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Specifications for VARI3D — A Multidimensional Reactor Design Sensitivity Code

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Specifications for VARI3D — A Multidimensional Reactor Design Sensitivity Code

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Specifications are outlined for a computer code, VARI3D, which will perform sensitivity calculations for reactor design studies. Generalized perturbation theory will be used to calculate perturbations to ratios of reaction rates and reactivity worths. For diffusion theory models the input to the code can be in terms of the engineering design of a reactor. Besides the user-specified model changes VARI3D will, optionally, determine additional changes subject to a certain number of simple constraints. The output will be in the form of sensitivities of performance parameters to changes in the original reactor model.

I. INTRODUCTION

The traditional method of calculating the sensitivity of parameters of interest in reactor design and analysis with respect to changes in the reactor model has been to calculate those parameters for each change and to determine the sensitivities by subtraction. This straightforward approach is satisfactory when only a few changes are involved and when design models are fairly simple. It becomes expensive in terms of both human and computer time, however, in studies including many model changes, when the models are complicated, or when convergence requirements on each physics calculation must be tight.

A wide class of design parameters are defined as, or can be defined in terms of, ratios of weighted integral reaction rates. The eigenvalue and ordinary, first-order perturbation theory reactivity worths can be expressed as adjoint-weighted, integral reaction rate ratios. The instantaneous breeding ratio and region power fractions are unity-weighted reaction rate ratios. For this class of parameters generalized perturbation theory provides a method of calculating first-order perturbations accurately and inexpensively.[1-4]

A program, VARI-1D, is available which applies generalized perturbation theory in one dimension to neutron diffusion problems.[5] The code has been used in a number of applications for reactor physics analysis.[6-9]

These specifications describe a computer program, VARI3D, which is intended to meet two general objectives:

(1) to extend the sensitivity analysis capabilities already available in VARI-1D to two and three dimensions; and

(2) to integrate the sensitivity calculation into core design procedures by the addition of input and output routines which read design model descriptions and edit sensitivities in terms of the engineering design changes to the core.

The primary goal is a set of program blocks which treats the open-loop system: the plant components outside the reactor and the associated operating economics will not be included in the first-generation code.

The sensitivities produced by the code can, of course, be used in subsequent plant calculations. We feel it is important to limit the scope of the initial calculation to the reactor alone, at least until experience with the code is accumulated.

The initial code will be written for time-independent calculations. This will mean, for example, that only instantaneous breeding ratios will be treated directly; definitions of breeding ratio which require inventories at different times in a fuel cycle cannot be handled explicitly by a time-independent calculation. VARI3D can be used, however, to do static, branch calculations at several times in a fuel cycle to determine instantaneous sensitivities of isotope production and destruction rates to design model changes. In this way the code can be used to estimate sensitivities for time-dependent (fuel cycle) problems. A methods development effort is planned to establish procedures for applying VARI3D output to burnup calculations.

Generalized perturbation theory can be extended to time-dependent problems, but this will require a major effort beyond the time-independent case. If it turns out to be unduly difficult to treat fuel cycles adequately with the first version of VARI3D the time-dependent calculation, and a certain amount of associated methods development, would be given high priority for a second-generation code.

The diffusion-theory difference equations treated by the code will be the mesh-block-centered form and will, therefore, be compatible with other codes used by the LMFBR community (DIF2D, 2DB, 3DB, VENTURE). The communication of data will be by CCCC (Committee on Computer Code Coordination) file structures, and the CCCC coding conventions will be observed.[10]

II. CODE USAGE AND GENERALIZED PERTURBATION THEORY

A sensitivity calculation is the determination of the effect on what we will call a performance parameter of a change, or a set of changes, to a model of a design. Performance parameters which will be treated by

VARI3D are discussed in Section IV and include such quantities as breeding ratio, cell power fraction, peak temperature, and a variety of reactivity coefficients. In several cases they require data from both physics and thermal-hydraulics calculations.

The model changes involved in sensitivity calculations will be divided into two categories: Independent model changes are specified directly by the code user and might be a change in a pin diameter, the isotopic composition of the fuel, the microscopic cross sections, etc. Dependent model changes are additional changes determined by the code itself in order to satisfy certain constraints specified by the user. Two such constraints might be conservation of flow rate and conservation of reactivity, and the corresponding dependent model changes might be, respectively, a change in the cell size to preserve coolant volume and a change in the fuel loading. Model changes and constraints are listed in Section V.

The nature of generalized perturbation theory is such that the number of neutron diffusion-theory calculations required depends only on the number of performance parameters of interest, not on the number of model changes. For each individual performance parameter (e.g. a breeding ratio or reactivity worth) one or two additional neutron diffusion problems must be run to generate special adjoint functions. Each subsequent model change requires only the evaluation of a set of numerical integrals. Compared with that of a diffusion theory calculation, the computer time required for a set of integrals is relatively small. The break-even point in comparing the economics of using perturbation theory or simply rerunning an entire problem is probably two or three changes.

Figure 1 shows schematically the flow of a hypothetical VARI3D calculation in terms of input and output quantities. Suppose a base model has been specified and it is of interest to determine the sensitivity of the instantaneous breeding ratio to simultaneous changes in clad thickness and fuel pellet diameter. These are two independent model changes; the magnitudes, M_1 and M_2, are specified by the user. To preserve the original eigenvalue the user directs VARI3D to alter the ^{239}Pu volume fraction in the fuel to compensate for the net reactivity worth of the first two

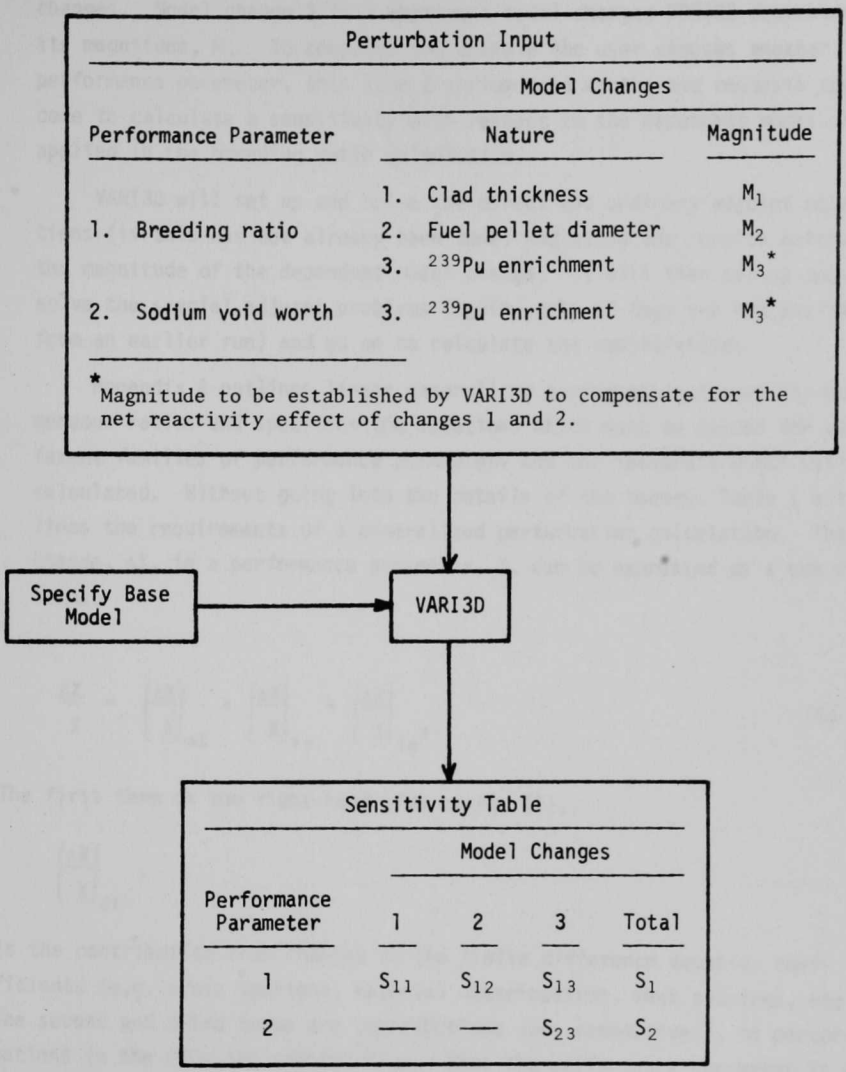


Fig. 1. The flow of a hypothetical VARI3D run. The sensitivity table lists the change (S_{ij}) in a performance parameter (i) due to a change in the model (j). S_{21} and S_{22} were not requested in the input. Model change 3 is a dependent model change. The net sensitivity (S_i) of each performance parameter to all model changes is the sum over the columns in the table.

changes. Model change 3 is a dependent model change; VARI3D determines its magnitude, M_3. To complete the example the user chooses another performance parameter, this time a sodium-void worth, and requests the code to calculate a sensitivity with respect to the dependent model change applied in the breeding ratio calculation.

VARI3D will set up and solve the direct and ordinary adjoint equations (if this has not already been done) and using the results determine the magnitude of the dependent model change. It will then set up and solve the special adjoint problems (again, only if they are not available from an earlier run) and go on to calculate the sensitivities.

Appendix A outlines linear generalized perturbation theory for homogeneous ratios and specifies the equations which must be solved for different families of performance parameters and the integrals which must be calculated. Without going into the details of the theory, Table I outlines the requirements of a generalized perturbation calculation. The change, ΔX, in a performance parameter, X, can be expressed as a sum of terms:

$$\frac{\Delta X}{X} = \left(\frac{\Delta X}{X}\right)_{\delta\Sigma} + \left(\frac{\Delta X}{X}\right)_{\delta\phi} + \left(\frac{\Delta X}{X}\right)_{\delta\phi^*} . \qquad (1)$$

The first term on the right-hand side of Eq. (1),

$$\left(\frac{\Delta X}{X}\right)_{\delta\Sigma} ,$$

is the contribution from changes in the finite difference equation coefficients (e.g. cross sections, material distributions, mesh spacings, etc.). The second and third terms are contributions due, respectively, to perturbations in the flux and adjoint flux. When the performance parameter is a simple reaction rate ratio (e.g. instantaneous breeding ratio), the ordinary adjoint does not enter the problem and the third term does not exist. In ordinary perturbation theory, where the object is to calculate the change in an eigenvalue, the second and third terms vanish to first-order.

TABLE I

Requirements for Calculating Changes to a Performance Parameter, X, Using Generalized Perturbation Theory

Parameter	$\frac{\Delta X}{X} = \left(\frac{\Delta X}{X}\right)_{\delta\Sigma} + \left(\frac{\Delta X}{X}\right)_{\delta\phi} + \left(\frac{\Delta X}{X}\right)_{\delta\phi^*}$ Require Functions			Required Integrals
Eigenvalue	ϕ^*,ϕ	——	——	$\int \phi^{*T}\delta\Sigma\phi$
Reaction rate ratios (e.g. breeding ratio, capture-to-fission ratios)	ϕ	Γ^*,ϕ	——	$\int \delta\Sigma\phi$, $\int \Gamma^{*T}\delta\Sigma\phi$
Reactivity worths (e.g. sodium-void worth)	ϕ^*,ϕ	ϕ^*,Γ	Γ^*,ϕ	$\int \phi^{*T}\delta\Sigma\phi$, $\int \phi^{*T}\delta\Sigma\Gamma$, $\int \Gamma^{*T}\delta\Sigma\phi$

Table I lists three families of performance parameters and the additional functions required to calculate perturbations. ϕ is the direct flux solution of the base case (unperturbed) model. ϕ^* is the ordinary adjoint function for the base case model. Both ϕ and ϕ^* are currently available from most diffusion theory codes. Γ^* and Γ are special adjoint functions associated with each performance parameter. A Γ^* associated with a breeding ratio is entirely different, and must be calculated separately, from a Γ^* associated with a sodium-void reactivity coefficient. On the other hand, the more familiar ϕ and ϕ^* are always the same and are calculated only once.

It is important to emphasize that generalized perturbation theory is a linear approximation (linear in changes to the coefficients of the neutron diffusion equation, that is) and to understand some of the consequences. Because of the linearity, perturbations in performance parameters due to any number of simultaneous model changes (independent and/or dependent) are additive. Permitting dependent model changes is a convenience to the VARI3D user and is not an essential element of the calculation. A dependent model change could as well be determined outside of VARI3D (e.g. by calculating a compensating reactivity change using an ordinary perturbation theory code) and supplied to VARI3D as an additional independent model change.

To illustrate this point consider the following sequence of calculations. Suppose that the user wishes to calculate the consequences of changing a particular cross section by 5%. At the same time he wants to change the fuel loading so that the net effect of the cross section and loading changes is to conserve the eigenvalue. VARI3D will use ordinary, first-order perturbation theory to determine the reactivity perturbation caused by the 5% cross-section change. Similarly, VARI3D will calculate the reactivity perturbation for a loading change on a per-unit basis and then, by scaling, determine a specific loading change to exactly balance the reactivity perturbation of the cross-section change. There will be no iterations; the assumption is made that linear perturbation theory is valid. Now if the user wants to make a 10% cross-section change under the same constraint he simply doubles all the performance parameter sensitivities calculated in the first pass through the code. There is no need to return to VARI3D to repeat any part of the calculation.

VARI3D is not intended to perform an optimization of a core design; it is probably not possible to write an optimization code that would satisfy a significant fraction of the requirements of all the design groups in the fast reactor community. VARI3D is intended to provide data, in the form of sensitivities, that can be used in individual optimization studies.

III. INPUT AND OUTPUT CONSIDERATIONS

Discussions with designers and analysts have made it clear that VARI3D must be flexible in the way it accepts model descriptions and model changes. We have identified four separate, optional procedures for inputting geometry and loading data. Figure 2 shows a flow diagram of the proposed code, including how the four input options interface.

Under the first option the user would describe the reactor in terms of the engineering design. The dimensions and isotopic compositions of the fuel pins, clad, coolant, fuel assembly can, and other basic components will be input on cards, along with the specification of how the assemblies are put together to form a core. The program will convert this description into a neutronics model by homogenizing the fuel assemblies and superimposing a finite-difference mesh. A neutronics model will be defined for the unperturbed case and for each model change and will be represented by a set of binary files (GEØDST, NDXSRF and ZNATDN) in the formats defined by the CCCC (Committee on Computer Code Coordination). Admittedly, this means a proliferation of data files, but it also allows one to define the interfaces in the code in a way which accommodates the other input options.

The second input option permits the neutronics description to be input directly on cards; in this mode of operation the code avoids all reference to an engineering description of the core. The homogenization of the model is done externally by the user, and the description of the core model and model changes is given in terms of the kinds of data required currently by standard, stand-alone diffusion theory codes. The sensitivity code will convert the card input into sets of GEØDST, NDXSRF and ZNATDN binary data files.

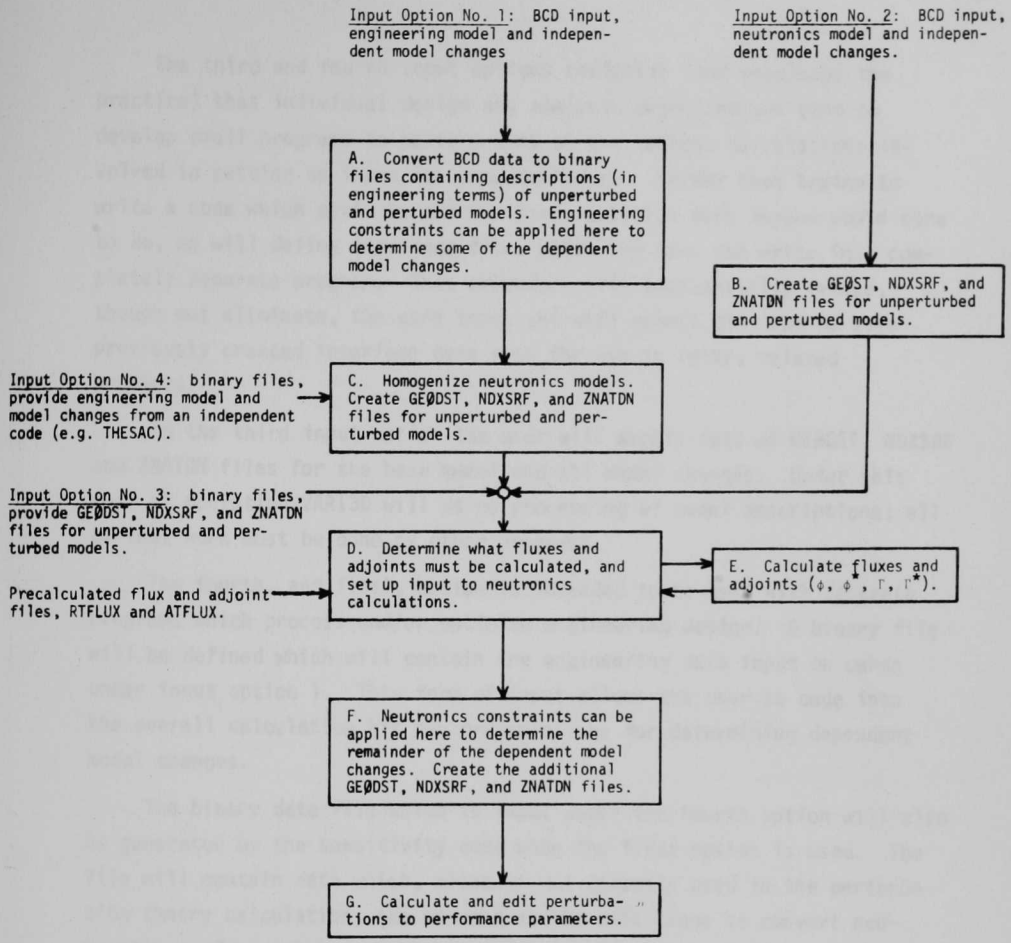
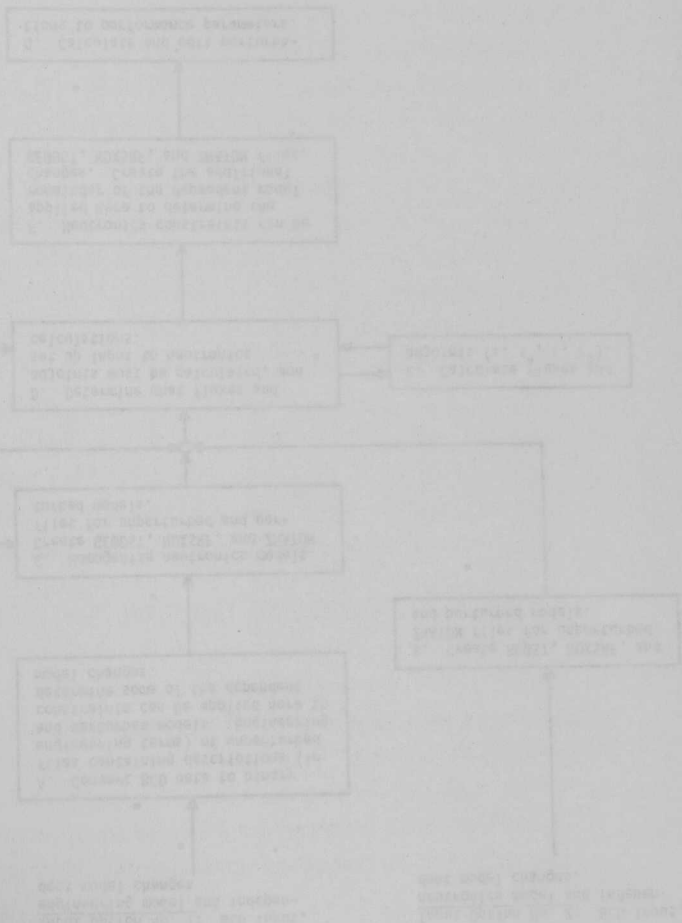


Fig. 2. Flow diagram of the proposed core performance sensitivity code VARI3D.



The third and fourth input options recognize (and encourage the practice) that individual design and analysis organizations tend to develop small programs to perform many of the tedious calculations involved in setting up input for computer codes. Rather than trying to write a code which performs all the precalculation work anyone would care to do, we will define interface files which the user can write in a completely separate program. This procedure will substantially reduce, though not eliminate, the card input and will permit the user to save previously created interface data sets for use in later, related problems.

In the third input option the user will supply sets of GEØDST, NDXSRF and ZNATDN files for the base model and all model changes. Under this mode of operation VARI3D will do no processing of model descriptions; all of that work must be done by other programs.

The fourth, and final, option is intended to be used with separate programs which process and/or optimize engineering design. A binary file will be defined which will contain the engineering data input on cards under input option 1. This form of input allows the user to code into the overall calculation his own prescriptions for determining dependent model changes.

The binary data file which is input under the fourth option will also be generated by the sensitivity code when the first option is used. The file will contain data which, although not directly used in the perturbation theory calculation, can be used at the edit stage to convert neutronics performance parameters to thermal-hydraulic equivalents. For example, total power and inlet coolant temperatures will not normally affect the perturbation calculation of cell or local power fractions but can be used to translate the result into changes in temperature and heat flux.

The calculated sensitivities can be edited by detailed distribution, by region, by zone (composition) or over the full core. At the user's option the pertubation can be broken down by components of the change (leakage, absorption, fission, etc.). Detailed edits of this nature are

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sometimes useful in analysis in understanding the physics associated with a model change. All but the most basic output will be optional, with the user in control. The edits associated with the input processing will include complete inventories and a description of the base model, and the output will include fuel destruction and production rates.

IV. PERFORMANCE PARAMETERS

The following is a list of performance parameters whose sensitivities to model changes are of interest in various phases of core design and analysis and which should be included in a first-generation code. The first three parameters are mathematically similar; they are ratios of integral reaction rates. The next four are all reactivity worths of one sort or another.

(1) The ratios of local or region reaction rates, by isotope or zone and by reaction type. Measurements of this type are routinely made in critical experiments and used to evaluate the accuracy of calculational methods (e.g. capture-to-fission ratios).

(2) Breeding ratios, by region or over the whole model. Discussions with designers and analysts indicate some disagreement over a useful definition of breeding ratio. Since this code is time-independent, and, therefore, cannot explicitly treat the fuel cycle, we will use the following definition for an instantaneous breeding ratio:

$$BR = \frac{^{238}U + ^{240}Pu \text{ Capture Rate}}{^{239}Pu + ^{241}Pu \text{ Absorption Rate}} .$$

Users who prefer other definitions will be able to specify their own breeding ratio by using the general reaction rate ratio option given in paragraph (1). There seems to be nearly total disagreement about a definition for doubling time. The only legitimate number a time-independent code can produce is an instantaneous, core doubling time based on breeding gain (BG = BR - 1), the rate at which fissile material is consumed and the core inventory of fissile material.

$$DT = \frac{^{239}Pu \text{ and } ^{241}Pu \text{ Core Inventory}}{(BG) \times (^{239}Pu + ^{241}Pu \text{ Absorption Rate})} .$$

Losses due to reprocessing can be included as a single, multiplicative constant. The corresponding compound core doubling time and inventory doubling times (which will require fuel cycle parameters supplied by the user) will also be edited.

(3) The ratio of a local reaction rate to a model-wide integral reaction rate, by isotope or zone and by reaction type. Depending on the reaction type chosen, this parameter might represent a peak-to-average power or pin heat flux, the irradiation of a component of the core or (if we extend "local" to include an entire region) a power fraction. Performance parameters of this type are important in thermal-hydraulic analysis and can be related directly to thermal-hydraulic parameters.

(4) Small sample reactivity worths at particular locations. These quantities are of interest in critical experiment analysis.

(5) Reactivity worths associated with physical changes (e.g. due to temperature) to the materials making up the core. These include Doppler reactivity worths.

(6) Reactivity worths associated with the removal or addition of material. Sodium-void worths for LMFBRs and helium and steam worths for GCFRs fall under this category, as do fuel and clad worths of interest in safety studies and assembly replacement worths.

(7) Control rod worths.

(8) β_{eff} and other kinetics-related parameters.

(9) Changes to the eigenvalue will be calculated. In this case the generalized perturbation theory reduces to the usual, first-order perturbation theory.

V. MODEL CHANGES

Model changes of several types may be of interest. The most frequently studied are deliberate design changes and include:

(1) Loading changes within a fixed geometry leading to changes in the number densities of isotopes.

(2) Changes to the geometry itself, such as modifications of fuel pin dimensions, clad thickness or even the overall size of fuel assemblies.

Other changes arise in sensitivity studies of the modeling procedure itself:

(1) Uncertainties in the dimensions and compositions of the core components due to manufacturing tolerances, swelling, and creep. These might affect the physics model not only through number density changes but also through changes in the size of the finite-difference mesh used in the calculations.

(2) Uncertainties in the microscopic, broad-group cross-section data by isotope, energy group, and reaction type.

Finally, there are feedback mechanisms which alter the model; for example, changes in isotopic number densities due to thermal expansion.

Particularly the first class of changes may be subject to criticality or thermal-hydraulic constraints. Dependent model change options planned for VARI3D include:

(1) Preservation of the eigenvalue. The code will determine by ordinary, first-order perturbation theory the magnitude of the dependent model change necessary to assure that there is no net reactivity change. The code will then calculate the effect on the performance parameter of both the dependent and independent model changes.

(2) Preservation of cross-sectional flow area in an assembly. The user will specify the nature of the dependent model change (e.g. the fuel assembly dimensions and the code will determine the magnitude.

We clearly cannot anticipate all the combinations of constraints that are desirable in design studies; VARI3D will be structured to make it as easy as possible for users to supply their own coding to do these calculations. This is the main reason for the fourth input option (see Section III).

Two quantities which will <u>not</u> be allowed to change are the number of energy groups and the number of finite-difference mesh intervals.

VI. CODE COMPONENTS

The code structure breaks down into three areas. These are relatively independent code blocks, or sets of code blocks, which communicate by a combination of CCCC standard files and scratch files. A schematic diagram of the logic flow of the code is given in Fig. 2.

(1) The input processor (boxes A, B, and C). This coding reads the model description, either in terms of the engineering design or in terms of the homogenized neutronics model, as well as the specifications of performance parameters and model changes. Under input options 1 and 4 it will perform the material homogenization and set up the physics calculational model.

(2) Flux and adjoint solutions (boxes D and E). This coding sets up and solves the flux and adjoint equations required by generalized perturbation theory and is the most time-consuming part of the calculation. However, if the resulting functions are saved, perturbations to the same performance parameter due to several different types of model changes can be calculated without returning to this part of the code. At the core of this code block is a diffusion theory calculation.

(3) Edits (boxes F and G). This code block performs two types of calculations in addition to editing the results. First, it determines the sensitivities of the performance parameters for specific model changes. In the process the code will, at the user's option, determine and include reactivity-compensating, dependent model changes intended to preserve the critical eigenvalue. Second, it converts those sensitivities, which initially are in terms of the physics model, into thermal-hydraulic parameters where prescriptions or correlations are available.

A suggestion has been made (Ref. 11) to include an iteration between boxes F and G to perform an optimization of a user-specified, nonlinear set of constraint relations. The function that this type of calculation would provide is, in large part, already permitted by the code structure shown in Fig. 2.

In the first place, Section II points out that, since generalized perturbation theory is a linear approximation, the sensitivities can easily be scaled up and down with the magnitudes of the model changes.

VARI3D can be used to supply one set of sensitivities (on a per-unit-change basis) which can be used in constraint equations in a stand-alone code; it is not necessary to include VARI3D inside the optimization loop.

Secondly, if for any reason it is necessary to return to VARI3D in a loop it may be simplest to loop back to the beginning of the code and to employ the fourth input option. Coding could be added to an optimization program to change the contents of the appropriate binary files. With the fluxes and adjoints already calculated, only boxes C, F, and G will be accessed.

As stated earlier, it is not our intention to write optimization procedures into the first version of VARI3D. We do intend to structure the input and output in such a way as to facilitate linkages with other codes used in design procedures.

APPENDIX A

The Generalized Perturbation Theory Equations

The following development of linear generalized perturbation theory was suggested by Martin Becker of RPI and is the most straightforward derivation available. What is presented here is not a complete treatment of the theory; our purpose is to show the genesis of the special adjoint functions and the nature of the required perturbation integrals. The total sensitivities (i.e. single numbers representing the changes in performance parameters brought about by model changes) will be available from VARI3D in both the linear form shown below and as the difference between variational estimates of the unperturbed and perturbed performance parameters as derived by Stacey.[3] Stacey's formulation includes some higher-order effects not included in the linear theory but which seem to be important only for very substantial model changes.

Definition of Terms. Treating the neutron diffusion difference equations as a matrix equation, the usual direct and adjoint eigenvalue equations are written,

$$[R - \lambda F]\phi = 0 , \tag{A-1}$$

$$[R - \lambda F]^T \phi^* = 0 . \tag{A-2}$$

The matrix R includes leakage, scattering, and absorption; F is the fission neutron source matrix; and λ is 1/k. When a change in made to the model R and F are perturbed,

$$R \rightarrow R + \delta R , \tag{A-3}$$

$$F \rightarrow F + \delta F . \tag{A-4}$$

As a consequence,

$$\phi \rightarrow \phi + \delta\phi , \tag{A-5}$$

$$\phi^* \rightarrow \phi^* + \delta\phi^* , \tag{A-6}$$

$$\lambda \rightarrow \lambda + \delta\lambda , \tag{A-7}$$

and, to first order, Eqs. (A-1) and (A-2) become,

APPENDIX A

The Generalized Perturbation Theory Equations

$$[R - \lambda F]\delta\phi + [\delta R - (\delta\lambda)F - \lambda(\delta F)]\phi = 0 , \tag{A-8}$$

$$[R - \lambda F]^T\delta\phi^* + [\delta R - (\delta\lambda)F - \lambda(\delta F)]^T\phi^* = 0 . \tag{A-9}$$

Reaction Rate Ratios. Consider the homogeneous functional,

$$X = \frac{H^T\phi}{G^T\phi} . \tag{A-10}$$

H and G are vectors and $H^T\phi$ and $G^T\phi$ represent numerical integrations. When H and G are perturbed the result, again to first order, can be written

$$\delta X\left[G^T\phi\right] = [\delta H - X(\delta G)]^T\phi + \delta\phi^T[H - XG] . \tag{A-11}$$

Now multiply (on the left) Eq. (A-8) by a yet-to-be-defined vector Γ^{*T} and transpose the first term.

$$\delta\phi^T[R - \lambda F]^T\Gamma^* + \Gamma^{*T}[\delta R - (\delta\lambda)F - \lambda(\delta F)]\phi = 0 . \tag{A-12}$$

Add Eqs. (A-11) and (A-12).

$$\delta X\left[G^T\phi\right] = \left\{\delta H^T - X(\delta G)^T + \Gamma^{*T}[\delta R - (\delta\lambda)F - \lambda(\delta F)]\right\}\phi$$

$$+ \delta\phi^T\left\{H - XG + [R - \lambda F]^T\Gamma^*\right\} . \tag{A-13}$$

We can eliminate all references to the perturbation in the flux, $\delta\phi$, by requiring that Γ^* be the solution of

$$[R - \lambda F]^T\Gamma^* = -H + XG , \tag{A-14}$$

in which case the perturbation to the ratio X is given by

$$\delta X = \frac{\left\{\delta H^T - X(\delta G)^T + \Gamma^{*T}[\delta R - (\delta\lambda)F - \lambda(\delta F)]\right\}\phi}{\left[G^T\phi\right]} , \tag{A-15}$$

If one has specified the model change in such a manner that there is no net reactivity change, the term involving $\delta\lambda$ in Eq. (A-15) identically vanishes. If not, $\delta\lambda$ can be evaluated by ordinary, first-order perturbation theory.

The operator in Eq. (A-14) represents a critical system, and so it is necessary that the fixed source -H + XG be orthogonal to the fundamental mode, ϕ. That this is true can easily be seen by multiplying $[-H + XG]^T$ (on the right) by ϕ and recalling the definition of X [Eq. (A-10)]. Because of roundoff this orthogonality condition cannot be precisely met in a numerical calculation, and this situation must be watched as a potential source of problems.

Bilinear Ratios. Consider the homogeneous functional,

$$X = \frac{\phi^{*T} H \phi}{\phi^{*T} G \phi} . \tag{A-16}$$

H and G are now matrices. The derivation proceeds as in the case of the reaction rate ratio, but an additional special adjoint must be used. To first-order, a perturbation to Eq. (A-16) yields

$$\delta X\left[\phi^{*T} G \phi\right] = \left(\delta\phi^{*T}\right)[H - XG]\phi + \phi^{*T}[\delta H - X(\delta G)]\phi + \phi^{*T}[H - XG](\delta\phi) . \tag{A-17}$$

Multiply Eq. (A-8) by Γ^{*T}, multiply Eq. (A-9) by Γ^{T}, and combine the results with Eq. (A-17). The perturbation to X is given by

$$\delta X = \left\{\phi^{*T}[\delta H - X(\delta G)]\phi + \phi^{*T}[\delta R - (\delta\lambda)F - \lambda(\delta F)]\Gamma + \Gamma^{*T}[\delta R - (\delta\lambda)F - \lambda(\delta F)]\phi\right\} \Big/ \left[\phi^{*T} G \phi\right] , \tag{A-18}$$

where Γ and Γ^{*} are the solutions to

$$[R - \lambda F]\Gamma = -[H - XG]\phi , \tag{A-19}$$

$$[R - \lambda F]^{T}\Gamma^{*} = -[H - XG]^{T}\phi^{*} . \tag{A-20}$$

Note that when the bilinear ratio is the eigenvalue, λ,

$$H = R \tag{A-21}$$

$$G = F \tag{A-22}$$

and the generalized perturbation theory expression [Eq. (A-18)] reduces to ordinary, first-order perturbation theory.

$$\delta\lambda = \frac{\phi^{*T}[\delta R - \lambda\delta F]\phi}{\phi^{*T}F\phi} . \tag{A-23}$$

Reaction Rate Ratios for Subcritical Systems. When a system is subcritical and is represented by an inhomogeneous equation,

$$[R - F]\phi = S , \tag{A-24}$$

the derivation remains essentially the same. The perturbation in a reaction rate ratio [Eq. (A-10)] is given by

$$\delta X = \left\{\left[\delta H^T - X\delta G^T + \Gamma^{*T}(\delta R - \delta F)\right]\phi - \Gamma^{*T}(\delta S)\right\} \Big/ \left[G^T\phi\right] , \tag{A-25}$$

where Γ^* is the solution of

$$[R - F]^T\Gamma^* = -H + XG , \tag{A-26}$$

and δS is the change to the fixed source vector, S.

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