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Development of Depletion Perturbation Theory for Coupled Neutron/Nuclide Fields

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OAK RIDGE NATIONAL LABORATORY
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ABSTRACT

A perturbation formulation is developed for the space-energy dependent burnup equations describing depletion and transmutation of nuclide densities in a coupled neutron-nuclide field, such as a reactor core. The formulation is developed in a form consistent with the computational methods used for depletion analysis. The analysis technique currently employed in most burnup calculations is first reviewed as a method for describing the nonlinear coupling between the flux and nuclide fields. It is shown that based on the present formulation three adjoint equations (for flux shape, flux normalization, and nuclide density) are required to account for the coupled variations arising from variations in initial conditions and nuclear data. The adjoint equations are derived in detail using a variational principle, and an algorithm is suggested for solving the coupled equations backward through time.

Perturbation expressions are used to define sensitivity coefficients for responses that depend on the coupled interaction between the neutron and nuclide fields. The relation between coupled and noncoupled sensitivity theory is illustrated. Finally, two analytic example problems are solved that determine the sensitivity of some final nuclide concentration to changes in initial conditions. Results obtained from direct calculation and from the coupled perturbation theory are compared.

I. INTRODUCTION

The area of nuclear engineering known as burnup analysis is concerned with predicting the long-term isotopic changes in the material composition of a reactor. Analysis of this type is essential in order to determine optimum fissile loading, efficient refueling schedules, and a variety of operational characteristics that must be known to ensure safe and economic reactor performance. Burnup physics is unique in that it is concerned not only with computing values for the neutron flux field within a reactor region, but also with computing the time-dependent behavior of the nuclide-density field. In general the flux and nuclide fields are coupled nonlinearly, and solving the so-called burnup equations is quite a formidable task which must be approached with approximate techniques.

It is the purpose of this study to develop a general perturbation theory for one of the common approximations used in burnup analysis. Based on such a technique, a sensitivity methodology will be established which seeks to estimate the change in various computed quantities when the input parameters to the burnup calculation are varied. A method of this type can be a very powerful analysis tool, applicable to several areas of practical interest. Two of the important areas are (a) in assessing the sensitivity of computed parameters to data uncertainties, and (b) in determining the effect of design changes at beginning-of-life on a parameter evaluated at some time in the future.

Several previous studies have employed burnup sensitivity theories of one type or another. Gandini first suggested the application of perturbation theory to the zero-dimensional nuclide-field equation,[1] and Tondinelli[2] and Gandini[3] have applied his equations to the question of actinide buildup in a LMFBR. Williams and Weisbin have applied a similar equation to the question of plutonium production in a thermal reactor, with an emphasis on uncertainty analysis.[4] However, these studies did not consider the nonlinear interaction between the neutron and nuclide fields.

Kallfelz, et al.,[5] addressed this problem by linking the perturbation theory for the nuclide field with static generalized perturbation theory (GPT) for the flux field. This method has given good results, but has the disadvantage of requiring a separate GPT calculation for each cross section in the nuclide field equation. Harris and Becker have derived perturbation expressions for general nonlinear systems of equations, and have applied the technique to simple models for depletion to examine uncertainties in fuel cycle costs.[6]

At present, however, there exists a need for a unifying theory which starts from the general burnup equations and derives perturbation expressions applicable to problems of arbitrary complexity. In particular, the physical and mathematical consequences of approximate treatments for the time-dependent coupling interaction between the nuclide and flux fields should be examined, and the role of perturbation theory in defining sensitivity coefficients for generic "responses" of the flux and nuclide fields should be clarified. This study attempts to provide a general theoretical framework for burnup sensitivity theory which is compatible with existing methods for treating the time dependence of the neutron field.

From a theoretical viewpoint it is convenient to categorize burnup perturbation analysis into two types. In this text these types are called the uncoupled and the coupled formalisms. The distinction lies in how the interaction between the nuclide and neutron fields is treated.

In the uncoupled perturbation method, it is assumed that a perturbation in the nuclide-field equation does not affect the flux field, and vice versa. In effect, the nonlinear coupling between the two field equations is ignored; or alternatively, one might say that for the depletion perturbation analysis, the flux field is treated as an input quantity, and not as a dependent variable. With this assumption, it is legitimate to consider the flux field as data, which can be varied independently along with the other data parameters.

In the coupled formalism, the nuclide and neutron fields cannot vary independently. Any data perturbation which changes one will also change the other, because the two fields are constrained to "move" only in a fashion consistent with their coupled field equations. In developing a workable sensitivity theory for the case of coupled neutron/nuclide fields, one must immediately contend with the specific type of formulation assumed in obtaining solutions to the burnup equations--the perturbation expressions themselves should be based on the approximation equations rather than the actual burnup equations, since the only solutions that exist for practical purposes are the approximate solutions.

The specific approximation addressed in this study will be the commonly used "quasi-static" burnup equations, discussed in detail in the text. This is the form of the equations solved by the more sophisticated burnup computer codes presently in use. The development in this study will assume the validity of this method as a hypothesis, and will find the associated perturbation expressions, which will then be related to depletion sensitivity analysis.

II. THE NONLINEAR SYSTEM OF BURNUP EQUATIONS

The purpose of this section is to review the burnup equations, expressing them in the operator form which will be followed throughout this study. We are interested in the interaction between the neutron flux field and the nuclide density field, both of which change with time and both of which influence the other.

A material reactor region is completely described by its nuclide density vector, which is defined by

$$\underline{N}(\hat{r},t) = \left(N_1(\hat{r},t),\ N_2(\hat{r},t),\ \ldots,\ N_n(\hat{r},t)\right) \tag{1}$$

where $N_i(\hat{r},t)$ = atom density of nuclide i at position $\hat{r}$ and time t.

While in operation, the reactor volume will also contain a population of neutrons whose distribution is described by the neutron flux field $\phi(\hat{\rho})$, where

$\hat{\rho}$ = vector in the 7-dimensional phase space of $(\hat{r}, t, \hat{\Omega}, E)$.

Note that the phase space over which $\underline{N}$ is defined is a subdomain of ρ-space.

Given an initial reactor configuration that is described by $\underline{N}_0(\hat{r})$ at $t = 0$, and that is exposed to the neutron flux field for $t \geq 0$, all future reactor configurations, described by the nuclide field $\underline{N}(\hat{r},t)$, will obey the nuclide transmutation equation (Bateman equation)*

$$\frac{\partial}{\partial t}\underline{N}(\hat{r},t) = [\phi(\hat{\rho})\underline{\underline{R}}(\sigma)]_{E,\Omega}\,\underline{N}(\hat{r},t) + \underline{\underline{D}}(\Lambda)\underline{N}(\hat{r},t) + \underline{C}(\hat{r},t) \qquad (2)$$

where

$\underline{\underline{R}}$ is a cross section matrix whose elements are

$\sigma_{ij}(\hat{r},E)$ = microscopic cross section and yield data for production of nuclide i by nuclide j, and

$\sigma_{ii} = -\sigma_{ai}$ = absorption cross section for nuclide i

$\underline{\underline{D}}$ is a decay matrix whose elements are

Λ_{ij} = decay constant for decay of nuclide j to nuclide i, and

$\Lambda_{ii} = -\Lambda_i$ = total decay constant for nuclide i

$\underline{C}(\hat{r},t)$ is an external source of nuclides, accounting for refueling, control rod motion, etc.

We will find it convenient to define a transmutation operator by

---

*$[\ ]_{x,y,\ldots}$ indicates integration over x,y,... .

$$\underline{\underline{M}} = \underline{\underline{M}}(\phi(\hat{\rho}),\ \sigma(\hat{r},E),\ \Lambda) = [\phi(\hat{\rho})\underline{\underline{R}}(\sigma)]_{E,\Omega} + \underline{\underline{D}}(\Lambda)\ . \tag{3}$$

Then the equation for the nuclide field vector becomes

$$\frac{\partial}{\partial t}\underline{N}(\hat{r},t) = \underline{\underline{M}}(\phi,\sigma,\Lambda)\underline{N}(\hat{r},t) + \underline{C}(\hat{r},t) \tag{4}$$

The neutron flux field obeys the time-dependent transport equation expressed by

$$\begin{aligned} 1/v\ \frac{\partial}{\partial t}\phi(\hat{\rho}) + \hat{\Omega}\cdot\nabla\phi(\hat{\rho}) + \underline{N}(\hat{r},t)\cdot\underline{\sigma}_t(\hat{r},E)\phi(\hat{\rho}) = \\ \underline{N}(\hat{r},t)\cdot\left[\underline{\sigma}_s(\hat{r},E'\rightarrow E,\Omega'\rightarrow\Omega) + (1-\beta)\ \frac{\chi(E)}{4\pi}\ \underline{\nu\sigma}_f(E')\phi(\hat{\rho})\right]_{E',\Omega'} \\ + \sum_i \chi_{Di}(E)\ \lambda_i d_i(\underline{N}) \end{aligned} \tag{5}$$

where

$\underline{\sigma}_t$ is the total cross-section vector, whose components are the total microscopic cross sections corresponding to the components of $\underline{N}$,

and similarly defined are

$\underline{\sigma}_s$, as the differential scatter cross-section vector
$\underline{\nu\sigma}_f$, as the fission-production cross-section vector,

and

$\chi(E)$ = prompt neutron fission spectrum
$\chi_{Di}(E)$ = delayed neutron fission spectrum for precursor group i
λ_i = decay constant for precursor group i
$d_i(\underline{N})$ = ith group precursor concentration, which is an effective average over various components of $\underline{N}$.
β = yield of all precursors, per fission neutron.

Defining the Boltzman operator in the indicated manner, $B = B[\underline{N}(r,t), \underline{\sigma}(r,E)]$, Eq. (5) becomes

$$1/v \frac{\partial}{\partial t} \phi(\hat{\rho}) = B(\underline{N},\sigma)\phi(\hat{\rho}) + \sum_i \chi_{Di}(E)\lambda_i d_i(\underline{N}) \qquad (6)$$

Equations (4) and (6) are the desired field equations for the nuclide and neutron fields within the reactor. In addition to these conditions, there may also be external constraints placed on the system, such as minimum power peaking, or some specified power output from the reactor. In general these constraints are met by adjusting the nuclide source $\underline{C}$ in Eq. (4), for example by moving a control rod. For this development we will consider only the constraint of constant power production:

$$[\underline{N}(\hat{r},t)\cdot\underline{\sigma}_f(\hat{r},E)\phi(\rho)]_\rho = P \qquad (7)$$

In this study the system of coupled, nonlinear equations given by Eqs. (4), (6) and (7) are referred to as the burnup equations. The unknowns are the nuclide and neutron fields, and the nuclide control source which must be adjusted to maintain criticality. These equations are obviously quite difficult to solve; in reality some suitable approximation must be used. One common approximation assumes that the Boltzman operator can be replaced by the diffusion operator, thus reducing the dimension of ρ-space from 7 to 5. Even with the diffusion approximation, however, the system is still coupled nonlinearly. In the next section we will examine assumptions which will decouple Eqs. (4) and (6) at a given instant in time, but first let us consider an alternate formulation for the flux-field equation which is useful in numerical calculations.

Suppose that $\phi(\rho)$ is slowly varying in time. Then at a given instant, the term $1/v\ \partial/\partial t\ \phi$ can be neglected. We will also assume that for the long exposure times encountered in burnup analysis, the fluctuations about critical arising from delayed neutron transients are unimportant (i.e., on the average the reactor is critical so that the precursors are at steady state). With these assumptions Eq. (6) can be approximated by

$$B(\underline{N})\phi(\hat{\rho}) = 0 \ , \tag{8}$$

if the prompt fission spectrum in Eq. (5) is modified to $(1 - \beta)\chi(E) + \sum \beta_i \chi_{Di}(E)$.

Equation (8) is homogeneous and thus at any given time will have nontrivial solutions only for particular values (an infinite number) of $\underline{N}$. To simulate the effect of control-rod motion, we will single out one of the components of $\underline{N}$ which will be designated the control nuclide N_c. Also we will express the B operator as the sum of a fission operator and a loss plus inscatter operator:

$$B = L - \lambda F \ , \tag{9}$$

so that Eq. (8) becomes

$$L(\underline{N},N_c) - \lambda F(\underline{N},N_c)\ \phi(\rho) = 0 \ , \tag{10}$$

where

$$\lambda = \frac{1}{k_{eff}} = \text{instantaneous lambda mode eigenvalue.}$$

The value for N_c is usually found indirectly by adjusting its magnitude until $\lambda = 1$. The concentration of the control nuclide is thus fixed by the eigenvalue equation and does not need to be considered as an unknown in the transmutation equation.

An alternate method of solving Eq. (8) is to directly solve the lambda mode eigenvalue equation (given $\underline{N}$, λ is sought from Eq. 10). In this case λ may or may not equal one. For both of these techniques, only the flux shape can be found from Eq. (10). The normalization is fixed by the power constraint in Eq. (7).

It is important to realize that both of these methods are approximations, and that in general they will yield different values for the flux shape. The former case is usually closer to "reality"

(i.e., to the burnup equations) while the latter is usually faster to solve numerically. For many problems concerned only with nuclide densities, results are not extremely sensitive to the approximation used.[7,8]

III. THE QUASI-STATIC APPROXIMATION

There are various methods to obtain numerical solutions to the space energy-dependent burnup equations. Nearly all approximations are based on decoupling the calculation for the flux and nuclide fields at a given instant in time. The simplest decoupling method is to treat the flux as totally separable in time and the other phase space variables over the entire time domain of interest

$$\phi(\hat{\rho}) = \Phi(t)\psi_0(\hat{r},E,\hat{\Omega}) \qquad \text{for } 0 < t < t_f \ , \tag{11}$$

where Φ is a time-dependent normalization, and ψ_0 is some shape function.

The "shape function" ψ_0 can be determined from a time-independent calculation at t = 0 using one of the eigenvalue equations discussed in the previous section. It is normalized such that

$$[\psi_0(\hat{r},E,\hat{\Omega}]_{E,\Omega,V} = 1 \tag{12}$$

Substituting Eq. (11) into Eq. (2),

$$\frac{\partial}{\partial t}\,\underline{N}(\hat{r},t) = \Phi(t)\,[\psi_0\underline{\underline{R}}(\sigma)]_{E,\Omega}\,\underline{N} + \underline{\underline{D}}\,\underline{N} + \underline{C} \tag{13}$$

Equation (13) can be simplified by writing the first term on the RHS as

$$\Phi(t)\,\underline{\underline{R}}_0(\sigma_0)\,\underline{N}(\hat{r},t) \ , \tag{14}$$

where $\underline{\underline{R}}_0$ is a one-group cross-section matrix whose components have the form

$$\sigma_o(\hat{r}) = [\psi_o(\hat{r},E,\Omega)\sigma(\hat{r},E)]_{E,\Omega} \tag{15}$$

Thus the cross-section matrix is rigorously composed of space-dependent, one-group microscopic data which can be evaluated once and for all at t = 0. In reality, detailed space-dependent depletion calculations are rarely performed due to prohibitive computing cost. Usually the $\underline{\underline{R}}$ matrix is averaged over some limited number of spatial zones (for example, a core zone, a blanket zone, etc.); in this case of "block depletion" the solution to the transmutation equation approximates the average nuclide field over each spatial region. The cross-section elements of $\underline{\underline{R}}$ for region z are given by

$$\sigma_o(z) = [\psi_o(z,E,\Omega)\sigma(z,E)]_{E,\Omega} \tag{16}$$

where $\psi_o(z,E,\Omega) \equiv [\psi_o(\hat{r},E,\Omega)]_{V_z}$

which has a normalization

$$\sum_z [\psi_o(z,E,\Omega)]_{E,\Omega} = 1$$

Throughout the remainder of this paper we will not explicitly refer to this region-averaging procedure for the nuclide field equation. This should cause no confusion since the spatial variable "r" in Eq. (13) can refer to either the region or spatial interval, depending on the case of interest. There is no coupling between the various r-points in the transmutation equation except through the flux-shape function, and therefore the equation for the region-averaged nuclide field appears the same as for the point-dependent field; only the cross-section averaging is different.

The value for the flux normalization in Eq. (13) is computed from the power constraint in Eq. (7):

$$\Phi(t) = P/[\underline{\sigma}_f(\hat{r},E)\ \underline{N}(\hat{r},t)\psi_o(\hat{r},E,\Omega)]_{E,V,\Omega} \tag{17}$$

For numerical calculations this normalization calculation is only done at discrete time intervals in the time domain,

$$\Phi_i = \frac{P}{[\underline{\sigma}_f(r,E)\ \underline{N}_i(r)\psi_o]_{E,V,\Omega}}\ , \quad \text{where } \underline{N}_i \equiv \underline{N}(\hat{r},t_i) \tag{18}$$

and is then held constant over some "broad time interval" (t_i, t_{i+1}).

One should realize that the broad time intervals at which the flux calculation is performed do not usually correspond to the finer time intervals over which the nuclide field is computed. To avoid confusion on this point, we will continue to represent $\underline{N}$ as an explicit function of time, rather than in its finite-difference form.

Note the discontinuity in Φ_i at each of the time intervals: at $t = t_i^-$, $\Phi = \Phi_{i-1}$, while at $t = t_i^+$, $\Phi = \Phi_i$. There is no corresponding discontinuity in the nuclide field; i.e.,

$$\underline{N}(\hat{r},t_i^+) - \underline{N}(\hat{r},t_i^-)\ ,$$

but there is discontinuity in the derivative of $\underline{N}$ at t_i.

With all the preceding assumptions, the nuclide-field equation becomes

$$\frac{\partial}{\partial t}\underline{N}(\hat{r},t) = \Phi_i \underline{\underline{R}}_U\ \underline{N}(\hat{r},t) + \underline{\underline{D}}\ \underline{N}(\hat{r},t) + \underline{C}(\hat{r},t)\ , \tag{19}$$

for $t_i < t < t_{i+1}$ with

$$\underline{N}(\hat{r},t_i^+) = \underline{N}(\hat{r},t_i^-) \tag{20}$$

as the initial condition of the broad time interval.

At a given value of r (either a region or a point), Eq. (19) depends only on the time coordinate; i.e., it is an ordinary differential equation. The assumption of total separability in the time variable of the flux field has completely eliminated the need for solving the transport equation, except for the initial eigenvalue calculation at t = 0 which was required to collapse the cross-section data.

In summary, the calculation usually proceeds as follows:

i) Solve Eq. (10) at t = 0 for flux shape
ii) Integrate cross-section data using Eqs. (15) or (16)
iii) Solve Eq. (18) for flux normalization at $t = t_i$
iv) Solve Eq. (19) for $\underline{N}(\hat{r},t)$ over the broad time interval $t_i < t < t_{i+1}$
v) Go to iii

The quasi-static depletion approximation, as used in this investigation,* essentially consists of a series of the above type calculations.[9] Instead of assuming that the flux field is totally separable in time over the domain of interest, it is only required that ψ be constant over some finite interval (t_i, t_{i+1}). The flux-shape function for each broad time interval is obtained from an eigenvalue calculation at the "initial" state t_i,

$$\left\{L(\underline{N}_i) - \lambda F(\underline{N}_i)\right\} \psi_i(\hat{r},E,\hat{\Omega}) = 0 \qquad (21)$$

at $t = t_i, \ldots,$ (i = 1, through number of time intervals) and the flux normalization is obtained from the power constraint at $t = t_i$,

$$\Phi_i \left[\psi_i(\hat{\rho})\underline{N}_i\underline{\sigma}_f\right]_{E,V,\Omega} = P_i \ , \qquad (22)$$

*Beware of difference in terminology from kinetics studies.

at $t = t_i, \ldots,$ where i ranges from 1 to the number of broad time intervals. Thus the time-dependent flux is approximated by the stepwise continuous function

$$\phi(\rho) \sim \Phi_i \psi_i(\hat{r},E,\hat{\Omega}) , \qquad t_i^+ < t < t_{i+1}^- . \tag{23}$$

After each eigenvalue calculation, a new set of one-group cross sections can be generated using the new value of ψ_i, resulting in a new cross-section matrix

$$\underline{\underline{R}}_i(\sigma_i) \equiv [\psi_i \underline{\underline{R}}]_{E,\Omega} , \tag{24}$$

with components

$$\sigma_i(\hat{r}) = [\sigma(\hat{r},E)\psi_i(\hat{r},E,\Omega)]_{E,\Omega} \tag{25}$$

The transmutation equation is then solved over the next time interval using the "constant" matrix $\underline{\underline{R}}_i$,

$$\frac{\partial}{\partial t} \underline{N}(\hat{r},t) = \Phi_i \underline{\underline{R}}_i \underline{N}(\hat{r},t) + \underline{\underline{D}}\underline{N}(\hat{r},t) + \underline{C}(\hat{r},t), \qquad t_i^+ < t < t_{i+1}^- \tag{26}$$

Note that the time-dependent flux given in Eq. (23) is again discontinuous at the boundaries of the broad time intervals, while the nuclide field is continuous (its derivative is discontinuous). The basic procedure for the quasi-static approximation is as follows:

i) solve flux eigenvalue equation for ψ_i at t_i
ii) integrate cross-section data using Eq. (25)
iii) solve Eq. (22) for normalization at t_i
iv) solve Eq. (26) between t_i and t_{i+1}
v) go to (i)

There are variations of this basic procedure presently in use. For example, some computer programs[10] iterate on the initial and final conditions of a broad time interval until the average power production over the interval (as opposed to the end-point values) meets some specified value; however, these refinements will not be considered in this study.

In Eqs. (21), (22) and (24), we have developed the quasi-static burnup equations. The approximations that were made have reduced the original coupled nonlinear equations to a series of equations which appear linear at any given instant. In reality, of course, the equations still approximate a nonlinear process, since a change in the value of ψ_i is ultimately fed back as a perturbation in the Boltzman operator for the calculation of ψ_{i+1}. It is this nonlinearity which will make the adjoint burnup equations derived shortly quite interesting.

Having reviewed the approximations used in burnup analysis, we can now address the subject of interest, which is the development of a perturbation theory for the quasi-static equations.

IV. SENSITIVITY THEORY FOR COUPLED NEUTRON/NUCLIDE FIELDS

The desired end result of virtually all design calculations is an estimated value for some set of reactor performance parameters. Each such parameter will be called a "response" in this study. For the case of burnup analysis, the generic response will be an integral of the flux and nuclide fields; i.e., it is mathematically a functional of both fields, which in turn are coupled through the respective field equations. As an example, the desired response may be the final ^{239}Pu mass at shutdown (a pure nuclide response); it may be the time-integrated damage to some non-depleting structural component (a flux response); or it may be some macroscopic reaction rate (a nuclide and flux functional). These functionals all take the general form of

$$R = R(\phi(\hat{\rho}), \underline{N}(\hat{r},t), \underline{h}) \ , \tag{27}$$

For future reference, we also note that the quasi-static formulation of Eq. (27) is

$$R_{QS} = R(\Phi_i, \psi_i, \underline{N}, \underline{h}) \ . \tag{28}$$

In these expressions $\underline{h}$ is a "realization vector" which can have the form of a cross section or of some unit vector which determines the response of interest. A discussion of some explicit forms for response functionals and their associated realization vectors appears in ref. 4.

It is the goal of sensitivity analysis to find the effect that varying some nuclear data parameter (e.g. a cross section, a decay constant, a branching ratio, etc.) will have on the response R. This will be accomplished by defining a "sensitivity coefficient" for the data in question, which will relate the percent change in R to the percent change in the data.

For example, let α_k be a nuclear data parameter contained in either or both the B and the $\underline{\underline{M}}$ operators. Then the sensitivity of R to α_k is given by

$$\delta R/R = \left[S_k(\hat{\rho}) \frac{\delta\alpha_k}{\alpha_k} (\hat{\rho}) \right]_\rho + \text{second-order terms} \tag{29}$$

For small $\delta\alpha_k$, we obtain the familiar linear relation between $\delta R/R$ and $\delta\alpha_k/\alpha_k$, with $S_k(\hat{\rho})$ serving as the sensitivity coefficient at position $\hat{\rho}$ in phase space. A change in the value of α_k in general will perturb both the nuclide and flux fields in some complex manner, depending on the specific $\delta\alpha_k(\hat{\rho})$.

Treating the response as an implicit function of α_k, we can expand R in a first-order Taylor series about the unperturbed state (see Appendix I for explanation of vector derivative notation):

$$R' \cong R + \left[\left(\frac{\partial R}{\partial \alpha_k}\right)\delta\alpha_k(\hat{\rho}) + \left(\frac{\partial R}{\partial \underline{N}}\right)\frac{d\underline{N}}{d\alpha_k}\,\delta\alpha_k(\hat{\rho}) + \left(\frac{\partial R}{\partial \phi}\right)\frac{d\phi}{d\alpha_k}\,\delta\alpha_k(\hat{\rho})\right]_\rho \quad (30)$$

$$\delta R/R \cong \left[\frac{\alpha_k}{R}\left(\frac{\partial R}{\partial \alpha_k} + \frac{\partial R}{\partial \underline{N}}\frac{d\underline{N}}{d\alpha_k} + \frac{\partial R}{\partial \phi}\frac{d\phi}{d\alpha_k}\right)\frac{\delta\alpha_k}{\alpha_k}(\hat{\rho})\right]_\rho \quad (31)$$

From this expression it is evident that

$$S_k(\hat{\rho}) = \alpha/R\left(\frac{\partial R}{\partial \alpha_k} + \frac{\partial R}{\partial \underline{N}}\frac{d\underline{N}}{d\alpha_k} + \frac{\partial R}{\partial \phi}\frac{d\phi}{d\alpha_k}\right) . \quad (32)$$

It is important to realize that the derivatives $d\underline{N}/d\alpha_k$ and $d\phi/d\alpha_k$ are <u>not independent</u>, since they must be computed from the constraint conditions (i.e., the field equations) which are coupled in $\underline{N}$ and ϕ.[11]

In order that this statement is clear, consider the coupled field equations in Eqs. (4) and (8) (the time-continuous eigenvalue form of the flux equation is used for simplicity, and the power constraint is neglected for this illustration). Taking the derivative of both equations with respect to α_k gives

$$\frac{d}{d\alpha_k}\left[B(\underline{N})\phi\right] = \left[\frac{\partial B}{\partial \underline{N}}\frac{d\underline{N}}{d\alpha_k} + \frac{\partial B}{\partial \alpha_k}\right]\phi + B(\underline{N})\frac{d\phi}{d\alpha_k} = 0$$

$$\frac{d}{d\alpha_k}\left[\left(\underline{\underline{M}} - \frac{\partial}{\partial t}\right)\underline{N}\right] = \left[\frac{\partial \underline{\underline{M}}}{\partial \phi}\frac{d\phi}{d\alpha_k} + \frac{\partial \underline{\underline{M}}}{\partial \alpha_k}\right]\underline{N} + \left(\underline{\underline{M}} - \frac{d}{dt}\right)\frac{d\underline{N}}{d\alpha_k} = 0 \quad (33)$$

Writing in matrix form, we have

$$\begin{pmatrix} B(\underline{N}) & \dfrac{\partial B}{\partial \underline{N}} \\ \dfrac{\partial \underline{\underline{M}}}{\partial \phi} & \underline{\underline{M}} - \dfrac{d}{dt} \end{pmatrix} \begin{pmatrix} \dfrac{d\phi}{d\alpha_k} \\ \dfrac{d\underline{N}}{d\alpha_k} \end{pmatrix} = - \begin{pmatrix} \dfrac{\partial B}{\partial \alpha_k}\phi \\ \dfrac{\partial \underline{\underline{M}}}{\partial \alpha_k}\underline{N} \end{pmatrix} = Q(\underline{N}, \phi, \alpha_k) \quad (34)$$

The interdependence of the sought-after derivatives is apparent in these equations. In theory Eq. (34) can be solved simultaneously for the required values, but in practice it is more advantageous to solve the adjoint system, as will be shown in the next section, because in Eq. (34) the source Q must be computed for each individual α_k.

The so-called "direct method" for sensitivity analysis consists of explicitly varying the data appearing in the burnup equations and estimating $dR/d\alpha$ with a finite difference scheme. For simple reactor models, this method can be effectively utilized (for example, see ref. 12). However, the procedure can be very laborious and expensive for more complex problems; therefore we are motivated to establish some sort of perturbation theory for burnup analysis, analogous to the generalized perturbation theory employed in static calculations. The method is founded on the development of an appropriate adjoint system for the burnup equations, which allows one to estimate the sensitivity coefficient independent of the specific data perturbation. These equations will obviously depend on the particular approximation assumed in solving the forward burnup system. The next section will derive the adjoint equations for the quasi-static approximation.

V. ADJOINT EQUATIONS FOR THE QUASI-STATIC BURNUP EQUATIONS

Before attempting to derive adjoint quasi-static equations, it will be instructive to consider the simpler case of point-depletion. Point-depletion corresponds to the first approximation described in Section III, with all space dependence of the nuclide field equation "averaged out," i.e., it is a zero-dimensional approximation. Gandini has previously addressed this problem under the further restriction that there be no variation in the flux field when the data is altered. This excludes perturbations both in flux shape at the initial condition and in normalization. Williams and Weisbin later showed that this amounts to neglecting a first-order error,[4] but one which may be small for many cases of interest.

The assumption of point-depletion with no flux perturbation simplifies Eq. (32) in two ways. First, the derivative $d\phi/d\alpha_k$ vanishes in the equation for S_k; and second, the derivative $d\underline{N}/d\alpha_k$ can be found independent of $d\phi/d\alpha_k$ [i.e., it also eliminates the $d\phi/d\alpha_k$ term in Eq. (34)]. It was shown in ref. 4 that under these restrictions, Eq. (32) is equivalent to

$$S_k(t) = \left(\frac{\alpha_k}{R} \frac{\partial R}{\partial \alpha_k} + \underline{N}^{*T} \frac{\partial \underline{\underline{M}}}{\partial \alpha_k} \underline{N} \right), \tag{35}$$

where $\underline{N}^*$ is the "uncoupled nuclide adjoint" obeying the final value equation

$$\underline{\underline{M}}^T \underline{N}^* = - \frac{\partial}{\partial t} \underline{N}^* - \frac{\partial R}{\partial \underline{N}}, \qquad \text{for } 0 \leq t < t_f \tag{36}$$

$$\underline{N}^*(t_f) = 0 \tag{37}$$

For the special case where R is a delta function in time at t_f (as assumed by Gandini), Eqs. (36) and (37) are equivalent to

$$\underline{\underline{M}}^T \underline{N}^* = - \frac{\partial}{\partial t} \underline{N}^* \qquad 0 \leq t < t_f \tag{38}$$

$$\underline{N}^*(t_f) = \frac{\partial R}{\partial \underline{N}} \tag{39}$$

These are the original "adjoint burnup equations" derived by Gandini, and are valid if the effect of flux perturbation on the response is small. The method of sensitivity theory for the noncoupled, point-depletion equations has been successfully applied in several studies;[2,4] however, the assumption of small flux variation warrants further investigation.

Note that even if the response is not an explicit function of ϕ (such as for a nuclide density response), there will still be a change

in R arising from $\delta\phi$, since this term will appear in Eq. (34). A priori, this indirect effect of the flux variation is difficult to evaluate. Studies by Kallfelz, et al.[5] [using a combination of static generalized perturbation theory for the flux field, and using Eq. (38) for the nuclide field], seem to indicate that for many responses the effect of changes in flux shape may be small, while the effect of changes in normalization may be significant. It was this apparent deficiency in the uncoupled adjoint equations which motivated development of a quasi-static perturbation theory in which the coupling in the burnup equations is explicitly treated (albeit approximately). Therefore let us now focus attention on obtaining the appropriate adjoint equations for the second approximation described in Section III.

For the derivation, we will use a variational technique described by Pomraning[13] and Stacy.[14] With this method, the quasi-static burnup equations in (21), (22), (26), and (12) are treated as constraints on the response defined in Eq. (28), and as such are appended to the response functional using Lagrange multipliers. We will specifically examine the case in which the shape function is obtained by solving the lambda mode eigenvalue equation, rather than the case in which ψ is obtained from a control variable ("N_c") search. The two cases are quite similar, the only difference being a "k-reset." (Eq. (54b) illustrates the mathematical consequence of the reset.) Let us consider the following functional

$$K[\underline{N}, \psi_i, \Phi_i, \alpha, \lambda, h] = R[\underline{N}, \psi_i, \Phi_i, h]$$

$$+ \sum_{i=1}^{T} \int_{t_i^+}^{t_{i+1}^-} \left[dt\, \underline{N}^*(\hat{r},t) \left([\psi_i \underline{\underline{R}}]_{E,\Omega}\, \Phi_i + \underline{\underline{D}} - \frac{\partial}{\partial t} \right) \underline{N}(\hat{r},t) + \underline{C} \right]_V dt$$

$$- \sum_{i=1}^{T} \left[\Gamma_i^*(\hat{\rho}) \left(L(\underline{N}_i) - \lambda_i F(\underline{N}_i) \right) \psi_i(\hat{\rho}) \right]_{\Omega,E,V}$$

$$- \sum_{i=1}^{T} P_i^* \left([\psi_i\, \underline{\sigma}_f\, \underline{N}_i]_{\Omega,E,V}\, \Phi_i - P_i \right) - \sum_{i=1}^{T} a_i \left([\psi_i]_{\Omega,E,V} - 1 \right) \qquad (40)$$

where

T = number of broad time intervals in the quasi-static calculation,

$\underline{N}_i = \underline{N}(\hat{r},t_i)$, and

$\underline{N}^*(\hat{r},t)$, $\Gamma_i^*(\rho)$, P_i^* are the Lagrange multipliers.

If P_i^* and Γ_i^* are set to zero and space dependence ignored, then the functional in Eq. (40) reduces to the same one discussed in ref. 4, which was used to derive the uncoupled, point-depletion adjoint equation in Eq. (36).

Note that if $\underline{N}$, ψ_i, and Φ_i are exact solutions to the quasi-static burnup equations, then

$$K = R \, . \tag{41}$$

In general, an alteration in some data parameter α will result in

$$K \rightarrow K'[\underline{N}', \psi_i', \Phi_i', \alpha', \lambda', h'] \, , \tag{42}$$

where the prime variables refer to their perturbed values. Again, if $\underline{N}'$, ψ_i', Φ_i' are exact solutions to the perturbed quasi-static equations,

$$K' = R' \, . \tag{43}$$

Expanding K' about the unperturbed state, and neglecting second-order terms,

$$K' = K + \left[\frac{\partial K}{\partial \alpha}\,\delta\alpha + \frac{\partial K}{\partial \underline{N}}\,\delta\underline{N} + \frac{\partial K}{\partial \underline{h}}\,\delta\underline{h} + \sum_i \left(\frac{\partial K}{\partial \psi_i}\,\delta\psi_i + \frac{\partial K}{\partial \Phi_i}\,\delta\Phi_i + \frac{\partial K}{\partial \lambda_i}\,\delta\lambda_i\right)\right] \tag{44}$$

If we can force the quantities $\partial K/\partial \underline{N}$, $\partial K/\partial \psi_i$, $\partial K/\partial \Phi_i$, $\partial K/\partial \lambda_i$ to vanish, then using Eqs. (41), (43), and (44),

$$\delta R = \left[\frac{\partial K}{\partial \alpha}\,\delta\alpha + \frac{\partial K}{\partial \underline{h}}\,\delta\underline{h}\right]_{\rho}, \tag{45}$$

or

$$\delta R/R = \left[\frac{\alpha}{R}\left(\frac{\partial K}{\partial \alpha} + \frac{\partial R}{\partial \underline{h}}\,\frac{\partial \underline{h}}{\partial \alpha}\right)\frac{\delta\alpha}{\alpha}\right]_{\dot{\rho}}. \tag{46}$$

From Eq. (46), it is obvious that the sensitivity coefficient for α is simply

$$S(\dot{\rho}) = \frac{\alpha}{\bar{R}}\left(\frac{\partial K}{\partial \alpha} + \frac{\partial \bar{R}}{\partial \underline{h}}\,\frac{\partial \underline{\dot{h}}}{\partial \alpha}\right). \tag{47}$$

The partial derivatives in Eq. (47) are trivial to evaluate, and therefore the problem of sensitivity analysis for the quasi-static burnup equations reduces to finding the appropriate stationary conditions on the K-functional. We will now set upon determining the required Euler equations, which will correspond to the adjoint field equations.

Consider first the functional derivative with respect to Φ_i (see Appendix I for functional derivative notation):

$$\frac{\partial K}{\partial \Phi_i} = \frac{\partial R}{\partial \Phi_i} + \int_{t_i^+}^{t_{i+1}^-} \left[\underline{N}^*[\psi_i \underline{\underline{R}}]_{E,\Omega}\,\underline{N}\right]_V dt - P_i^*[\psi_i\,\underline{\sigma}_f\,\underline{N}_i]_{E,\Omega,V} \tag{48}$$

In order for this expression to vanish, we should choose

$$P_i^* = \frac{\displaystyle\int_{t_i^+}^{t_{i+1}^-} \left[\underline{N}^*[\psi_i \underline{\underline{R}}]_{\Omega,E}\,\underline{N}\right]_V dt + \frac{\partial R}{\partial \Phi_i}}{[\psi_i\,\underline{\sigma}_f\,\underline{N}_i]_{\Omega,E,V}} \tag{49}$$

Now examine the term $\partial K/\partial \psi_i$, employing the commutativity property of adjoint operators,

$$\frac{\partial K}{\partial \psi_i} = \left\{ \frac{\partial R}{\partial \psi_i} - \left(L^*(\underline{N}_i) - \lambda_i F^*(\underline{N}_i) \right) \Gamma_i^* - P_i^* \, \Phi_i \, \underline{\sigma}_f \, \underline{N}_i + \Phi_i \int_{t_i^+}^{t_{i+1}^-} \underline{N}^* \, \underline{\underline{R}} \, \underline{N} \, dt - a \right\} \tag{50}$$

with L^*, $F^* \equiv$ adjoint operators to L and F, respectively. The vanishing of this term implies that (assuming the "standard" adjoint boundary conditions)

$$\left\{ L^*(\underline{N}_i) - \lambda_i F^*(\underline{N}_i) \right\} \Gamma_i^*(\hat{\rho}) = Q_i^* \, , \tag{51}$$

where

$$Q_i^*(\hat{\rho}) = \frac{\partial R}{\partial \psi_i} + \Phi_i \int_{t_i^+}^{t_{i+1}^-} \underline{N}^*(\hat{r},t) \, \underline{\underline{R}}(\sigma) \, \underline{N}(\hat{r},t) dt - \Phi_i P_i^* \, \underline{\sigma}_f \, \underline{N}_i - a \tag{52}$$

At this point it should be noted that Eqs. (51) and (21) demand that the flux shape function be orthogonal to the adjoint source; i.e.,

$$[\psi_i \, Q_i^*]_{\Omega,E,V} = 0 \, , \text{ at all } t_i \, .$$

From Eqs. (52) and (49) it is easily shown that this condition requires

$$\left[\psi_i \, \frac{\partial R}{\partial \psi_i} \right]_{E,\Omega,V} - \Phi_i \left[\frac{\partial R}{\partial \Phi_i} \right]_{E,\Omega,V} = a \tag{53}$$

which fixes the value of "a". For most cases of practical interest, this term is zero. For example if R is bilinear in ψ_i and Φ_i, or is a bilinear ratio, then "a" will vanish.

The term $\partial K/\partial \lambda_i$ is evaluated to be

$$\frac{\partial K}{\partial \lambda_i} = [\Gamma_i^*(\hat{\rho}) \, F(\underline{N}_i) \, \psi_i]_{\Omega,E,V} = 0 \, , \tag{54a}$$

which forces $\Gamma_i^*(\hat{\rho})$ to be orthogonal to the fission source at $t = t_i$.

This condition requires that Γ_i^* contain no fundamental mode from the homogeneous solution. More specifically, if Γ_p^* is a solution to Eq. (51) and $\Gamma_p^* \perp \phi_H^*$, where ϕ_H^* is the fundamental solution to the homogeneous equation, then $\Gamma_p^* + b\phi_H^*$ is also a solution <u>for all b</u>. However, Eq. (54) fixes the value of "b" to be zero, so that $\Gamma_i^* = \Gamma_p^*$.

However, this is true <u>only</u> for the case in which there is no k-reset (i.e., λ is allowed to change with data perturbations). For the case in which λ is made invariant by adjusting a control variable N_c, it is easily shown that the proper orthogonality condition is

$$\left[\Gamma_i^*(\hat{\rho}),\ \frac{\partial}{\partial N_c}\left(L(\underline{N}_i) - \lambda_i F(\underline{N}_i)\right)\psi_i\right]_{\Omega,E,V} = \frac{\partial K}{\partial N_c} = 0 \qquad (54b)$$

Now the value of "b" is <u>not</u> zero, but is given by

$$\frac{\left[\Gamma_p^* \frac{\partial}{\partial N_c}(L - \lambda P)\psi\right]_{\Omega,E,V}}{\left[\phi^* \frac{\partial}{\partial N_c}(L - \lambda P)\psi\right]_{\Omega,E,V}}$$

Thus the effect of adjusting a control variable is to "rotate" Γ_i^* so that it will have some fundamental component. The specific projection along ϕ^* depends on the specific control variable.

The Euler condition corresponding to a variation in $\underline{N}(r,t)$ is slightly more complex than for the other variables. Rather than simply taking the partial functional derivative, it will be more instructive to consider the differential (variation) of K with respect to $\delta\underline{N}$ (see Appendix I)

$$\delta K[\delta \underline{N}] = \left[\frac{\partial \underline{R}}{\partial \underline{N}} , \delta \underline{N}\right]_\rho$$

$$+ \sum_{i=1}^{T} \int_{t_i^+}^{t_{i+1}^-} dt \left[\delta \underline{N}(\hat{r},t) \left([\psi_i \underline{\underline{R}}^*]_{\Omega,E} \Phi_i + \underline{\underline{D}}^* + \frac{\partial}{\partial t}\right) \underline{N}^*\right]_V$$

$$- \sum_{i=1}^{T} [(\underline{N}_{i+1}^{*-} \delta \underline{N}_{i+1}^- - \underline{N}_i^{*+} \delta \underline{N}_i^+)]_V$$

$$- \sum_{i=1}^{T} \left[\delta \underline{N}_i \left[\Gamma_i^* \frac{\partial}{\partial \underline{N}_i} \left(L(\underline{N}_i) - \lambda F(\underline{N}_i)\right) \psi_i\right]_{\Omega,E}\right]_V$$

$$- \sum_{i=1}^{T} P_i^* \Phi_i \left[\delta \underline{N}_i [\psi_i \underline{\sigma}_f]_{\Omega,E}\right]_V , \qquad (55)$$

where $\underline{N}_{i+1}^{*-} = \underline{N}^*(\hat{r},t_{i+1}^-)$, etc.; and $\underline{\underline{R}}^* \equiv$ transpose $\underline{\underline{R}}$, $\underline{\underline{D}}^* \equiv$ transpose $\underline{\underline{D}}$ (i.e., $\underline{\underline{R}}^*$ and $\underline{\underline{D}}^*$ are the adjoint operators to $\underline{\underline{R}}$ and $\underline{\underline{D}}$).

This variation will be stationary if the following conditions are met. The first two expressions on the RHS of Eq. (55) will vanish if

$$\Phi_i [\psi_i \underline{\underline{R}}^*]_{E,\Omega} \underline{N}^* + \underline{\underline{D}}^* \underline{N}^* = - \frac{\partial}{\partial t} \underline{N}^* - \left[\frac{\partial \underline{R}}{\partial \underline{N}}\right]_{\Omega,E} , \text{ for } t_i^+ < t < t_{i+1}^- , \qquad (56)$$

which can be written

$$\underline{\underline{M}}^* \underline{N}^* + \underline{C}^* = - \frac{\partial}{\partial t} \underline{N}^* , \qquad (57)$$

where

$$\underline{C}^* = \left[\frac{\partial \underline{R}}{\partial \underline{N}}\right]_{\Omega,E} \qquad (58)$$

This equation is valid for the open interval (t_i, t_{i+1}). But the question of the behavior of $\underline{N}^*(\hat{r},t)$ at the time boundaries t_i has not yet been answered. The remaining terms in Eq. (55) will provide the necessary boundary conditions for each broad time interval. These terms may be written as

$$\sum_{i=1}^{T} \left[\delta\underline{N}_i \left\{ \underline{N}_i^{*+} - \left[\Gamma_i^* \frac{\partial}{\partial \underline{N}_i} (L - \lambda F)\psi_i \right]_{\Omega,E} - \Phi_i \, P_i^* [\psi_i \, \underline{\sigma}_f]_{\Omega,E} \right\} - \delta\underline{N}_{i+1} \underline{N}_{i+1}^{*-} \right]_V \tag{59}$$

where we have employed the continuity condition on the nuclide field,

$$\underline{N}_i = \underline{N}_i- = \underline{N}_i+ \, .$$

Expanding the summation, we get

$$\left[\delta\underline{N}_0 \left\{ \underline{N}_0^* - \left[\Gamma_0^* \frac{\partial}{\partial \underline{N}_0} (L - \lambda F)\psi_0 + P_0^* \, \Phi_0 \, \psi_0 \, \underline{\sigma}_f \right]_{\Omega,E} \right\} \right.$$
$$+ \delta\underline{N}_1 \left\{ \left(\underline{N}_1^{*+} - \underline{N}_1^{*-} \right) \cdot \left[\Gamma_1^* \frac{\partial}{\partial \underline{N}_1} (L - \lambda F)\psi_1 + P_1^* \, \Phi_1 \, \psi_1 \, \underline{\sigma}_f \right]_{\Omega,E} \right\}$$
$$\left. + \ldots - \delta\underline{N}_f \, \underline{N}_f^{*-} \right]_V \tag{60}$$

By allowing a discontinuity in the nuclide adjoint field we can make all the terms containing $\delta\underline{N}_i$ vanish, except at the end points $t = 0$ and $t = t_f$. Therefore we assert the following property of $\underline{N}^*(r,t)$ at the time boundaries,

$$\underline{N}^*(\hat{r},t_i^-) = \underline{N}^*(\hat{r},t_i^+) - \left[\Gamma_i^* \frac{\partial}{\partial \underline{N}_i}(L - \lambda F)\psi_i + \Phi_i\, P_i^*\, \underline{\sigma}_f\, \psi_i\right]_{\Omega,E}$$

$$= \underline{N}^*(\hat{r},t_i^+) - [\Gamma_i^*\, \underline{\beta}_i + P_i^*\, \underline{\Pi}_i]_{\Omega,E} \ , \tag{61}$$

where

$$\underline{\beta}_i = \frac{\partial}{\partial \underline{N}_i}\left(L(\underline{N}_i) - \lambda_i\, F(\underline{N}_i)\right)\psi_i$$

$$\underline{\Pi}_i = \Phi_i\, \underline{\sigma}_f\, \psi_i \tag{62}$$

The second term on the RHS of Eq. (61) represents a "jump condition" on $\underline{N}^*$ at $t = t_i$; its value depends on the magnitude of the other adjoint variables Γ_i^* and P_i^*. Essentially, $\Gamma_i^*\, \underline{\beta}_i$ and $P_i^*\, \underline{\Pi}_i$ are sensitivity coefficients to changes in $\underline{N}_i$.

The term in Eq. (60) containing $\delta \underline{N}_f$ will vanish if we fix the final condition of $\underline{N}^*$ to be

$$\underline{N}^*(\hat{r},t_f) = 0 \ . \tag{63}$$

(For responses which are delta functions in time, the final condition will be inhomogeneous--see next section.)

With all these restrictions placed on $\underline{N}^*$, the summation in Eq. (60) reduces to a single expression,

$$\left[\delta \underline{N}_o \left\{\underline{N}_o^* - [\Gamma_o^*\, \underline{\beta}_o + P_o^*\, \underline{\Pi}_o]_{\Omega,E}\right\}\right]_V \ . \tag{64}$$

From this equation we can define a sensitivity coefficient for the initial condition of nuclide m to be

$$S_o^m = N_o^m\left\{N_o^{m*} - [\Gamma_o^*\, \beta_o^m + P_o^*\, \Pi_o^m]_{\Omega,E}\right\} \tag{65}$$

For no change in the initial condition of the nuclide field, Eq. (64) will also vanish. To be general, however, we will not make this assumption, and will retain the expression in Eq. (65) as part of the sensitivity coefficient.

This rather involved development has provided the adjoint field equations for the quasi-static approximation. We have found that there exist adjoint equations corresponding to the nuclide transmutation equation, to the flux-shape equation (transport equation), and to the power-constraint equation. In addition, we have found that it is convenient to ascribe additional restrictions on the adjoint fields--namely, that Γ_i^* be orthogonal to the fission source and that $\underline{N}^*$ be discontinuous at each time boundary. The adjoint field equations are coupled, linear equations which contain the unperturbed forward values for $\underline{N}$, ψ_i, and Φ_i. These equations are repeated below:

Adjoint flux-shape equation

$$\left\{ L^*(\underline{N}_i) - \lambda_i F^*(\underline{N}_i) \right\} \Gamma_i^* = Q_i^* \tag{66}$$

at $t = t_i$.

Adjoint flux-normalization equation:

$$P_i^* = \frac{\int_{t_i^+}^{t_{i+1}^-} \left[\underline{N}^* [\psi_i \underline{\underline{R}}]_{\Omega,E} \underline{N} \right]_V dt + \frac{\partial R}{\partial \Phi_i}}{[\psi_i \underline{\sigma}_f \underline{N}_i]_{\Omega,E,V}}, \quad \text{at } t = t_i \tag{67}$$

Adjoint transmutation equation:

$$-\frac{\partial}{\partial t} \underline{N}^*(\hat{r},t) = \underline{\underline{M}}^*(\Phi_i, \psi_i) \underline{N}^*(\hat{r},t) + \underline{C}^*(\hat{r},t) \ , \ t \in (t_i, t_{i+1}) \tag{68}$$

$$\underline{N}^*(\hat{r},t_i^-) = \underline{N}^*(\hat{r},t_i^+) - [\Gamma_i^* \underline{\beta}_i + P_i^* \underline{\Pi}_i]_{\Omega,E} \text{ , at } t = t_i,\ i \neq f \quad (69)$$

$$\underline{N}^*(\hat{r},t_f) \equiv \underline{N}_f(\hat{r}) = 0 \text{ , at } t = t_f \quad (70)$$

In the limit, as the length of the broad time-step goes to zero, the flux becomes a continuous function of time and there is no jump condition on the nuclide adjoint. For this case, if the fundamental mode approximation is made for the spatial shape of the flux, the energy dependence expressed in few-group formalism, and the components of $\underline{N}$ limited to a few isotopes important to thermal reactor analysis, then the equations reduce to a form similar to those derived by Harris.[12] These equations are in fact simply the adjoint system to Eq. (34), with an appropriate adjoint source.[11]

The adjoint field equations previously derived were for an arbitrary response which satisfies the orthogonality requirement in Eq. (53). A specific type of response which is often of interest is some nuclide density evaluated at a specified time. This is the type of response originally considered by Gandini in his derivation of the uncoupled point-depletion nuclide adjoint equation, and was briefly discussed in Section V. Under this assumption,

$$R = R[\underline{N}_f,\underline{h}] = R[\underline{N}(\hat{r},t)\ \delta(t - t_f),\ \underline{h}] \quad (71)$$

i.e., the response is a delta function in time at $t = t_f$. In this case, the adjoint source is equivalent to a fixed final condition, and the adjoint field equations will simplify by

$$\underline{C}^*(\hat{r},t) = 0 \quad \text{for } t < t_f \quad (72)$$

$$\underline{N}_f^* = \frac{\partial R}{\partial \underline{N}_f} \qquad \text{at } t = t_f \quad (73)$$

$$\frac{\partial R}{\partial \Phi_i} = \frac{\partial R}{\partial \psi_i} = 0 \qquad \text{at } t = t_i \quad (74)$$

If the values for the variables P_i^* and Γ_i^* are also small (i.e., the effect of flux perturbation is negligible), then the discontinuity in $\underline{N}^*$ at t_i will be small, and the nuclide adjoint equation reduces to the uncoupled form in Eqs. (38) and (39).

VI. SOLUTION ALGORITHM FOR THE ADJOINT QUASI-STATIC EQUATIONS

As for the forward quasi-static equations, the practical utility of the adjoint equations depends on their ease of solution numerically. It turns out that the calculational flow for the adjoint solution is quite similar to that for the forward solution, except it proceeds backward in time. Therefore one would expect the computation requirements to be similar also. As an example of an algorithm for solving the adjoint quasi-static equations, we will consider the particular case discussed at the end of the previous section; i.e., the case in which the response is a nuclide functional at some final time t_f. Before outlining a computational flow chart, it may be helpful to make some preliminary observations.

First, it is shown in Eq. (52) that the flux adjoint source S_i^* at t_i depends on an integral of $\underline{N}^*$ over the <u>future</u> time interval (t_i, t_{i+1})--this fact is strong incentive for solving the adjoint equations backwards in time. We will not dwell on the difficulties encountered in solving the flux adjoint equation, other than to point out that the operator on the LHS of Eq. (51) is singular (hence the requirement that the fixed source be orthogonal to the fundamental forward eigenfunction). A discussion of the numerical methods required to solve these "generalized adjoint" equations can be found in ref. 15.

Second, notice that over any given time interval, (t_i, t_{i+1}), Eq. (57) for the coupled nuclide adjoint is identical to Eq. (36) for the uncoupled case; i.e., it is a final-value equation with constant coefficients. A method for solving this equation is described in ref. 4.

Finally, we see from Eq. (61) that the final value of $\underline{N}^*$ at the end of each time interval is fixed by the "jump" condition. Its

magnitude depends not only on the future behavior of $\underline{N}^*$, but also on Γ^* and p^* at the final time of the interval.

In summary, the adjoint quasi-static equations are coupled in the following manner:

a) the variables $\underline{N}^*$ and p^* appear in the source term of the equation for Γ^*,

b) the variable $\underline{N}^*$ appears in the defining equation for p^*,

c) the variables Γ^* and p^* appear in the "jump condition" for $\underline{N}^*$.

With these conditions in mind, we will now attempt to establish a suitable computational algorithm for numerical solution of the adjoint quasi-static equations. Toward this end, consider the following flow chart:

i) Starting with the Tth time interval (i.e., the last interval), solve Eq. (68) for the value of $\underline{N}^*$ between (t^+_{T-1}, t^-_f). The final value $\underline{N}^*_f$ is fixed by Eq. (73).

ii) Compute the value for p^*_{T-1} at t_{T-1} from Eq. (67)

iii) Compute Q^*_{T-1} using Eq. (52)

iv) Solve Eq. (66) for Γ^*_{T-1} at t_{T-1}

v) With the known values for p^*, Γ^*, and $\underline{N}^*$ at t^+_{T-1}, compute the value for $\underline{N}^*$ at t^-_{T-1} from Eq. (69)

vi) Using this new value for the final condition of $\underline{N}^*$, solve Eq. (68) for the behavior of $\underline{N}^*$ between (t^+_{T-2}, t^-_{T-1})

vii) etc.

This marching procedure is followed backward through all the time intervals until the values at t = 0 are obtained, at which time the adjoint calculation is complete. When all the adjoint values have been obtained, the sensitivity coefficient for data variations is computed with Eq. (47), and for initial value variations with Eq. (65).

As an example of a data sensitivity coefficient, consider the hypothetical data $\alpha(r,E)$. The sensitivity coefficient for α [using Eqs. (47) and (40)] is

$$S_\alpha(\hat{r},E) = \frac{\partial R}{\partial \alpha(r,E)} +$$

$$+ \sum_i \int_{t_i^+}^{t_{i+1}^-} \underline{N}^*(\hat{r},t) \frac{\partial}{\partial \alpha(r,E)} \underline{\underline{M}}_i \underline{N}(\hat{r},t)dt$$

$$- \sum_i [\Gamma_i^*(\hat{\rho}) \frac{\partial}{\partial \alpha(r,E)} B_i \psi_i(\hat{\rho})]_\Omega$$

$$- \sum_i P_i^* [\psi_i(\hat{\rho}) \frac{\partial}{\partial \alpha(r,E)} \underline{\sigma}_f \underline{N}_i(\hat{r})]_\Omega ,$$

where the operators $\underline{\underline{M}}$ and B [Eqs. (3) and (9)] were used to simplify notation. After computing the sensitivity coefficients for all important data, these are folded with data covariance files to find the response variance. (See ref. 4 for more details concerning time-dependent uncertainty analysis.)

In describing the flow charts for the depletion calculations, we have made no reference to the specific numerical procedures to be employed in solving the derived adjoint equations. It has been assumed that the solution techniques used for solving the forward equations (multi-group, finite differencing, etc.) are also applicable to the adjoint equations. In the next section we will consider the application of quasi-static sensitivity theory to two simplistic examples in which the adequacy of the method can be examined.

VII. EXAMPLE CALCULATIONS

As an illustrative application of the adjoint quasi-static equations, we will first consider the simplest possible case of an infinite, single-nuclide medium in which the energy behavior of the flux is described by one energy group and will assume that the quasi-static calculation is to be performed in a single time step (thus technically this is a point-depletion calculation). Let us further assume that the purpose of the calculation is to determine the sensitivity of the nuclide concentration at time T_f to changes in the initial condition at time zero.

The burnup equations for this example are

$$N_o(\sigma_a - \lambda\nu\sigma_f)\psi_o = 0 \qquad \text{(flux shape equation)} \qquad (75)$$

$$\psi_o N_o \Phi_o \sigma_f = P \qquad \text{(flux normalization equation)} \qquad (76)$$

$$\frac{dN}{dt} = - \sigma_a \psi_o \Phi_o N \qquad \text{(transmutation equation)} \qquad (77)$$

$$N(o) \equiv N_o \qquad \text{(initial condition)} \qquad (78)$$

Because of the simplistic nature of this problem, the lambda eigenvalue is found independently of N or ψ,

$$\lambda = \frac{1}{k_\infty} = \frac{\sigma_a}{\nu\sigma_f} , \qquad (79)$$

and does not vary with time.

Equation (75), which is to be solved for the flux-shape function, is actually satisfied by <u>any</u> constant; however, from the normalization constraint, the value for ψ_o is fixed to be unity.

The flux magnitude is easily computed from Eq. (76):

$$\Phi_o = \frac{P}{N_o\sigma_f} , \qquad (80)$$

and the time-dependent nuclide concentration is found to be

$$N(t) = N_o e^{-\sigma_a \Phi_o t} = N_o e^{-\frac{\sigma_a P t}{N_o \sigma_f}} . \qquad (81)$$

For this example the response has been defined as the concentration of nuclide N at some specified time T_f (a "final-time nuclide response"),

$$R \equiv N(T_f) = \int_0^{T_f} \delta(t - T_f)N(t)dt = N_o e^{-\sigma_a \Phi_o T_f} . \qquad (82)$$

Now observe the consequences of perturbing the initial condition by $N_o \rightarrow N_o + \Delta N_o$

a) from Eq. (80),

$$\phi_o \rightarrow \frac{P}{(N_o + \Delta N_o)\sigma_f}$$

b) from Eq. (81),

$$N(t) \rightarrow N(t) + \Delta N(t) = (N_o + \Delta N_o)e^{-\frac{\sigma_a P t}{(N_o+\Delta N_o)\upsilon_f}}$$

c) from Eq. (82),

$$R \rightarrow R + \Delta R = (N_o + \Delta N_o)(e^{-\sigma_a \Phi_o T_f})(e^{-\sigma_a \Delta\Phi_o T_f}) \qquad (83)$$

The expression in (c) corresponds to the "exact" perturbed response, accurate within the limitations of the quasi-static formulation. Note that if the flux and nuclide fields were assumed to be uncoupled (as discussed at the beginning of Section V), a perturbation in N_o would not affect ϕ_o (i.e., $\Delta\phi_o = 0$). Equation (82) then reduces to

$$\Delta N(t) = \Delta N_o e^{-\sigma_a \Phi_o t} ,$$

and the response would be perturbed by

$$\frac{\Delta R}{R} = \frac{\Delta N_o}{N_o} \cdot \tag{84}$$

Therefore the initial-condition sensitivity coefficient for the uncoupled case is 1.

The effect of the flux perturbation in Eq. (82) can be approximated in the following manner: using the fact that $\Delta\Phi_o \sim -\Phi_o \, \Delta N_o/N_o$ (accurate to second order), Eq. (83) can be written as

$$R + \Delta R \sim (N_o + \Delta N_o) e^{-\sigma_a \Phi_o T_f} \cdot e^{\sigma_a \Phi_o \frac{\Delta N_o}{N_o} T_f} \tag{85}$$

Expanding the last exponential in a Maclaurin series, and neglecting all but first order terms,

$$\Delta R = \Delta N_o \left\{ e^{-\sigma_a \Phi_o T_f} + T_f \sigma_a \Phi_o e^{-\sigma_a \Phi_o T_f} \right\} \tag{86}$$

This implies that

$$\frac{\Delta R}{R} = \frac{\Delta N_o}{N_o} \left\{ 1 + T_f \sigma_a \Phi_o \right\} , \tag{87}$$

with the term in brackets serving as the sensitivity coefficient. Comparing the sensitivity coefficients for the coupled [Eq. (87)] and uncoupled [Eq. (84)] cases, we conclude that the term $T_f \sigma_a \Phi_o$ arises from the coupling between the flux and nuclide fields.

Now consider the adjoint system for this example. The value for Γ_o^*, the shape function adjoint, is obviously zero from the orthogonality condition in Eq. (54). The equation for the nuclide adjoint is

$$-\frac{dN^*}{dt} = -\sigma_a \Phi_o N^* , \qquad t < T_f \tag{88}$$

with

$$N^*(T_f) = \frac{\partial R}{\partial N} = 1 , \qquad t = T_f \tag{89}$$

This final-value problem has the solution

$$N^*(t) = e^{-\sigma_a \Phi_o (T_f - t)} \tag{90}$$

The value for the normalization adjoint at t = 0 is given by Eq. (67), with $\partial R/\partial \Phi_1 = 0$:

$$P^* = \frac{\int_0^{T_f} N^*(-\sigma_a) N dt}{\sigma_f N_o} = - \frac{\sigma_a N(T_f) T_f}{\sigma_f N_o} , \tag{91}$$

and the value for Π in Eq. (62) is

$$\Pi_o = \Phi_o \sigma_f . \tag{92}$$

Substituting Eqs. (92), (91), and (90) into Eq. (65) for the sensitivity coefficient gives, after simplification

$$S_o = \{1 + T_f \sigma_a \Phi_o\} , \tag{93}$$

which is the same value as in Eq. (87). Thus we see that the coupled adjoint equations provide a first-order estimate of the effect of the nonlinear coupling between the flux and nuclide fields, which does not appear in the uncoupled case. Of course, if the nuclide/flux coupling were ignored, then p^* would be zero; and the sensitivity coefficient in Eq. (93) would reduce to the uncoupled value of 1.

This example was obviously a very simple case, and yet it has provided some very important insight into the physical role of p^*--the

normalization adjoint corresponds to the importance of the flux normalization to the response. In ref. 4, the nuclide adjoint N^* was shown to play the role of "nuclide importance" for the noncoupled, point-depletion equation; and it can be shown to have a similar interpretation for the coupled quasi-static equations. Therefore, one might expect that Γ^* represents the importance of the flux shape (in both space and energy) to the response. The next example will focus on computing Γ^*.

For a second example, we will consider a problem described by two energy groups, and an infinite homogeneous medium composed of one fuel nuclide and one poison nuclide (the infinite-medium restriction can be relaxed if the flux is separable in space, and if the buckling term corresponding to the finite system is added to the absorption cross section in the flux equation). For simplicity we again only consider one time step. The response considered is the concentration of the fuel nuclide after 600 days of exposure. In this example the following notation will be employed:

σ_{xj}^{k} = micro-cross-section of type x; for nuclide k, group j. Cross-section types are indicated by r for removal, a for absorption, c for capture, f for fission, and s for scatter

$N_1(t)$ = atom density of fuel nuclide

$N_2(t)$ = atom density of poison nuclide

$\zeta(t) = N_2(t)/N_1(t)$

$\underline{N}_o$ = initial condition = $\begin{pmatrix} 1 \\ 0 \end{pmatrix} \times 10^{24}$ atoms/cm^3

The burnup equations describing the system are assumed to be the following:

Flux-shape equation

$$\begin{pmatrix} N_1(t)\ \sigma^1_{r1} & 0 \\ -N_1(t)\ \sigma^1_{s,1-2} & N_1(t)\ \sigma^1_{a2} + N_2(t)\ \sigma^2_{c2} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} - \lambda \begin{pmatrix} 0 & N_1(t)\ \nu\sigma^1_{f2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0 \tag{94}$$

which can be written

$$\begin{pmatrix} \sigma^1_{r1} & 0 \\ -\upsilon^1_{s,1-2} & \sigma^1_{a2} + \xi(t)\ \sigma^2_{c2} \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} - \lambda \begin{pmatrix} 0 & \nu\sigma_{f2} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \end{pmatrix} = 0 \tag{95}$$

Flux normalization equation

$$N_1\ \sigma^1_{f2}\ \psi_2\ \Phi = P\ ,$$

$$\Phi = \frac{P}{N_1\ \sigma^1_{f2}\ \psi_2} \tag{96}$$

Nuclide transmutation equation

$$\begin{pmatrix} -(\sigma^1_{a1}\ \psi_1 + \sigma^1_{a2}\ \psi_2)\cdot\Phi & 0 \\ \gamma\sigma^1_{f2}\ \psi_2\cdot\Phi & -(\Phi\sigma^2_{c2}\ \psi_2 + \Lambda) \end{pmatrix} \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} = \frac{d}{dt} \begin{pmatrix} N_1 \\ N_2 \end{pmatrix} \tag{97}$$

where

γ = yield of nuclide 2 from fission,

Λ = decay constant of nuclide 2

It is a straightforward, though somewhat laborious task, to obtain closed form solutions to Eqs. (95), (96), and (97). For the general case of several time-steps in the quasi-static calculation, the expressions are very involved; however, if we stay with our original assumption and use only a single time-step, the resulting expressions are more manageable. The solutions are summarized below:

$$\lambda = \frac{\sigma_{r1}^1(\sigma_{a2}^1 + \zeta(t)\ \sigma_{c2}^2)}{(\nu\sigma_{f2}^1)(\sigma_{s,1-2}^1)} \tag{98}$$

$$\psi_1/\psi_2 = \frac{(\sigma_{a2}^1 + \zeta(t)\ \sigma_{c2}^2)}{\sigma_{s,1-2}^1} \tag{99}$$

$$\Phi = \frac{P}{N_1\ \sigma_{f2}^1\ \psi_2} \tag{100}$$

$$N_1(t) = N_1(o)e^{-a_{11}t} \tag{101}$$

$$N_2(t) = N_2(o)e^{-a_{22}t} + \frac{N_1(o)\ a_{21}}{a_{22} - a_{11}}\left[e^{-a_{11}t} - e^{-a_{22}t}\right] \tag{102}$$

where a_{ij} refers to the elements of the matrix in Eq. (97).

The nuclide adjoint equation is obtained by simply transposing the matrix in Eq. (97). The resulting nuclide adjoint solutions are

$$N_1^*(t) = N_1^*(T_f)e^{-a_{11}(T_f-t)} - \frac{a_{21}}{a_{22} - a_{11}} N^*(T_f)\left\{e^{-a_{22}(T_f-t)} - e^{-a_{11}(T_f-t)}\right\}$$

$$N_2^*(t) = N_2^*(T_f)e^{-a_{22}(T_f-t)} \tag{103}$$

where a_{ij} again refers to the matrix elements in Eq. (97).

The value for the flux normalization adjoint is given by

$$P^* = \frac{\int_0^{T_f} \left\{N_1^*(t)a_{11}N_1(t) + N_2^*(t)a_{21}N_1(t) + N_2^*(t)a_{22}N_2(t)\right\}dt}{\psi_2\ \sigma_{f2}^1} \tag{104}$$

which can be integrated analytically.

The equation for the shape adjoint function is obtained by transposing Eq. (95), and setting the result equal to the adjoint source defined in Eq. (52). For an infinite, homogeneous medium, in which Γ^* is orthogonal to the fission source the fission term can be ignored (see Appendix II), which makes the equation for Γ^* particularly simple:

$$\begin{pmatrix} \sigma_{r1}^1 & -\sigma_{s,1-2}^1 \\ 0 & \sigma_{a2}^1 + \zeta(t)\ \sigma_{c2}^2 \end{pmatrix} \begin{pmatrix} \Gamma_1^* \\ \Gamma_2^* \end{pmatrix} = \begin{pmatrix} Q_1^* \\ Q_2^* \end{pmatrix} \tag{105}$$

where

$$Q_1^* = \Phi \int_0^{T_f} dt N_1^*(t)(-\sigma_{a1}^1)N_1(t)$$

$$Q_2^* = \Phi \int_0^{T_f} dt\left\{N_1^*(t)(-\sigma_{a2}^1)N_1(t) + N_2^*(t)(\gamma\sigma_{f2}^1)N_1(t) + N_2^*(t)(\sigma_{c2}^2)N_2(t)\right\}$$

$$- \Phi\ P^* N_1(o)\sigma_{f2}^1 \tag{106}$$

These expressions can be evaluated analytically using the terms in Eqs. (100), (101), and (102). For this example the various data values were assumed to be those given in Table 1. These values are not

Table 1. Assumed values for nuclear data in example 2

Parameter	Value
σ^1_{r1}	9 barns
σ^1_{c1}	3 b
$\sigma^1_{1,1-2}$	6 b
σ^1_{c2}	1 b
σ^1_{a2}	2b
σ^1_{f2}	1b
μ	2b
σ^2_{c2}	10b
χ_1	1
χ_2	0
γ	.5
P	2.0×10^{14} $\frac{\text{fissions}}{\text{sec-cm}^3}$
Λ	4.0×10^{-9} sec^{-1}

particularly realistic, and were chosen arbitrarily to illustrate the technique. Using this data, the values for Φ, ψ and $\underline{N}$ were computed "semi-analytically" (i.e., a computer program was written to evaluate the analytic expressions and couple the results), and are listed in Column 1 of Table 2.

The response considered in this particular example was the concentration of nuclide 1 after 600 days of exposure. Therefore, the appropriate final condition for the nuclide adjoint is

$$N_1^*(600) = 1$$

$$N_2^*(600) = 0$$

The results of the adjoint calculations for this response are given in Table 3.

Now consider the change in the final concentration of the fuel nuclide, due to varying the initial concentration of the poison nuclide. A change in the concentration of nuclide 2 does not directly affect nuclide 1, since nuclide 1 is not produced by nuclide 2 (note that $N_2^*(t) = 0$). The poison nuclide was also assumed to have a zero fission cross section, and hence does not affect the flux normalization directly. Therefore the only mechanism by which a change in the concentration of nuclide 2 will affect the final concentration of nuclide 1 is through a change in the flux spectrum.

Column 2 of Table 2 shows the results of the perturbed calculation, for a change in the initial condition of the poison nuclide equal to $.1 \times 10^{24}$ atoms/cm^3. As one would expect, the addition of the poison nuclide hardens the spectrum, which increases the rate of depletion of nuclide 1, because nuclide 1 was assumed to have a higher absorption cross section in group 1 than in group 2. Consequently, after 600 days exposure the concentration of nuclide (i.e., the response) is slightly lower for the perturbed case than for the reference case. The amount of the response perturbation is -.52%.

Table 2. Results of forward calculation in example 2

	Reference case		Perturbed case ($\Delta N_2 = .1$)	
	t = 0	t = 600 days	t = 0	t = 600 days
N_1	1.0×10^{24}	$.96937 \times 10^{24}$	1.0×10^{24}	$.96436 \times 10^{24}$
N_2	0.0	$.17533 \times 10^{23}$	$.10 \times 10^{24}$	$.95125 \times 10^{23}$
$\Phi \cdot \psi_1$	$.6667 \times 10^{14}$	$.74992 \times 10^{14}$	$.1000 \times 10^{15}$	$.10323 \times 10^{15}$
$\Phi \cdot \psi_2$	$.2000 \times 10^{15}$	$.20632 \times 10^{15}$	$.2000 \times 10^{15}$	$.20739 \times 10^{15}$
k_{eff}	1.500	1.380	1.000	1.005

Table 3. Results of adjoint calculation[α] in example 2

	t = 0	t = 600
N_1^*	.96937	1.0
N_2^*	0.0	0.0
Γ_1^*	5.0164×10^{17}	
Γ_2^*	6.7008×10^{21}	
p^*	1.5076×10^{8}	

[α]For a response of $R = N_1$ (600 days)

We would now like to predict the response change using perturbation theory, and compare with the direct calculation. For the perturbation of

$$\Delta N = \begin{pmatrix} 0 \\ .1 \end{pmatrix} \times 10^{24} ,$$

Eq. (64) reduces to

$$\Delta R/R = \frac{-.1 \times 10^{24}}{.96937 \times 10^{24}} (\Gamma_2^* \sigma_{c2}^2 \psi_2) = .52\%$$

From this result we see that the perturbation method is very accurate for this example.

Both of the preceding examples have considered the sensitivity of some final nuclide concentration to changes in various initial conditions. It should be stated that the perturbation technique has also been applied in Example 2 to estimate the change in the response due to changes in cross sections and the decay constant of nuclide 2. Equally satisfactory results were obtained for these cases.

Because the example problems were relatively simple, the true power of the quasi-static perturbation method was not fully realized--it was actually an easy task to recompute the perturbed response analytically. However, such is not the case in realistic problems! The reader should be aware that with perturbation theory, a change in some response (for these examples, a nuclide concentration) due to a change in the initial condition or in any nuclear data can be estimated (to first order accuracy) without requiring a new burnup calculation. When one considers the cost of many burnup calculations, the power of burnup perturbation theory is evident.

CONCLUSION

Sensitivity theory expressions have been derived for functionals dependent upon coupled neutron and nuclide fields, as encountered in burn-up analysis. Equations for the adjoint functions appearing in the sensitivity coefficients were developed, based on a common approximation (called the quasi-static" formulation in this study) used in such computer codes as CITATION and VENTURE-BURNER.

After obtaining sensitivity coefficients, changes in a specified response due to changes in nuclear data or in the initial reactor configuration can be easily estimated without requiring new burn-up calculations. The numerical algorithm for solving the adjoint system of equations appears to require a comparable amount of computation as a single forward calculation. The method appears to have the greatest potential for application in the areas of uncertainty analysis and design scoping studies.

Appendix I

It is assumed that the reader has an elementary understanding of vector and functional analysis, or at least a knowledge of the basic definitions. This appendix will simply describe the mathematical notation employed in the text, without dwelling on any theoretical aspects.

A.1.1. Vector Notation. For this study, vector fields are denoted by underlining the variable, such as $\underline{N}(\hat{r},t)$. Vectors denoting points in a phase space (i.e., independent variables) are denoted with a caret, such as $\hat{r} = (x,y,z)$. Matrices are denoted with two underlines, such as $\underline{\underline{M}}$.

A.1.2. Inner Product of Vectors and Functions. All vector multiplication used in this work refers to the inner product operation. For example,

$$\underline{A}\,\underline{B} = A_1B_1 + A_2B_2 + \ldots + A_nB_n \ .$$

If we think of a function as being an infinite dimensional vector, the inner product of two functions is defined analogously:

$$[g(x)\cdot f(x)]_x = \int g(x)\cdot f(x)\, dx \ .$$

A.1.3. Vector Derivative (gradient). The derivative of a scalar function with respect to a vector is defined by

$$\frac{\partial f}{\partial \underline{A}}(\underline{A}) = \left(\frac{\partial f}{\partial A_1}, \frac{\partial f}{\partial A_2}, \ldots, \frac{\partial f}{\partial A_n}\right) \qquad (A.1\text{-}1)$$

This operation maps a scalar into a vector (note that if $\underline{A}$ is a position vector, the vector derivative is the familiar gradient operator).

A.1.4. Functional Derivative (gradient). This is a generalization of the concept of a vector derivative. If one considers a function to be an infinite dimensional vector, the generalization follows quite naturally--this operator transforms a functional (a scalar) into a function (a vector). If $K[f(x)]$ is a functional defined by $K = \left[F[f(x)]\right]_x$, where F is some composite function of $f(x)$, then we have (see ref. 16 for details)

$$\frac{\partial K}{\partial f(x)} = \frac{\partial F}{\partial f(x)} \tag{A.1-2}$$

A.1.5. Functional Variation (differential). A functional variation is a generalization of the concept of a differential (which of course is closely related to a directional derivative) in finite dimensional vector analysis. It is defined by

$$\delta K[f(x)] = \left[\frac{\partial K}{\partial f} \cdot \Delta f\right]_x = \left[\frac{\partial F}{\partial f} \cdot \Delta f\right]_x . \tag{A.1-3}$$

In this expression it is assumed that Δf is small, such that second-order terms can be ignored. A functional is called stationary at some function $f_0(x)$ if the functional gradient (and hence the variation) vanishes there. At such a point, K will either have an extremum or an inflection point.

A.1.6. Functional Taylor Series. Using the definitions in A.1.4 and A.1.5, a Taylor series expansion of a functional is defined completely analogously to a Taylor series for a function of a finite dimensional vector:

$$K[f + \Delta f] = K[f] + \left[\frac{\partial K}{\partial f} \cdot \Delta f\right]_x + \frac{1}{2}\left[\frac{\partial^2 K}{\partial f^2} \cdot \Delta f^2\right]_x + \ldots \tag{A.1-4}$$

Appendix II

The purpose of this appendix is to prove that for an infinite homogeneous medium the value for $\Gamma^*(E)$, which is orthogonal to the forward fission source, is given by the first term in a Neumann series expansion; i.e., $\Gamma^*(E)$ can be found from a fixed-source calculation without considering any multiplication. This proof was suggested to the author by R. L. Childs.[17]

The equation for the shape adjoint function, as derived in the text, is given for an infinite homogeneous medium by

$$L^*\Gamma^*(E) - \lambda F^*\Gamma^*(E) - Q^*(E) \qquad (A.2\text{-}1)$$

along with the constraint conditions

$$\int_0^\infty \psi(E)Q^*(E)dE = 0 \ , \qquad (A.2\text{-}2)$$

and

$$\int_0^\infty \Gamma^*(E)F\psi(E)dE = 0 \qquad (A.2\text{-}3)$$

The forward equation for the flux shape is

$$L\psi(E) - \lambda F\psi(E) = 0 \qquad (A.2\text{-}4)$$

The adjoint shape function can be expressed as a Neumann series by

$$\Gamma^*(E) = \Gamma_0^*(E) + \Gamma_1^*(E) + \ldots \ , \qquad (A.2\text{-}5)$$

where the terms in the infinite series are found from

$$L^*\Gamma_0^*(E) = Q^* \qquad (A.2\text{-}6)$$

$$L^*\Gamma_1^*(E) = \lambda F^*\Gamma_0^*(E) \qquad (A.2\text{-}7)$$

$$\vdots$$

Multiply Eq. (A.2-4) by Γ_0^*, and Eq. (A.2-6) by ψ, integrate both over energy and subtract:

$$\lambda \int_0^\infty \Gamma_0^*(E) F\psi(E) dE = \int_0^\infty \psi(E) Q^*(E) dE \tag{A.2-8}$$

Therefore, from Eq. (A.2-2) we see that

$$\int_0^\infty (\Gamma_0^* F\psi) dE = 0 = \int_0^\infty \psi(E) \nu\Sigma_f(E) dE \cdot \int \chi(E') \Gamma_0^*(E') dE' \tag{A.2-9}$$

This equation shows that $\Gamma^*(E) \perp \chi(E)$, since

$$\int_0^\infty \chi(E') \Gamma_0^*(E') dE' = 0 \tag{A.2-10}$$

Now consider the term on the RHS of Eq. (A.2-7):

$$F^* \Gamma_0^* = \nu\Sigma_f(E) \int_0^\infty \chi(E') \Gamma_0^*(E') dE' = 0 \ , \tag{A.2-11}$$

by Eq. (A.2-10). Since L^* is a nonsingular operator, we conclude that $\Gamma_1^*(E) = 0$. This argument is easily extended to the higher iterates, and the result is that

$$\Gamma^*(E) = \Gamma_0^*(E) \ , \tag{A.2-12}$$

where Γ_0^* is the solution to Eq. (A.2-6).

REFERENCES

1. A. Gandini, "Time-Dependent Generalized Perturbation Theory for Burn-up Analysis," CNEN RT/FI(75) 4, CNEN, Rome (1975).

2. L. Tondinelli, "Sensitivity of Actinide Concentration during Burn-up with Respect to Nuclear Data," CNEN RT/FI(76) 1, CNEN, Rome (1976).

3. A. Gandini, et al., "New Developments in Generalized Perturbation Theory in the Nuclide Field," *Nucl. Sci. Eng.*, 62, 339 (1977).

4. M. Williams, C. Weisbin, "Sensitivity and Uncertainty Analysis for Functionals of the Time-Dependent Nuclide Density Field," ORNL-5393 (1978).

5. J. Kallfelz, et al., "Burn-up Analysis with Time-Dependent Generalized Perturbation Theory," *Nucl. Sci. Eng.* 62(2), 304 (1977).

6. D. R. Harris and M. Becker, "Nonlinear Perturbation Theory for the Nuclear Fuel Cycle," *Trans. Am. Nuc. Soc.*, 23, 534 (1976).

7. M. Williams, et al., "Preliminary Neutronic Study of Actinide Transmutation in an LMFBR," ORNL/TM-6309 (In press).

8. G. Oliva, et al., "Trans-Uranium Elements Elimination with Burn-up in a Fast Power Breeder Reactor," *Nuc. Tech.*, (1978), Vol. 37, No. 3.

9. T. Fowler, D. Vondy, "Nuclear Reactor Core Analysis Code: CITATION," ORNL/TM-2496, Rev. 2 (1971).

10. D. Vondy, G. Cunningham, "Exposure Calculation Code Module: Burner," ORNL-5180, to be published.

11. M. Williams, et al, "Sensitivity Theory for Depletion Analysis," Proceedings from Sensitivity Theory Workshop sponsored by ORNL Radiation Shielding Information Center, Oak Ridge, Tennessee (August 1978).

12. D. R. Harris, "Sensitivity of Nuclear Fuel Cycle Costs to Uncertainties in Data and Methods," Ph.D. thesis, Rensselaer Polytechnic Institute, 1976.

13. G. Pomraning, "Variation Principle for Eigenvalue Equations," *J. Math. Phys.* 8, 149 (1967).

14. W. Stacy, *Variational Methods in Nuclear Reactor Physics*, Academic Press, N.Y., 1974.

15. E. Oblow, "Reactor Cross Section Sensitivity Studies Using Transport Theory," ORNL TM/4437 (1974).

16. E. Oblow, "Sensitivity Theory from a Differential Viewpoint," *Nucl. Sci. Eng.* 59, 187-189 (1976).

17. R. Childs, personal communication, 1977.

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