CONF-800942--15

ON THE IMPLEMENTATION, VERIFICATION, AND APPLICATION OF MULTICYCLE DEPLETION PERTURBATION THEORY

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ABSTRACT

Several application-oriented features of generalized depletion perturbation theory (DPT) are analyzed from the viewpoint of the reactor designer. The detailed theory is first reduced to some new terminology necessary for an adequate understanding of DPT. Using this terminology, the main features and computational accuracy of this new technique are illustrated through representative DPT calculations utilizing a CDS-type heterogeneous reactor model. Several examples are presented that indicate the potential of DPT methods as an alternate computational tool for certain types of reactor physics analyses.

INTRODUCTION

Over the past several years static generalized perturbation theory (GPT) methods have been increasingly used for reactor analyses in lieu of more detailed and costly direct computations. The usefulness of these methods in the area of data sensitivity and uncertainty analysis, as well as in parametric and design optimization studies, is well documented.[1-3] Recent theoretical developments in time-dependent perturbation theory methods[4-7] have greatly extended the potential applications of GPT to include areas such as fuel depletion and reactor kinetics.

Williams,[6] in particular, has developed a coupled neutron/nuclide depletion perturbation theory (DPT) applicable to multidimensional and multigroup reactor analysis problems. He has shown that three adjoint equations (for the flux shape, flux normalization, and nuclide density) are required to fully account for variations in both the neutron and nuclide fields arising from variations in initial nuclide concentrations and nuclear data. This base theory has recently been modified[8-9] to include nuclide discontinuities such as fuel shuffling and discharge, thus extending DPT to be applicable to multicycle burnup analyses.

Although much work has gone into the theoretical development, prior to the present study,[8-9] little effort has been expended in the way of implementation, verification, and realistic application of multicycle DPT. Therefore, the purpose of this paper is to emphasize these latter areas. Thus, after a brief review of the terminology of DPT, the remainder of this paper discusses the status of the current calculational capability, illustrates the

main features and computational accuracy of this new technique through its application to representative reactor depletion problems, and lastly, outlines the use of DPT in some new and interesting areas of application.

DPT TERMINOLOGY

Before discussing the application side of DPT, it is necessary to define some new terminology. This can be accomplished by considering the definition of a typical response utilized in perturbation theory analyses. A response of interest is generally a final-time functional of both the independent and dependent variables describing the reference reactor system, and can be written using the notation of ref. 9 as,

$$R(t_f) = \int f[\underline{N}(\vec{r},t), \underline{\beta}(\vec{r},\varepsilon,t), \alpha(t), \psi(\vec{r},\varepsilon,\tau)]\ \delta(t-t_f)d\vec{r}d\varepsilon dt \qquad (1)$$

where $\underline{N}$, $\underline{\beta}$, α and ψ are the nuclide density vector, data vector, flux normalization, and neutron flux shape function, respectively.

From eqn. (1) one sees that there are only four possible ways in which R can be altered:

1. Variation in $\underline{N}(\vec{r},t)$ —— direct `N* effect'

$$\Delta R = \int \frac{\partial R(t_f)}{\partial \underline{N}(t)} * \Delta\underline{N}(t)d\vec{r} \qquad (2)$$

2. Variation in $\alpha(t_i)$ —— direct or indirect `P* effect'

$$\Delta R = \frac{\partial R(t_f)}{\partial P(t_i)} * \Delta P(t_i) + \int \frac{\partial R(t_f)}{\partial P(t_i)} * \frac{\partial P(t_i)}{\partial \underline{N}(t_i)} * \Delta\underline{N}(t_i)d\vec{r} \qquad (3)$$

where P = reactor power = $f(\alpha)$

3. Variation in $\psi(\vec{r},\varepsilon,t_i)$ —— indirect `Γ effect'

$$\Delta R = \int \frac{\partial R(t_f)}{\partial Q(t_i)} * \frac{\partial Q(t_i)}{\partial \underline{N}(t_i)} * \Delta\underline{N}(t_i)d\vec{r}d\varepsilon \qquad (4)$$

where $Q(\vec{r},\varepsilon,t_i)$ = neutron source strength = $f(\psi)$

4. Variation in $\underline{\beta}(\vec{r},\varepsilon,t)$ —— `direct' or indirect `β* effect'

$$\Delta R = \int \frac{\partial R(t_f)}{\partial \underline{\beta}(t_i)} * \Delta\underline{\beta}(t_i)d\vec{r}d\varepsilon + \int \frac{\partial R(t_f)}{\partial \underline{\beta}(t_i)} * \frac{\partial \underline{\beta}(t_i)}{\partial \underline{N}(t_i)} * \Delta\underline{N}(t_i)d\vec{r}d\varepsilon \qquad (5)$$

Finally, adding eqns. (2)-(5) gives the total perturbed response,

$$\Delta R_{total} = N^*_{effect} + P^*_{effect} + \Gamma^*_{effect} + \beta^*_{effect} \qquad (6)$$

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Now, in the design and operation of a reactor, the independent variables most commonly employed to optimize system performance are the reactor power and nuclide density field. Thus, in perturbation studies it is necessary to relate variations in these independent variables to the performance parameters of interest. Equations (2)-(5) indicate that the desired relationships can be obtained by simply taking the partial time-dependent derivatives of the response definition with respect to the four variables in eqn. (1) and by using the chain rule to relate ΔR to the independent system perturbations, ΔP and $\Delta \underline{N}$.

At this point it should be mentioned that the time scale of interest in the present study is characteristic of burnup calculations rather than kinetics problems. For this class of problems, the neutron flux is assumed to vary slowly with time. Therefore, a `quasi-static' solution algorithm, in which the flux shape is assumed constant during some finite time step, is usually employed. Under this formulation the flux shape and power constraint equations in the reference problem are applied only at the time-step boundaries, giving rise to a discontinuous time behavior and the discrete time notation (t_i) used in eqns. (3)-(5). Furthermore, in eqn. (5) the $\Delta\underline{\beta}$ term is zero for typical design perturbation studies (data sensitivity theory in which $\Delta\underline{\beta}$ is not zero is discussed briefly later in this paper), and the $\partial\underline{\beta}/\partial\underline{N}$ term is usually assumed to be negligible. Therefore, eqn. (6) with the β^* effect term set to zero is the generalized perturbation theory formulation utilized in this work for both static and time-dependent (quasi-static) analyses.

To distinguish between static and time-dependent perturbation theory, one need only specify the time at which the perturbation is made. If $t = t_i = t_f$, static perturbation theory results. If however, t and $t_i < t_f$, the $\partial R/\partial \underline{N}$, $\partial R/\partial P$, and $\partial R/\partial Q$ derivatives in eqns. (2)-(4) become time-dependent functions and thus relate the change in the final-time response to perturbations made prior to t_f.

This rather simplified explanation and rationalization of DPT will hopefully serve as a bridge between the detailed theory[6,9] and the terminology necessary for an adequate understanding of the application of DPT. A detailed derivation of the adjoint depletion equations shows that the $\underline{N}^*(\vec{r},t)$, $P^*(t_i)$ and $\Gamma^*(\vec{r},\varepsilon,t_i)$ adjoint functions are just the $\partial R/\partial \underline{N}(\vec{r},t)$, $\partial R/\partial P(t_i)$, and $\partial R/\partial Q(\vec{r},\varepsilon,t_i)$ time-dependent derivatives needed in the perturbation expression of eqn. (6). Not only does this simple comparison define the desired terminology but it also provides a physical basis for the three adjoint functions of DPT.

Although the detailed structure of the three adjoint equations is not required for application purposes, it is important to note that a one-to-one correspondence exists between the forward and adjoint `quasi-static' burnup equations.[9] This similarity indicates that the same computational methods used to solve the forward burnup equations can be utilized with only moderate modifications to calculate the three adjoint functions of DPT. Therefore, in principle, solution of the adjoint equations is no more difficult than solution of the forward burnup problem.

THE DPT CALCULATIONAL SYSTEM

Based on the similarity of the forward and adjoint equations, a time-dependent sensitivity capability was developed and integrated within the VENTURE[10] modular code system. The new DEPTH (for DEpletion Perturbation THeory) module solves for the adjoint nuclide density vector and normalization adjoint, $\underline{N}^*(\vec{r},t)$ and $P^*(t_i)$, respectively. It then calculates the generalized adjoint source necessary for the adjoint flux calculation. Using this source, the VENTURE module solves for the adjoint shape function, $\Gamma^*(\vec{r},\varepsilon,t_i)$, and evaluates several integrals involving both the forward and adjoint shape functions. Calculational control is then returned to DEPTH where the time-step jump conditions are applied using the previously computed adjoint functions. This procedure is repeated for each depletion time step, backwards through time, until the initial time (in the forward sense) has been reached.

Once the importance functions have been calculated, the effect of a design variation from the reference state on a given final time response can be estimated by the evaluation of the simple integral expression given in eqn. (6). Also, since the adjoint functions are independent of the specific perturbation (arbitrary $\Delta\underline{N}$ and ΔP), a single adjoint calculation allows the investigation of the effects of any number of design perturbations. Thus DPT allows a considerable savings in time and cost when several design variations or a general sensitivity analysis are to be performed.

To make the DPT computational system complete, several utility routines for general data manipulation purposes were also written and incorporated into the CHARGE module. Most noteworthy are: 1) a generalized source generation routine which calculates the adjoint sources required as input to DEPTH for several types of response functionals, and 2) a flexible code block for the calculation of perturbed responses using the nuclide sensitivity coefficients calculated in DEPTH and any number of user-defined nuclide perturbations to the reference system.

The DEPTH-CHARGE system for the calculation and subsequent use of the time-dependent adjoint functions of DPT is essentially complete. With only minor restrictions, time- and space-dependent sensitivities to all the nuclides in the system can be obtained for any problem that can be modeled using the VENTURE system. Thus, the present capability is very general and can handle most any problem of interest. The DEPTH-CHARGE system provides, for the first time, a complete generalized first-order perturbation theory capability for both static and time-dependent analyses of realistic multidimensional reactor models.

VERIFICATION AND APPLICATION OF DPT

A wide variety of numerical calculations have been performed to verify the accuracy of the coding within the DEPTH-CHARGE system, as well as the adequacy and generality of multicycle DPT. The detailed examples discussed in ref. 9 covered the range from 1-group, 1-D reactor models to more complex multigroup 2-D calculational representations. In addition, several multicycle calculations were performed as a test of the adjoint formulation for problems involving discontinuous nuclide fields. The comparison of predicted responses with direct computations for this large calculational data base

clearly demonstrates the remarkable predictive capability of DPT. However, as a further verification of the method and as a representative application of DPT, a set of new calculations utilizing a CDS-type heterogeneous reactor model[11] has been performed.

The specific computational model employed for this work is shown in Fig. 1. As indicated, this $PuUO_2/UO_2$ LMFBR configuration is a representative heterogeneous design with three discrete inner blanket and fuel driver regions surrounded by three rows of radial blanket assemblies. The indicated regions were then further subdivided into subzones. The driver, axial blanket, and inner blanket zones have two subzones while the first, second, and third radial blanket rows have three, four, and five subzones, respectively. The purpose of the subzone modeling is to allow for fuel management operations in multicycle calculations. For example, the zones having two subzones have a two-cycle refueling schedule, with one subzone in each zone being discharged and refueled annually.

Utilizing an equilibrium version of this model (with 10-group cross sections), time-dependent sensitivity analyses were performed for two responses of general interest in reactor design studies. The main goals of these realistic examples are to 1) verify the applicability of DPT methods for heterogeneous reactor models, 2) illustrate the type of problems that can be solved, 3) emphasize the large amount of useful information available from such an analysis, and 4) discuss several key features of the method.

Nuclide Inventory Response

The first response for which sensitivity coefficients were calculated was the ^{239}Pu inventory in the reactor at various times during the equili-

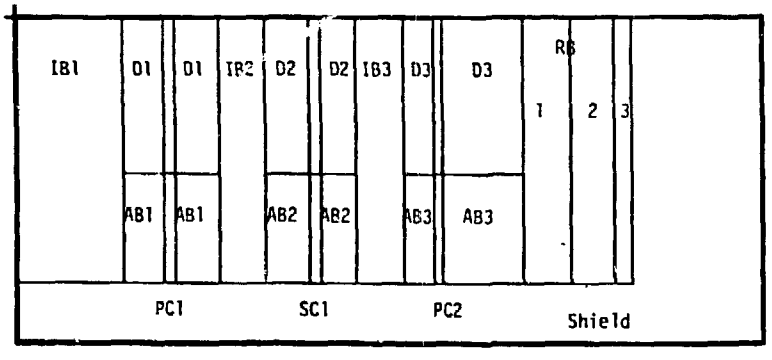

Fig. 1. RZ Model of GDS-Type Heterogeneous LMFBR.

brium cycle. This choice of response was somewhat arbitrary in that the fissile inventory in the equilibrium discharge or any subset of the reactor volume may be equally appropriate for some applications. In any case, knowledge of the fissile inventory in the reactor (or some subset thereof) is important for the calculation of fissile gain, doubling time, growth rate, or fuel-cycle cost.

Therefore, with this justification, two adjoint depletion calculations were performed; one for the middle-of-cycle (MOC) ^{239}Pu inventory and another for the EOC inventory. These DEPTH calculations produced sensitivity coefficients as a function of time to all the nuclides for which cross section data were supplied. In particular, sensitivity information was generated that relates a change in the desired final-time response to a BOC design variation.

The benefit of perturbation theory methods can now be realized by performing as many parametric design studies as desired. For example, assume that one wanted to investigate the effect of a pin diameter change in the design of the equilibrium feed assemblies. This design variation from the reference calculation manifests itself as a nuclide perturbation in the feed stream. With the data calculated in DEPTH and the desired $\Delta\underline{N}$, one can easily obtain an estimate of the change in the ^{239}Pu inventory with use of the CHARGE module to evaluate the perturbation expression in eqn. (6).

This procedure was followed for several perturbations for both the MOC and EOC ^{239}Pu inventory responses. Table 1 compares DPT methods with direct

Table 1. Comparison of DPT Results with Direct Computations for the ^{239}Pu Inventory Response

	BOC	MOC			EOC		
Case	Direct ΔR(kg)	DPT ΔR	Direct ΔR	% Diff.	DPT ΔR	Direct ΔR	% Diff.
1A	0.0	8.32	8.21	1.3	15.49	15.23	1.7
1B	0.0	4.72	4.59	2.0	9.43	9.16	3.0
1C	0.0	1.00	0.98	2.0	1.94	1.88	3.2

Note: Perturbation cases 1A-1C refer to a 10% increase in the ^{238}U reload concentrations for the driver, inner blanket and radial blanket regions, respectively.

2A	-281.7	-259.4	-257.6	0.7	-240.2	-237.1	1.3
2B	- 89.1	- 81.2	- 80.8	0.4	- 74.3	- 73.8	0.8
2C	104.6	95.2	95.3	-0.1	87.2	87.4	-0.1

Note: Perturbation cases 2A-2C refer to variations in the fuel and coolant volume fractions in the driver reload assemblies. Cases 2A-2C represent fuel volume fractions of .35, .40, and .45, respectively, compared to .423 for the reference model. Fuel plus coolant fractions were kept constant.

calculations for these two responses. Although some interesting effects are apparent (compare ΔR at MOC and EOC), the important point to note here is the excellent agreement between DPT and direct methods. The percent error in the predicted ΔR is generally in the range of a few percent or less. These are extremely good results when one notes that six forward depletion calculations were required to obtain the 'Direct' results given in Table 1.

It should also be noted that Table 1 contains only the composite results of each perturbation to the system. Although in many instances this is all that is required, the DEPTH-CHARGE system can provide much more detailed information if desired. For example, the change in the response by perturbed nuclide and spatial region are also easily obtained, thus providing the reactor designer more useful information about the system of interest.

Another detail worthy of mention is the ability to break up the perturbed response into its N*, P*, and Γ^* effect components. The Γ^* effect, in particular, is a unique feature of coupled neutron/nuclide depletion perturbation theory and has been shown to be a major part of the total ΔR for many perturbation/response pairs.[9] In the present example, the percent contribution of the Γ^* effect to the total ΔR (Γ^* effect/Total effect) for the MOC ^{239}Pu inventory was -6.9%, -53.7%, and -203.0% for the driver, inner blanket, and radial blanket ^{238}U perturbations, respectively. As apparent, the relative contribution of the Γ^* effect is very large in regions away from the main neutron source of the reactor (driver regions). Thus, the Γ^* effect becomes an essential part of DPT if perturbations are to be made in regions other than the fissile driver zones.

Since the Γ^* effect is generally quite important, it is instructive to examine the distributional behavior of $\Gamma^*(\vec{r},\epsilon,t_i)$. Figure 2 displays the group 5 generalized adjoint flux calculated at BOC for the MOC ^{239}Pu inventory response. As indicated, the addition of a source neutron into group 5 at t_o in either the axial, radial, or inner blankets will increase the response, while increased source strength in the driver regions has both positive and negative contributions to the ^{239}Pu inventory at t_f. These observations also support the previous conclusions that the relative ^{238}U Γ^* effect was small in the driver regions but resulted in a large negative effect in the blankets due to the negative removal source introduced with an increase in the ^{238}U reload density.

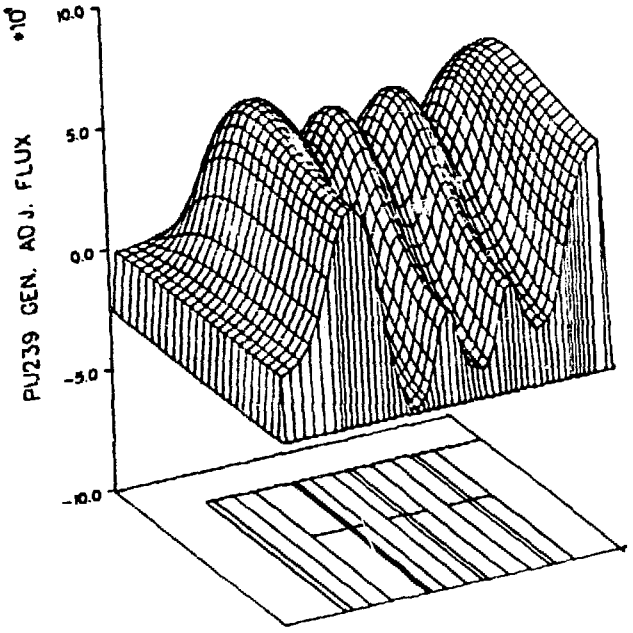

Fig. 2. BOC Generalized Adjoint Flux (Energies 2.6-31.8 keV) for the MOC ^{239}Pu Inventory Response.

Reactivity Response

The above nuclide inventory response has demonstrated the application of DPT in straightforward parametric design studies as well as in detailed analyses of the physics underlying a particular observed behavior. To further illustrate the usefulness of time-dependent perturbation theory, consider the task of determining the reactivity perturbation associated with various design options (i.e., fissile enrichments, volume fractions, fuel shuffling strategies, or control patterns, etc.). Typically, the variations in both the BOC and EOC reactivities are desired. The most direct solution method for this problem is to perform a complete burnup analysis for each design variation to be considered. For realistic calculational models, however, direct solutions such as this quickly become prohibitively expensive, even for only a small number of design variables.

Static perturbation methods have alleviated the problem of determining the effect of BOC design variations on the BOC reactivity. Likewise, the effect of EOC perturbations on the EOC K-eff could also be determined with static methods. However, what is needed in this case is a sensitivity function that relates the EOC state of the reactor to design variations at the beginning of the cycle. DPT can be utilized to bridge this time gap and provide the necessary importance functions.

Table 2 illustrates the difference between the sensitivity coefficients just described for the CDS-type heterogeneous reactor model discussed earlier. The first two columns represent static perturbation theory results at the BOC and after 292 days of full power operation. Differences in the nuclide importance to K-eff for these two cases can be attributed to shifts in the nuclide field and flux distribution during the 292-day burn. The last

Table 2. Comparison of Static and Time-Dependent K-eff Sensitivity Coefficients to Driver Reload Concentrations

Nuclide	Case 1 $\frac{(\Delta K/K)t_o}{(\Delta N/N)t_o}$	Case 2 $\frac{(\Delta K/K)t_f}{(\Delta N/N)t_f}$	Case 3 $\frac{(\Delta K/K)t_f}{(\Delta N/N)t_o}$	% Diff. $\frac{\text{Case 3-Case 2}}{\text{Case 2}}$
U-235	1.72-3	1.42-3	1.36-3	-4.0
U-238	-5.22-2	-5.13-2	-2.72-2	-47.0
Pu-238	1.98-3	1.65-3	1.77-3	7.3
Pu-239	2.23-1	2.07-1	1.80-1	-13.0
Pu-240	1.00-2	1.02-2	1.17-2	14.7
Pu-241	4.74-2	3.84-2	3.50-2	-8.9
O-16	-1.38-2	-1.73-2	-1.54-2	-11.0
Na	-3.39-3	-4.42-3	-4.13-3	-6.6
Cr	-1.33-3	-1.58-3	-1.56-3	-1.3
Ni	-2.72-3	-2.98-3	-2.97-3	0.3
Mo	-1.01-3	-1.02-3	-1.06-3	3.9
Fe	-6.52-3	-7.80-3	-7.42-3	-4.9

column of sensitivity coefficients, calculated using DPT with $(\Delta K/\Delta N)t_f$ as the initial condition for the adjoint equations, represent the percent change in the EOC K-eff due to a 1% perturbation in the BOC driver reload concentrations. The difference between case 2 and case 3 sensitivities represents the time-integrated importance of the depletion process to the response of interest. As shown in the last column of Table 2, this contribution can be quite significant in some cases.

The nuclides that immediately stand out in Table 2 are the main fertile and fissile species present in the reactor, particularly ^{238}U and ^{239}Pu. This is due primarily to the fact that these isotopes account for most of the changes that occur during the burnup process. To understand some of the differences noted in Table 2, consider the sensitivity of K-eff to the ^{238}U concentration. Table 2 indicates that at t_o a 1% increase in the ^{238}U driver reload density would result in an immediate reactivity decrease of about .05% relative to the reference case. However, if one considers the effect of a BOC perturbation on the EOC reactivity, a somewhat different scenario can be rationalized. An initial increase in ^{238}U also results in an increased ^{239}Pu concentration at future times due to neutron captur reactions. Thus, as observed, one would expect the time-dependent sensitivity coefficient to be less negative than the static case.

In addition to this direct "N* effect", the indirect flux effect due to the BOC ^{238}U perturbation also needs to be considered. Figure 3 displays

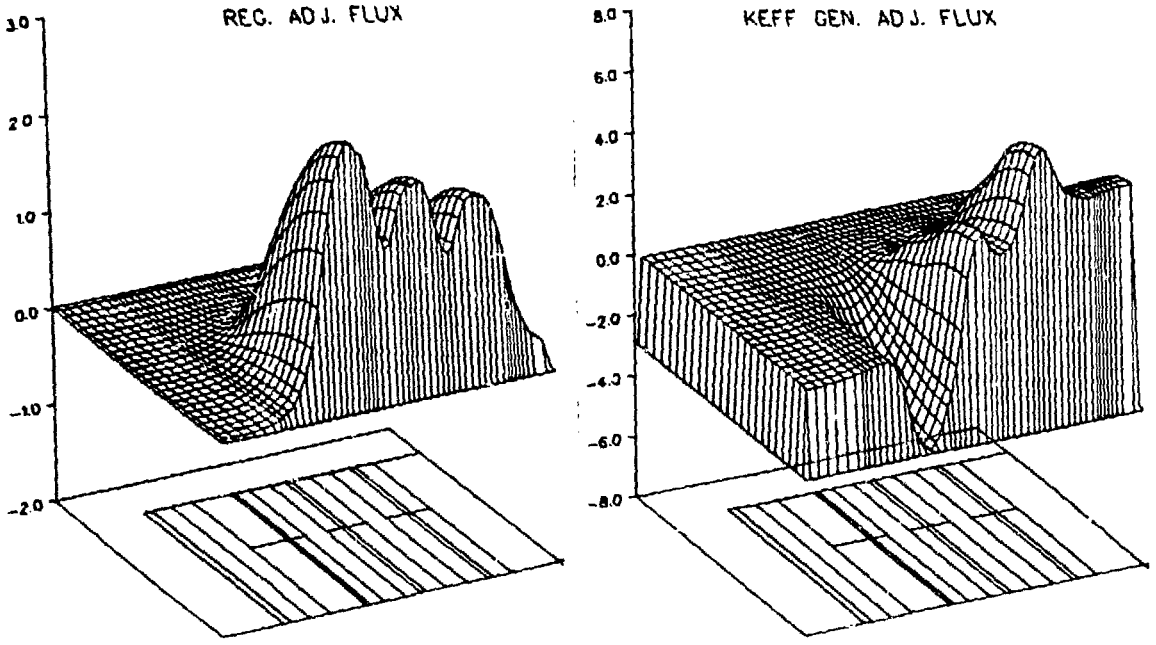

Fig. 3. BOC Regular and Generalized Adjoint Fluxes (Energies 2.6-31.8 keV) for the EOC Reactivity Response.

both the static and time-dependent adjoint fluxes for group 5, indicating the importance of a change in the BOC neutron source distribution to the BOC and EOC reactivities, respectively. Close observation shows that the non-negative regular (static) adjoint flux peaks in the three driver zones, while the generalized adjoint importance function has maxima in the inner blankets and minima in the drivers. Thus, the negative neutron source introduced via a BOC ^{238}U perturbation in the drivers causes a decrease in the BOC reactivity and an increase or decrease in the EOC K-eff depending on driver location. A ^{238}U increase in D1 and D2 decreases the EOC reactivity while a similar variation in D3 increases K-eff at t_f.

For the present example, the composite N^* and Γ^* effects (and small P^* effect) reduce the time-dependent ^{238}U sensitivity coefficient to about one-half the static value. This is a significant difference for such an important nuclide as ^{238}U. An accurate accounting of the time- and space-dependent nuclide sensitivities to the EOC reactivity (and several other responses) should be of considerable use in many reactor design analyses. The ability to quantify these sensitivities is an important characteristic of DPT.

FUTURE APPLICATIONS OF DPT

This paper cannot be properly concluded without emphasizing the fact that there is still a considerable amount of research to be performed in the relatively new field of time-dependent perturbation theory. The present investigation has only verified the generality and accuracy of the theory through its use in some simple, but illustrative applications. Hopefully, the capability demonstrated in these problems will arouse the interest of the reactor design community, since only through the use of DPT methods in a variety of application areas will the full potential of time-dependent sensitivity theory be realized. Two particular areas having an enormous potential for future application will be mentioned here.

The first topic to be discussed is the area of data sensitivity and uncertainty analysis. Until recently, most sensitivity analyses have been restricted to time-independent problems due to the limitations of static generalized perturbation theory.[1-2] However, the introduction of DPT methods removes this restriction and opens up the new area of time-dependent data sensitivity theory.

This new application area requires the evaluation of the $\partial R(t_f)/\partial \underline{\beta}(t_i)$ data derivative given in eqn. (5). However, the computation of this time-dependent data derivative does not require much additional work since it can be expressed in terms of the previously calculated $\underline{N}^*(\vec{r},t)$, $P^*(t_i)$, and $\Gamma^*(\vec{r},\varepsilon,t_i)$ adjoint functions. Thus only a slight revision of the present DEPTH-CHARGE system is required to implement this new capability, with the necessary modifications currently being made.

Some preliminary results are available from this data sensitivity work.[12] Comparison of static and time-dependent sensitivity coefficients for several nuclides in a simplified 1-D reactor model indicates that the effect of the burnup process may be an important consideration in the calculation of data sensitivity coefficients for realistic EOC responses. Thus, the future application of DPT methods in data sensitivity studies appears to be an interesting and informative area of research.

A second and more futuristic application of static and time-dependent perturbation theory is its use in computer-automated core design studies.[3] The design of a nuclear reactor from neutronic, thermal-hydraulic, structural, and economic viewpoints obviously require that compromises in the material configuration of the reactor be made. Now that time-dependent effects can be treated, perturbation theory methods can generate sensitivity coefficients that reflect the importance of these material compromises on several important performance parameters. A library of nuclide sensitivity coefficients for the performance indicators along with a set of user-defined system constraints could be utilized in an optimization package to provide a best estimate design in a single computer calculation. The possibilities of such a system as outlined here are enormous.

The first realistic application of design optimization on this scale may be in determining the optimum fuel shuffling pattern for an operating light water reactor. In this case the design variations may be limited to reload enrichment and fuel location. Since perturbation theory can predict the changes in the desired responses due to an interchange of assemblies (nuclide perturbation), in principle at least, the optimum location of each assembly based on certain system constraints can be determined. Thus, an automated optimization package based on static and time-dependent perturbation theory, as indicated here, could prove to be an invaluable aid for core design and fuel management analyses.

In conclusion, it should be emphasized that the application areas discussed throughout this paper by no means represent an exhaustive list. The primary goal of the illustrations utilized was to indicate that time-dependent perturbation theory (whose capability is presently available) represents an attractive alternate analytical and computational tool for certain types of reactor physics studies.

ACKNOWLEDGEMENTS

This research was sponsored by the Nuclear Energy Program, Reactor Research and Technology Division, U. S. Department of Energy under contract, W-7405-eng-26, with Union Carbide Corporation.

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