^*\Gamma^{*(N-1)} + S^* \end{aligned} \tag{40}$$

The solution is taken to be $\Gamma^* = \Gamma^{*(N)}$ when the following convergence criteria is met:

$$\left| \frac{\lambda B^*\Gamma^{*(N)} - \lambda B^*\Gamma^{*(N-1)}}{\lambda B^*\Gamma^{*(N)}} \right| \leq \varepsilon \tag{41}$$

Here, the superscripts represent successive iterates to the solution Γ^* and correspond to outer iteration counters in a fixed + fission source calculation in ANISN.

This solution approach which we will be using differs from both the Stacey and Gandini approaches in that (1) we solve the transport equation, not the diffusion equation, and (2) Stacey and Gandini use a Neumann series to solve for Γ^*. In the Neumann series approach, the solution is represented by:

$$\Gamma^* = \sum_{n=0}^{N} \psi^{*(n)} \tag{42}$$

where the $\psi^{*(n)}$'s solve the following set of equations:

$$\begin{aligned} A^*\psi^{*(0)} &= S^* \\ A^*\psi^{*(1)} &= \lambda B^*\psi^{*(0)} \\ &\vdots \\ A^*\psi^{*(N)} &= \lambda B^*\psi^{*(N-1)} \end{aligned} \tag{43}$$

It is easily shown that the method of successive approximations and the Neumann series approach are equivalent since the fluxes are related as follows:

$$\Gamma^{*(N)} = \sum_{i=0}^{N} \psi^{*(i)} \tag{44}$$

The method of successive approximations was chosen for the present work since it is the method used to solve fixed + fission source problems in ANISN.

C. Characterization of Convergence

The way in which the two solution schemes approach convergence is similar and can be characterized as follows. For the Neumann series, using the representation of the source given in Eq. (35), we can write the first iterate as:

$$A^*\psi^{*(0)} = \sum_{i=1}^{\infty} a_i \lambda_i B^* \phi_i^* \tag{45}$$

giving

$$A^*\psi^{*(0)} = \sum_{i=1}^{\infty} a_i A^* \phi_i^* \tag{46}$$

and therefore

$$\psi^{*(0)} = \sum_{i=1}^{\infty} a_i \phi_i^* \tag{47}$$

For the second and subsequent iterates, we get:

$$A^*\psi^{*(1)} = \lambda B^*\psi^{*(0)} = \lambda B^*\sum_{i=1}^{\infty} a_i\phi_i^*$$

$$\psi^{*(1)} = \sum_{i=1}^{\infty} a_i\left(\frac{\lambda}{\lambda_i}\right)\phi_i^*$$

$$\vdots \qquad (48)$$

$$\psi^{*(n)} = \sum_{i=1}^{\infty} a_i\left(\frac{\lambda}{\lambda_i}\right)^n \phi_i^*$$

As n gets larger, the fact that λ is the smallest eigenmode leads to the conclusion that the iteration process yields a $\psi^{*(n)}$ which approaches the first eigenmode solution to Eq. (32) since the fundamental mode has been taken out of the initial source by orthogonality considerations. That is:

$$\psi^{*(n)} \cong \phi_1^* \qquad (49)$$

The summation of the Neumann series has a convergence limit which is given by:

$$\Gamma^* = \sum_{n=0}^{\infty}\psi^{*(n)} = \sum_{n=0}^{\infty}\sum_{i=1}^{\infty} a_i\left(\frac{\lambda}{\lambda_i}\right)^n \phi_i^* \qquad (50)$$

which after exchanging summation orders and summing over n gives:

$$\Gamma^* = \sum_{i=I}^{\infty} a_i \frac{1}{(1-\lambda/\lambda_i)}\phi_i^* \qquad (51)$$

Its rate of convergence depends on the ratio λ/λ_1, since this determines how well the smallest term in the series representintation of $1-\lambda/\lambda_1$ is converged to the real value after N terms. The error is therefore given by:

$$\frac{1}{1-\lambda/\lambda_i} = \sum_{=0}^{N-1}\left(\frac{\lambda}{\lambda_i}\right)^n + \text{error of order}\left(\frac{\lambda}{\lambda_i}\right)^N \qquad (52)$$

For the method of successive approximations, we also get a final converged value of Γ^* given by Eq. (51) with a rate of convergence governed by Eq. (52). It should be noted that these convergence rates are of the same order as those for solving the fundamental mode equation, since in that case the solution is not converged until all higher eigenmodes die away. In the latter case, this also is governed by the separation between λ_1 and λ, and thus the error is of order $(\lambda/\lambda_1)^N$:

An upper limit to the number of iterations needed for convergence can be estimated by assuming Γ^* only has contributions from the first eigenmode. In this case:

$$\Gamma^* = a_i \phi_i^* \Big/ (1-\lambda/\lambda_i) \tag{53}$$

The error after N-1 iterations is gotten from the expansion of $(1-\lambda/\lambda_1)^{-1}$, as:

$$\Gamma^* = a_1 \phi_1^* \left[1 + \left(\frac{\lambda}{\lambda_1}\right) \cdots + \left(\frac{\lambda}{\lambda}\right)^{N-1} + \delta \right] \tag{54}$$

where the order of the error in the expansion is:

$$\delta \cong \left(\frac{\lambda}{\lambda_1}\right)^N \tag{55}$$

The result can be related to the convergence criteria given in Eq. (41) by the following manipulation:

$$\epsilon = \frac{\left\langle a_1 B^* \phi_1^* \right\rangle \delta}{\left\langle a_1 B^* \phi_1^* \left[1 + \frac{\lambda}{\lambda_1} + \cdots + \left(\frac{\lambda}{\lambda_1}\right)^{N-1} \right] \right\rangle} \cong \frac{\delta}{\left(1 - \frac{\lambda}{\lambda_1}\right)^{-1}} \cong \frac{\left(\frac{\lambda}{\lambda_1}\right)^N}{\left(1 - \frac{\lambda}{\lambda_1}\right)^{-1}} \tag{56}$$

Solving for N, we get finally:

$$N = \frac{\ell n \frac{1}{\epsilon} + \ell n \left(1 - \frac{\lambda}{\lambda_1}\right)}{\ell n \left(\frac{\lambda_1}{\lambda}\right)} \tag{57}$$

It is clear from Eq. (57) that as the separation between λ_1 and λ decreases the number of iterations increases logarithmically, a fact which should lead to quick solutions in "leaky" systems ($\lambda_1 >> \lambda$) and much slower convergence in large, absorption dominated systems ($\lambda_1 \cong \lambda$).

D. Fundamental Mode Contamination

From the preceding discussion, it should be clear that using the method of successive approximations restricts the solution of the generalized adjoint equation to only the particular solution within some error limits. This is easily seen from Eq. (50), if we allow $a_o \neq 0$. In this case:

$$\Gamma^* = \sum_{n=o}^{\infty}\sum_{i=o}^{\infty} a_i \left(\frac{\lambda}{\lambda_i}\right)^n \phi_i^*$$

$$= \sum_{n=o}^{\infty} a_o \phi^* + \sum_{i=1}^{\infty} a_i \frac{1}{1 - \lambda/\lambda_i} \phi_i^* \qquad (58)$$

After N iterations, the second term in Eq. (58) approximates the particular solution as before, but the first term, representing the buildup in the fundamental mode, is nonconvergent. That is:

$$\Gamma^{*(N)} = \sum_{n=0}^{N} a_o \phi^* + \sum_{i=1} a_i \phi_i^* \sum_{n=0}^{N} \left(\frac{\lambda}{\lambda_i}\right)^n$$

$$= N a_o \phi^* + \sum_{i=1}^{\infty} a_i \phi_i \left[\frac{1}{1 - \frac{\lambda}{\lambda_i}} + \delta_i\right] \qquad (59)$$

No matter how small the initial contamination (as measured by $|a_o|$), this mode builds up linearly with the number of iterations and eventually the solution degenerates into a fundamental mode adjoint solution which blows up as:

$$\lim_{N\to\infty} \Gamma^*(N) = Na_o\phi^* \tag{60}$$

Within the confine[illegible] the convergence criteria previously applied, the successive apprpxi[illegible]n scheme would indeed "converge" since the iteration procedure would terminate when:

$$\left| \frac{N\langle a_o B^*\phi^*\rangle - (N-1)\langle a_o B^*\phi^*\rangle}{N\langle a_o B^*\phi^*\rangle} \right| = \frac{1}{N} \leq \in \tag{61}$$

The solution, however, would be virtually a pure fundamental mode (i.e., $\Gamma^* \sim \phi^*$) and Γ^* would have no relationship whatsoever to the particular S^* used as the fixed source in this equation.

To guarantee a meaningful particular solution, the initial contamination must be made arbitrarily small so that after the N iterations needed to converge the particular solution, the fundamental contamination is still small. That is:

$$\left| N\langle a_o B^*\phi^*\rangle \right| << \in \tag{62}$$

A combination of Eqs. (36), (57), and (62) and some experience can be used to insure the initial contamination of the adjoint source S^* (its nonorthogonality to the fundamental mode) is small enough to insure convergence. However, since there are a number of sources of contamination, some of which are uncontrollable (numerical roundoff errors), it seems desirable to have an alternate way of handling this problem. The orthogonality condition given in Eq. (31) defining the stationary functional provides an easy method of eliminating fundamental mode contamination from Γ^*. To insure this orthogonality relationship with an arbitrarily contaminated adjoint Γ_a^*, one can simply apply an orthogonalization procedure to sweep out the contamination as follows:

$$\Gamma^* = \Gamma_a^* - \frac{\langle \Gamma_a^*, B\phi\rangle}{\langle \phi^*, B\phi\rangle}\phi^* \tag{63}$$

It is clear that Eq. (63) satisfies the orthogonality condition given in Eq. (31) irrespective of the nature or size of the contamination. This expression can be used to eliminate any contamination after a converged solution for Γ^* has been generated or it can be used in the iteration process itself to periodically sweep out any contamination which might have arisen in the course of the calculation. The latter sweep out is difficult to handle computationally and should only be done when it appears that the sources of contamination are large enough to prevent convergence from ever being achieved.

E. Adjoint S_n Equations

In the actual process of solving the generalized adjoint equation numerically, consideration has to be given to the present limitations of the S_n code ANISN. One point to note is that a great deal of effort has gone into eliminating negative fluxes and oscillations about zero from S_n solutions.[15] Both of these occurrences stem from the inadequacy of the diamond-difference scheme for flux extrapolations with course space and angle mesh spacings. Flux fixups involving hybrid-difference schemes are generally used in these cases.[15] For generalized adjoint problems, however, the very nature of the adjoint source (i.e., its being orthogonal to the fundamental mode, an everywhere positive function) requires the generalized flux to be both positive and negative in the solution space. This necessitates the elimination of flux fixup schemes and the use of only pure differencing techniques despite their drawbacks. The coarse mesh acceleration schemes must also be carefully checked and modified where necessary since they are sometimes ill behaved with fluxes that change sign. A tighter range of allowable coarse mesh rescaling coefficient values appears to be sufficient for our present needs in this regard. It is expected that as the need arises, development work can be undertaken to remove these restrictions. There is certainly nothing conceptually difficult, for instance, about separating positive and negative flux solutions arising from the positive and negative components of the fixed source in the actual solution process in each outer iteration. The two components can then be treated with the full S_n

capabilities available for any fixed source calculation with no complications. The process is simply laborious, and until the need arises we will not pursue such a course.

A more fundamental deficiency of the S_n method for solving the generalized equations is the non-adjointness of the difference equations which arise when a diamond-differencing scheme is applied to the leakage operator in the Boltzmann equation. This fundamental concern has been discussed in some detail by Carlson.[16] The consequence of concern to us of the non-adjointness of the equations is the fact that the errors involved give rise to unphysical boundary source terms in each space-angle mesh cell which contribute fundamental mode contamination to the solution. Carlson has investigated the order of magnitude of these terms and concluded that they are quite small for k calculations. The fact that we deal with distributed sources and reactor parameters that are spatially localized heightens our concerns over the adjointness of the equations. While k might be unaffected, the spatial flux itself is certainly orders of magnitude more sensitive to the difference scheme adjointness, and since contamination of the order of 10^{-3} is cause for alarm in our case (this is the order of the convergence criteria ε) the non-adjointness is a serious problem.

Three approaches can be taken to mitigate this problem. In the first place as is done in all shielding problems, the forward and adjoint flux runs can be converged to very stringent criteria with respect to the space and angular meshes used to model the system. This mesh convergence substantially reduces the order of the non-adjointness errors since these latter errors disappear in the limit of small mesh sizes.[16] For reactor sensitivity work, however, the order of error required for converged generalized solutions is much smaller and the meshes can become unreasonably fine. A second, and more practical alternative, involves the use of an anternate differencing scheme, "step mode" (available in ANISN) for solving reactor sensitivity problems. The "step mode" as will be shown below gives rise to adjoint difference equations, thus completely removing this cause of concern.

In the "step mode" the volume averaged flux $\overline{N}$ in a space-angle cell is assumed to be constant across the cell according to the following scheme:

$$\overline{N} = \begin{cases} N_{m+\frac{1}{2}} & \mu_{m>0} \\ N_{m+\frac{1}{2}} & \mu_{m<0} \end{cases} \tag{64}$$

Here conventional S_n notation[15] is used with m being an angular mesh point, i being a space mesh point, and the centered mesh point m, and i + (1/2) are left out of the equations to simplify the notation. Since the differencing scheme has no effect on the adjointness of any operator in the Boltamann equation other than the leakage operator and is independent of the energy variable,[16] we can illustrate the general result with a one-group leakage term only.

In S_n notation, the finite difference form of forward flux leakage term can be written as:

$$w\mu \left(A_{i+1} N_{i+1} - A_i N_i \right) + \alpha_{m+\frac{1}{2}} N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}} \tag{65}$$

The adjoint leakage is likewise given as:

$$- w\mu \left(A_{i+1} N^*_{i+1} - A_i N^*_{i+1} \right) - \alpha_{m+\frac{1}{2}} N^*_{m+\frac{1}{2}} + \alpha_{m-\frac{1}{2}} N^*_{m-\frac{1}{2}} \tag{66}$$

where ω and μ are quadrature weights and angles at the m^{th} centered angular point, the α's are the curvature coefficients, and the A's are the areas at the cell boundaries. Also, the α's and the A's satisfy the following condition:

$$\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} = -w\mu \left(A_{i+1} - A_i \right) \tag{67}$$

To check for adjointness, Eq. (65) is multiplied by $\overline{N}$ and Eq. (64) by $\overline{N}^*$, both are summed over all space and angle and then subtracted to get:

$$\sum_i \sum_m \Big\{ w\mu \bar{N}^* \left(A_{i+1} N_{i+1} - A_i N_i \right) + \alpha_{m+\frac{1}{2}} \bar{N}^* N_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} \bar{N}^* N_{m-\frac{1}{2}} \tag{68}$$

$$+ w\mu \bar{N} \left(A_{i+1} N^*_{i+1} - A_i N^*_i \right) + \alpha_{m+\frac{1}{2}} \bar{N} N^*_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} \bar{N} N^*_{m-\frac{1}{2}} \Big\}$$

Using the step difference relations given in Eq. (64) and their adjoint counterparts:

$$\bar{N}^* = \begin{cases} N^*_{m-\frac{1}{2}} = N^*_i & \mu_m > 0 \\ N^*_{m-\frac{1}{2}} = N^*_{i-1} & \mu_m < 0 \end{cases} \tag{69}$$

we can rewrite Eq. (68) as follows:

$$\sum_i \sum_m \left\{ w\mu \left(A_{i+1} N_{i+1} N^*_{i+1} - A_i N_i N^*_i \right) + w\mu \left(A_{i+1} - A_i \right) N_{i+1} N^*_i \right\} +$$

$\mu_m > 0$

$$\sum_i \sum_m \left\{ w\mu \left(A_{i+1} N_{i+1} N^*_{i+1} - A_i N_i N^*_i \right) + w\mu \left(A_{i+1} - A_i \right) N_i N^*_{i+1} \right\} + \tag{70}$$

$\mu_m < 0$

$$\sum_i \sum_m \left\{ \alpha_{m+\frac{1}{2}} N_{m+\frac{1}{2}} N^*_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} N_{m-\frac{1}{2}} N^*_{m-\frac{1}{2}} + \left(\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}} \right) N_{m+\frac{1}{2}} N^*_{m-\frac{1}{2}} \right\}$$

The first terms in all the expressions in braces when summed over i cancel out for all points internal to the system. In addition, with anti-symmetric boundary conditions (for the forward and adjoint fluxes), such as the conventional vacuum boundary conditions, the remaining surface terms cancel out. We finally are left with:

$$\sum_i \sum_m \left[w\mu \ (A_{i+1} - A_i) \begin{cases} N_{i+1} N_i^* & \mu_m > 0 \\ N_i N_{i+1}^* & \mu_m < 0 \end{cases} \right] + (\alpha_{m+\frac{1}{2}} - \alpha_{m-\frac{1}{2}}) N_{m+\frac{1}{2}} N_{m-\frac{1}{2}}^* \quad (71)$$

Using the expression for the α's given in Eq. (67), we can write:

$$\sum_i \sum_m w\mu \ (A_{i+1} - A_i) \begin{cases} N_{i+1} N_i^* - N_{m+\frac{1}{2}} N_{m-\frac{1}{2}}^* & \mu_m > 0 \\ N_i N_{i+1}^* - N_{m+\frac{1}{2}} N_{m-\frac{1}{2}}^* & \mu_m < 0 \end{cases} . \quad (72)$$

Converting back to expressions in $\overline{N}$ and $\overline{N}^*$ only, using the step difference relations, we see that everything cancels out:

$$\sum_i \sum_m w\mu \ (A_{i+1} - A_i) \ (\overline{NN}^* - \overline{NN}^*) = 0 \quad (73)$$

The step-difference scheme thus results in adjoint numerical equations as opposed to the conventional diamond-difference scheme in which terms similar to those in braces in Eq. (72) do not cancel out. This property of step-difference eliminates the numerical difference scheme as a source fundamental mode contamination in solving the generalized adjoint equation.

The final alternative, and the easiest of all to implement, involves using slab geometry models of the reactor system being studied. The adjoint difference equations in this geometry retain their adjointness property using any differencing scheme. This fact is discussed at some length by Carlson and will therefore not be repeated here. Since one-dimensional reactor mockups only are being discussed here, the slab model may be the least objectional of the alternatives for cylindrical reactors, with step differencing a possible alternative for spherical systems.

In conclusion, without further modification of any of the existing coding in ANISN, one can employ step-difference schemes or slab geometry and any differencing scheme, together with the method of successive approximations with a positive and negative valued source for reactor sensitivity analysis. A fundamental mode sweep-out at the end of an ANISN run is recommended to remove any unnecessary homogeneous equation solution terms from the answers. In addition, fairly tight convergence criteria are recommended for the critical forward and adjoint solutions (which must also be run in step-difference mode if the generalized flux solutions are run in this mode) so that the initial source contamination will not interfere with the convergence in the generalized forward and adjoint runs. For more advanced reactor studies, further development work on adjoint differencing schemes is indicated and should be pursued.

IV. UNCERTAINTY ANALYSIS

Having spelled out the procedures for determining sensitivity functions for reactor problems, it is now possible to discuss the methods by which this information is combined with cross-section uncertainty data to predict uncertainties in reactor parameters. This connection can be described most simply in terms of a statistical analog calculation for determining parameter variances based on statistical data uncertainties. Such an approach then leads directly to a discussion of deterministic methods using cross-section variances for estimating reactor parameter variances.

A. Analog Uncertainty Analysis

To estimate the variance in a computed result R, that depends on a data base which has statistical uncertainties in it, a statistical analog computation can be made to evaluate the following defining expression for the variance of the parameter R:

$$V_R = \left\{ (R_n - \{R_n\})^2 \right\} \tag{74}$$

Here the variance of R, denoted by V_R, is the expectation value, denoted by { }, of samplings of the value of R (the n^{th} sample having a value R_n), based on the statistical nature of the uncertainties in the data base, and $\{R_n\}$ is the average or expectation value of R for all the samples. In computational terms, a correlated sampling from uncertainty distributions for the whole data base is made and a transport calculation using the sampled cross sections is carried out to get each R_n. The sampling process consists of picking the energy dependent cross-section value for each partial cross section from a normal distribution having a specified variance V_{σ_i} and an average value $\{\bar{\sigma}_i\}$ for the i^{th} cross section element. Consideration of the correlated nature of the cross-section data would be taken into account in choosing from the data set.

In terms of differences between R and the average value $\{R_n\}$ resulting from using a particular sampled cross-section data base, Eq. (74) can be rewritten as:

$$V_R = \left\{ \delta R_n^2 \right\} \tag{75}$$

where

$$\delta R_n = R_n - \{R_n\} \tag{76}$$

Rewriting this expression in terms of the R_n's being explicit functions of cross sections resulting from the sampling procedure (i.e. the set of $\Sigma_{i,n}$):

$$\delta R_n = R_n(\Sigma_{i,n}) - \left\{R_n(\Sigma_{i,n})\right\} \tag{77}$$

where the i subscript refers to the elements of the cross-section set in the n^{th} sample.

If we assume a linear relationship to exist between the data base elements and the result (a condition that was carefully preserved in the derivation of the sensitivity functions), then we can express δR_n in terms of sensitivity coefficients as follows:

$$\delta R_n = \sum_i \frac{\partial R}{\partial \Sigma_i} \delta \Sigma_{i,n} \tag{78}$$

where $\delta \Sigma_{i,n}$ is given as:

$$\delta \Sigma_{i,n} = \Sigma_{i,n} - \left\{ \Sigma_{i,n} \right\} \tag{79}$$

and the partial derivative is assumed to be invariant with n and equal to the value of $\partial R/\partial \Sigma_i$ computed with all $\Sigma_i = \{\Sigma_{i,n}\}$.

With these assumptions, the variance in R can be computed from Eq. (75) as:

$$V_R = \left\{ \left(\sum_i \frac{\partial R}{\partial \Sigma_i} \partial \Sigma_{i,n} \right)^2 \right\} = \sum_i \sum_j \left\{ \frac{\partial R}{\partial \Sigma_i} \frac{\partial R}{\partial \Sigma_j} \delta \Sigma_{i,n} \delta \Sigma_{j,n} \right\} \tag{80}$$

$$= \sum_i \sum_j \frac{\partial R}{\partial \Sigma_i} \frac{\partial R}{\partial \Sigma_j} \left\{ \delta \Sigma_{i,n} \delta \Sigma_{j,n} \right\}$$

In terms of sensitivity coefficients, P, relative variances, U, and covariances C, and the relative covariance matrix V, we can finally write:

$$U_R = \sum_i \sum_j P_{\Sigma_i} P_{\Sigma_j} V_{\Sigma_i, \Sigma_j} \tag{81}$$

where

$$P_{\Sigma_i} = \frac{\partial R \Big/ \left\{ R_n \right\}}{\partial \Sigma_i \Big/ \left\{ \Sigma_{i,n} \right\}} \tag{82}$$

$$V_{\Sigma_i,\Sigma_j} = \begin{cases} \left\{\delta\Sigma_{i,n}\delta\Sigma_{j,n}\right\} \Big/ \left\{\Sigma_{i,n}\right\}\left\{\Sigma_{j,n}\right\} = C_{\Sigma_i\Sigma_j} & i\neq j \\ \left\{\delta\Sigma^2_{i,n}\right\} \Big/ \left\{\Sigma_{i,n}\right\}^2 = U_{\Sigma_i} & i=j \end{cases} \tag{83}$$

$$U_R = \left\{\delta R_n\right\} \Big/ \left\{R_n\right\} \tag{84}$$

The final problem variance is thus given in terms of sensitivity coefficients P and a covariance matrix V. The sensitivity coefficients are calculated in the course of solving the regular and generalized flux equations using a mean value set of cross section data (denoted by $\Sigma_i = \{\Sigma_{i,n}\}$). The partial derivatives at these mean values are the required mean sensitivity coefficients. The covariance matrix likewise is evaluated using variances and covariances of the basic data around their mean.

The task of evaluating the full covariance matrix from basic nuclear data is a sizeable one, since correlations between elements must be calculated. An initial attempt will be made to take into account only the strongest and most important of these correlations as determined by preliminary sensitivity studies. Additional evaluation will be left for future studies after more information is available on which to base judgments on the need for more detail and accuracy.

It should be pointed out again that the form of Eqs. (78) and (81) necessitate to the use of linear (second-order accurate) approaches to calculating sensitivity coefficients. A consistent extension of these methods to higher order uncertainty estimates would require the evaluation of not only higher order sensitivity coefficients but also higher order moments of the uncertainty distributions in the basic nuclear data. Non-linear effects involved in the sensitivity coefficients should be

used only if the data uncertainty moments can be extended to higher order accuracy (a monumental task) and we therefore choose to remain consistent in ignoring higher order effects for these studies.

B. Multigroup Methods

For deterministic evaluation of parameter uncertainties, the expression for the parameter variance [i.e., Eq. (81)] must be computed from energy group averaged cross-section data. This requirement places an added burden on the cross-section uncertainty evaluator in that an effort must be made to convert pointwise data variances and covariances into group averaged data. Two major limitations inherent in such an effort are (1) the problem-dependent nature of the energy group structures and (2) the additional variances and covariances in the averaged cross-section data elements arising from the particular choice of a weighting function for group averaging. This latter consideration could be quite significant if the weighting function were a realistic problem flux spectrum which would then have structure in it correlated to some cross-section behavior for the problem. The flux would thus be correlated with the data it was averaging as well as having its own uncertainty bounds. We will ignore this consideration for the first sensitivity studies taking the weighting function to be a fixed, precisely known independent variable for the problems studied. The effect of weighting function uncertainties will certainly appear in later studies, however, as we narrow down the major sources of uncertainty in reactor parameters arising from basic cross-section data.

The effect of group structure will likewise be dealt with only as necessity dictates, in that initial correlations will be taken to be longer range than the anticipated fine group structures to be used for the study. Broad range variances and covariances are all that will be required for the fine group library we will use.

V. SUMMARY

A complete summary of the sensitivity code system being developed at ORNL based on transport theory appears in Fig. 1. The central chain in this flow chart consists of the ANISN transport calculations of normal and generalized fluxes using the methods outlined in this report. Results from this sequence couple with the sensitivity analysis package SWANLAKE in two stages (indicated by SWANLAKE I and II). The first stage consists of a normal analysis of all relevant cross-section data and the second an analysis with k-reset options in effect.

The left-hand chain represents the flow of uncertainty estimation procedures, starting with evaluation of basic uncertainty data from cross-section measurements and leading to the creation of the ENDF/B-IV error file and the processing of these files into multigroup covariance matrices. Both of these chains link up in an uncertainty analysis package where estimates of reactor parameter uncertainties are made. This final stage will contain multiple analysis options to allow the overall parameter uncertainty to be broken down into various components while still maintaining all data correlation information.

Finally in the right-hand chain the linking up of processed cross-section information (including complete files of partial cross sections) and auxilliary codes for creating general operators is illustrated. Processed cross-section data and various cross-section operators are needed at all stages of calculation in the central chain.

It is hoped that when the transport sensitivity analysis capability is fully operating and some experience has been gained through analysis of several problems we will be able to eliminate many of the restrictions on the methods employed. Hopefully an alternative P_1-diffusion theory system can be deployed as a result of successful development of the transport system.

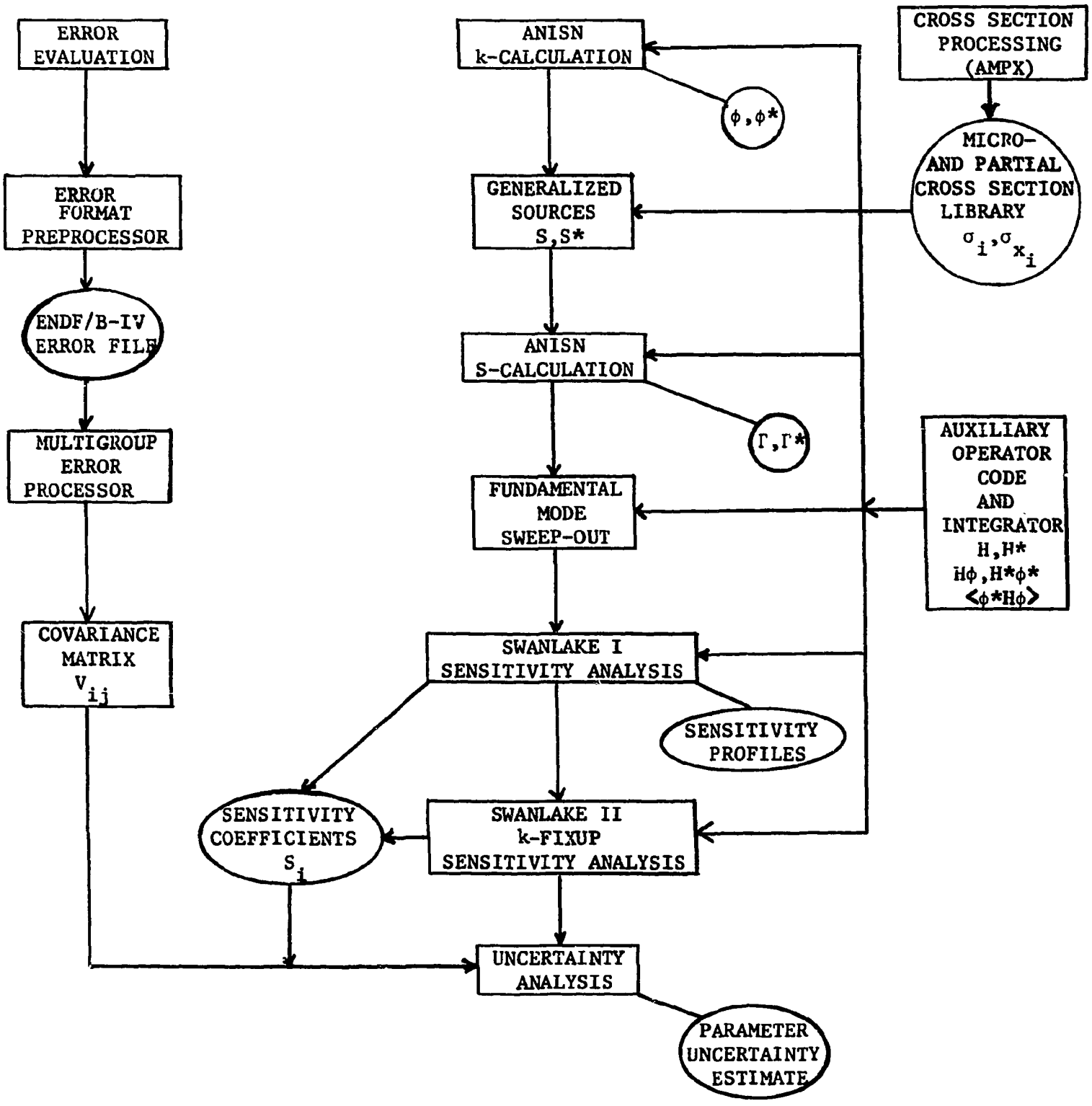

Fig. 1. Flow Diagram of Reactor Sensitivity Analysis Procedures

APPENDIX A. OPERATORS FOR PARTICULAR REACTOR PARAMETERS (R)

$$\text{Bilinear ratio:} \quad R = \frac{\langle \phi^* H_1 \phi \rangle}{\langle \phi^* H_2 \phi \rangle}$$

$$\text{Linear ratio:} \quad R = \frac{\langle H_1 \phi \rangle}{\langle H_2 \phi \rangle}$$

R	$H_1\phi$	$H_2\phi$
Breeding ratio (linear)	$\sum_i \Sigma_{c_i} \phi$ capture in fertile isotopes	$\sum_i (\Sigma_{f_i} + \Sigma_{a_i})\phi$ absorption and fission in fissile isotopes
Reactivity worth (bilinear)	$\Delta A\phi' - \lambda \Delta B\phi'$ Δ denotes material change involved in worth measurement *Note $\phi' \simeq \phi$	$B'\phi'$ perturbed fission source *Note $B' \simeq B$ and $\phi' \simeq \phi$
Doppler effect (bilinear)	$\Delta A\phi - \lambda \Delta B\phi$ Δ denotes temperature induced changes in all material cross sections based on two temperatures T_1 and T_2.	$B\phi$ fission source

Defining equations for transport operators in multigroup form are given as:[11,15]

$$A\phi = \Sigma_{T_g} \phi_g - \sum_\ell \sum_m \frac{2\ell+1}{4\pi} \sum_{g'} \Sigma^\ell_{g' \to g} \phi^{\ell m}_{g'} Y^{\ell m}(\bar{\Omega}) + \bar{\Omega} \cdot \nabla \phi_g \qquad \text{(A.1)}$$

$$B\phi = \chi_g \sum_{g'} (\nu \Sigma_f)_{g'} \phi^o_{g'} \qquad \text{(A.2)}$$

APPENDIX B. GENERALIZED PERTURBATION THEORY SOURCES

Forward source $S \equiv \frac{dR}{d\phi^*}$

Adjoint source $S^* = \frac{dR}{d\phi}$

R	S*	S
Breeding ratio (linear)	$R\left[\frac{\Sigma_1}{\langle\Sigma_1\phi\rangle} - \frac{\Sigma_2}{\langle\Sigma_2\phi\rangle}\right]$ *Note: $H_1 = \Sigma_1$ $H_2 = \Sigma_2$	NONE
Reactivity worth and Doppler effect (bilinear)	$R\left[\frac{H_1\phi}{\langle\phi^*H_1\phi\rangle} - \frac{H_2\phi}{\langle\phi^*H_2\phi\rangle}\right]$	$R\left[\frac{H_1^*\phi^*}{\langle\phi^*H_1\phi\rangle} - \frac{H_2^*\phi^*}{\langle\phi^*H_2\phi\rangle}\right]$

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