# Differential Sensitivity Analysis of Model Equation System

Summary and Results

TR-112100

Final Report, January 1999

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This report describes research sponsored by EPRI.

The report is a corporate document that should be cited in the literature in the following manner:

*Differential Sensitivity Analysis of Model Equation System: Summary and Results, EPRI, Palo Alto, CA: 1999. TR-112100.* 

## **REPORT SUMMARY**

Identification and quantification of the important parameters in mathematical models of physical processes continues to be a significant area of research. Differential Sensitivity Analysis (DSA) has been demonstrated to be a useful method for parameter sensitivity investigations. In this work, DSA has been applied to a system of model equations to determine if the methodology can be used effectively for sensitivity analysis.

#### Background

Questions almost always arise concerning which of the many parameters in models and codes are the most important. Various methods have been developed to try to determine sensitivity of models and codes to their parameters. In the absence of a formal methodology, the usual practice is to execute the code with several different values for each parameter to cover the range of expected values. Unfortunately, this approach must be carried out for each individual application of the model and software to both identify the important parameters and then to quantify their effects. Sensitivity theory is a methodology for assessing the effects and importance of parameter variations on selected results (usually referred to as 'responses') in any process that can be represented by mathematical models. DSA is a powerful method for identifying important parameters relative to design features in complex physical processes and engineering systems. The DSA method also quantifies the relative importance of all parameters in models and software.

#### **Objectives**

To study the ability of DSA to augment, guide, or ultimately reduce the effort required to determine model sensitivities.

#### Approach

In this work, the project team applied the concepts and methods explored by Cacuci and others at the Oak Ridge National Laboratory to a simple equation system (similar to that of RETRAN-3D code). The model included equations for transient fluid flow, heat conduction, and reactor kinetics. The team developed adjoint sensitivity equations and defined a response function.

#### Results

Results show that DSA produces reasonable predictions of forward equations within linear limitations and has potential as a tool for analysis of complex physical systems.

### **EPRI** Perspective

The models and results in this study are a first step in differential sensitivity analysis for RETRAN and other EPRI codes. The current trend in advanced codes is to move to more predictive or first-order sensitivity models; such a move will help users assess model uncertainty effects on the response being studied. EPRI believes this project will help in the evaluation of such models for its codes.

### TR-112100

## **Interest Category**

Exploratory research & new science

## Keywords

Differential sensitivity analysis Sensitivity analysis Uncertainty effects Adjoint response functions

# ABSTRACT

Identification and quantification of the importance of the parameters in mathematical models of physical processes continues to be an important area of research. Differential Sensitivity Analysis (DSA) has been demonstrated to be a useful method for parameter sensitivity investigations. DSA is directly applied to the model equations and performs both the identification and quantification of parameter sensitivity.

In this work, DSA has been applied to a system of model equations similar to that of the RETRAN-3D code to determine if DSA can be used effectively for sensitivity analysis. The results show that DSA produces reasonable predictions of the forward equations within the linear limitations and has the potential as a tool for analysis of complex physical systems.

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# **1** INTRODUCTION AND OBJECTIVE

Identification and quantification of the importance of parameters in complex mathematical models and computer software is an integral part of the software lifecycle. Two kinds of parameters are introduced into mathematical models; those that are well based in theory and those of a more empirical or heuristic nature. The former kind of parameter includes transport properties, for example, and although these are well founded in theory, the exact value could be uncertain for a variety of reasons. The second kind might be associated with engineering models or correlations of physical processes. The value or even the form of these parameters might be uncertain due to the basic nature of engineering correlations and modeling of complex physical phenomena. Additional parameters of interest are introduced by the use of software in analyses. The geometric properties of the system, usually represented as input values to the code, may be uncertain and the time-step size used for numerical integration of the equations is also a parameter.

Questions almost always arise concerning which of the many parameters in the models and codes are the most important and what are the effects of the uncertainty of the value of the important parameters in the results obtained from the models and computer codes. In the practice of everyday application of software to analyses of systems and processes, a single run of the code is almost never sufficient because of these issues. Various methods have been developed to try to determine the sensitivity of the model and codes to the parameters. In the absence of a formal methodology, the usual practice is to execute the code with several different values of the parameters in order to cover the range of expected values. Unfortunately, this approach must be carried out for each individual application of the model and software in order to both identify the important parameters and then to quantify the effects of these.

Sensitivity theory is a methodology for assessing the effects and importance of parameter variations on selected results (usually referred to as 'responses') in any process (e.g., physical, engineering, biological, etc.) that can be represented by mathematical models. It is important to note that sensitivity theory accomplishes both identification and quantification of the important parameters relative to the system response under consideration. Models based on partial and ordinary differential equations and algebraic equations, including finite difference equations, are candidates for application of sensitivity theory. Applications in the literature include hyperbolic,

#### Introduction and Objective

elliptic, and parabolic partial differential equation systems, systems of ordinary differential equations, algebraic systems, and combinations of these types.

Differential Sensitivity Analysis (DSA) is a powerful method for identification of important parameters relative to design features in complex physical processes and engineering systems. The DSA method also quantifies the relative importance of all parameters in the models and software. DSA was originally developed to analyze the sensitivity of reactor shield performance to design features such as shield material and geometry. DSA can also be use to optimize a system relative to parameters contained in the models of the physical processes. DSA theory is related to parameter estimation and optimization methods. Early references to the development and application of DSA are given in the books by Tomovic,[1] Radanovic,[2] and Tomovic and Vukoratic.[3]

The resurgence of interest in DSA in the nuclear power industry in the 1970s and early 1980s was lead by Cacuci, Oblow, and coworkers at the Oak Ridge National Laboratory. Some of the ORNL work during this time period was funded by EPRI. A sample of publications from the research at ORNL are given in References 4 through 12.

The methods examined in the research were advanced by Cacuci who formalized and extended a general sensitivity theory that applies to almost all problems of practical interest, especially problems which are motivated by physical phenomena. Application of the functional (Gateaux) differential to the model's equations, boundary and initial conditions, and the system's response gives an auxiliary system of equations for the sensitivities of the response to variations in the parameters. Cacuci has shown that existence and uniqueness of the solution of the model equations ensures the existence and uniqueness of the sensitivity equations.

In this work, we apply the concepts and methods that have been explored by Cacuci and others to a simple equation system. The model includes equations for transient fluid flow, heat conduction, and reactor kinetics. Adjoint sensitivity equations were developed and a response function is defined. The objective of this work is to study the ability of the method to augment, guide, or ultimately reduce the effort required to determine model sensitivities.

# **BACKGROUND AND LITERATURE REVIEW**

## **Previous Applications of DSA**

DSA is a powerful methodology for both identifying and quantifying the most important parameters in mathematical models of physical processes. Because many, if not all, mathematical models are ultimately developed into computer software, DSA is usually applied to the software containing the equations and numerical solution methods for the models.

There is a large body of research in which sensitivity analysis is under consideration or has been demonstrated to aid in calculating the uncertainty of a response. The application of these methods to the area of two-phase flow and coupled nuclear safety-related research was systematically investigated in the early 1980's.[8-10]

Applications exist in hydrology and geology[13-19] in which the modeling of transport and diffusion are examined in groundwater and aquifers. In these models of groundwater flow systems, performance indices include piezometric heads, velocities, or travel time in aquifers and ultimate mass discharge to the biosphere. These responses depend upon boundary heads or fluxes, aquifer recharge-discharge rates and hydraulic conductivities. One of the fortunate aspects of these models is that groundwater performance studies can usually be measured against test site data as a confirmation of the method.

Other related applications have been demonstrated in the characterization of storage sites for radioactive wastes and transport of radionuclides.[28-30] In these systems, the estimated radionuclide transport through various media depend upon soil and transporting fluid properties as well as the radionuclide half life.

Studies involving chemical reaction kinetics and diffusion,[20-27] open channel flow networks[31] and enhanced oil recovery have been reported. In the later work, the effect upon the displacement of oil in a porous medium by the injection of a mixture of water and polymer was investigated. Input parameters such as porosity, permeability, and absorption functions were some of the model uncertainties.

The implementation of adjoint based sensitivity analysis methods in large scale thermalhydraulic analysis codes has been demonstrated for COBRA-IV[33] and

#### Background and Literature Review

CATHARE.[34,35] The later work is aimed at developing automated methods to allow quantification of code uncertainties using a form of adjoint sensitivity analysis, DASM, the discrete adjoint sensitivity method.

Because many of the models and associated software to which DSA is applied were developed before consideration was given to sensitivity analysis, methods have been developed so that DSA can be applied to existing software. Oblow and coworkers have developed a computer code, GRESS,[36,37] to facilitate application of DSA to existing computer codes. GRESS and other codes of a similar nature, are designed to do the algebraic and numerical development of the system of sensitivity equations by use of computer algebra. Other computer algebra codes include ADIFOR,[38] ATOMCC,[39] and the code given by Douglas.[40] Special-purpose codes have also been written to directly include model sensitivities into the analysis. ODESSA,[25] which does analyses of chemical reactions, is an example of these codes. A review of almost all computer algebra codes is given in Reference 41. These codes are also used to develop implicit numerical solution methods for equation systems.

# 3 dsa methodology

Application of sensitivity theory comes in two varieties: forward sensitivity analysis and adjoint sensitivity analysis. Each has its advantages and disadvantages. Forward sensitivity analysis is best suited to problems in which there are few parameter variations and several responses. Adjoint sensitivity analysis is better suited to cases in which there are many parameter variations and few responses. One such situation is, for example, the large break loss of coolant accident, where a typically important response is simply the highest clad temperature attained during the incident, a single response. Note also that the system-wide computer codes used to analyze the transient response of nuclear steam supply systems to postulated incidents are also characterized by a large number of parameters but, in almost all cases, only a single response is identified with each postulated event: the minimum critical power ratio, the maximum allowable power increase, etc. The method of choice for the sensitivity analysis of such problems is again the adjoint method.

Some of the theoretical aspects of DSA are summarized in the following discussion.

Given a set of differential equations describing a physical system

$$HF = 0 \tag{3-1}$$

where

F = dependent variable vector.

If one defines an integral response or output from this set of equations given by

$$\mathbf{R} = \int_{\mathbf{s}} \mathbf{E}(\mathbf{F}(\mathbf{s}), \alpha) \, \mathrm{d}\mathbf{s} \tag{3-2}$$

where

- E=response function,s=phase space variable, and
- $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_n)$ , input or model parameters.

It is possible to define the sensitivity of the response to variations in the parameters which appear in the differential equation set. The sensitivity of the response, R, to a parameter,  $\alpha_i$ , is given by

$$\frac{\mathrm{dR}}{\mathrm{d}\alpha_{j}} = \left\langle \frac{\partial E}{\partial \alpha_{j}} \right\rangle_{\mathrm{s}} + \sum_{i} \left\langle \frac{\partial E}{\partial F_{i}} \frac{\partial F_{i}}{\partial \alpha_{j}} \right\rangle_{\mathrm{s}} . \tag{3-3}$$

The first integral evaluates the direct effect of parameter variations on R and the second integral accounts for the indirect effects through the model equations. For example, assume the response function is a weighted normalized power given by  $f(\alpha) n(t)$ . Then

$$\frac{\partial \mathbf{E}}{\partial \alpha} = \mathbf{n}(\mathbf{t}) \ \frac{\partial \mathbf{f}}{\partial \alpha}$$
(3-4)

and

$$\frac{\partial \mathbf{E}}{\partial \mathbf{n}} \frac{\partial \mathbf{n}}{\partial \alpha} = \mathbf{f}(\alpha) \frac{\partial \mathbf{n}}{\partial \alpha} \quad . \tag{3-5}$$

Equation 3-3 can be evaluated by differentiating Eq. 3-1 with respect to the parameters  $\alpha_i$  and solving the resulting sets of coupled equations for the new variables

$$\Phi_{ij} = \frac{\partial F_i}{\partial \alpha_j} \quad . \tag{3-6}$$

Using adjoint equation methods, the  $\phi_{ij}$ 's can be eliminated from Eq. 3-3 and all the sensitivities to a specified response derived from solving one set of linear equations for the adjoint functions. The sensitivities of the response integral to the parameters are then obtained by integration of known functions.

The equations for  $\phi_{ij}$ , obtained by differentiating Eq. 3-1 with respect to a parameter,  $\alpha_{j}$ , form an inhomogeneous, linear set given by

$$L[\Phi] = S \tag{3-7}$$

with the terms in the source vector known functions of the system variables. The source vector, S, is a function of the particular  $\alpha$  being evaluated. Since Eq. 3-7 is linear, there exists an operator  $M^*$  adjoint to L such that

$$\langle \Phi^{*T}, L[\Phi] \rangle = \langle \Phi^{T}, M^{*}[\Phi^{*}] \rangle + B.C.$$
 (3-8)

where

 $M^{*}[\Phi^{*}] = S^{*},$ B.C. = boundary conditions, and  $S^{*} = adjoint$  source to be defined.

The adjoint operator, M<sup>\*</sup>, can be determined by integrating the left side of Eq. 3-8 by parts to form terms equivalent to the right side of the equation. To evaluate S<sup>\*</sup>, form the equation

$$\langle \Phi^{*T}, L[\Phi] \rangle - \langle \Phi^{T}, M^{*}[\Phi^{*}] \rangle = B.C. = \langle \Phi^{*T}, S(\alpha) \rangle - \langle \Phi^{T}, S^{*} \rangle$$
(3-9)

or

$$\langle \Phi^{\mathrm{T}}, \mathrm{S}^{*} \rangle = \langle \Phi^{*\mathrm{T}}, \mathrm{S}(\alpha) \rangle - \mathrm{B.C.}$$
 (3-10)

Identifying  $S_i^*$  from Eq. 3-10 with the function  $\partial E/\partial F_i$  in the second term on the right side of Eq. 3-3 uniquely defines the adjoint sources for the particular response and Eq. 3-10 provides a prescription for evaluating Eq. 3-3 once the adjoint functions are determined. Applications of these general methods will be illustrated more completely in later sections of the report.

### **Examples**

A good way to demonstrate the power and advantage of the methods described above is to illustrate the techniques with a simple model that has an analytical solution. The advantage of the technique may be lost when applied to such simple systems but the results from simple models can be more intuitive.

### **Simple Motion Equation**

Consider a first order, linear, ordinary differential equation of the form

$$\frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}t} = \mathbf{g} - \tau \mathbf{v}(t) \tag{3-11a}$$

$$v(0) = 0$$
 . (3-11b)

The equation may be viewed as a simple equation of motion where g represents gravity or an accelerating force and  $\tau$  represents a friction or drag coefficient. In this model the parameter vector  $\alpha$  is very simple consisting of  $\tau$  and g.

The solution to Eq. 3-11 subject to the given boundary condition is

$$\mathbf{v}(\mathbf{t}) = \frac{\mathbf{g}}{\tau} \left( 1 - \mathbf{e}^{-\tau \mathbf{t}} \right) . \tag{3-12}$$

For illustration, an arbitrary response is defined, involving the solution, v(t)

$$R = \int_{0}^{t_{r}} f v(t) dt , \qquad (3-13)$$

f is an arbitrary weight factor. R then is a weighted integrated speed and thus represents an effective distance traveled in time  $t_f$ .

Now using this response function and concepts and definitions from the previous section, we define the sensitivity to R or the response derivative as

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\alpha} = \int_{0}^{t_{\mathrm{f}}} \frac{\partial \mathbf{f}}{\partial \alpha} \mathbf{v}(t) \,\mathrm{d}t + \int_{0}^{t_{\mathrm{f}}} \mathbf{f} \,\frac{\partial \mathbf{v}(t)}{\partial \alpha} \,\mathrm{d}t \quad . \tag{3-14}$$

The first term on the right-hand side of Eq. 3-14 represents the direct effect on R or the explicit dependence of R on  $\alpha$  and the second term is the implicit dependence of R on  $\alpha$  through the velocity. Note in Eq. 3-14 that the key term  $\frac{\partial v}{\partial \alpha}$  is a vector quantity consisting of  $\tau$  and g, and it is a time-dependent quantity.

One can gain an intuitive feel for the competing effects of the parameters on the solution by observing the behavior of the solution and the individual  $\partial v / \partial \alpha$ . The analytical expressions are plotted in Figure 3-1 illustrating the behavior over a 10.0 second interval.

As one would expect, the dominant parameter is  $\tau$ , but the early time behavior depends on both parameters. As the solution reaches an equilibrium value (near 5.0 seconds for this particular set of  $\tau$  and g) the effect of either coefficient approaches a constant. Note that the response function R is an integral value and is defined at  $t_{\rm f}$ .

In this example an analytical expression for Eq. 3-14 can be found. Since f is not a function of the  $\alpha$ 's in this case

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\alpha} = \int_{0}^{t_{\mathrm{f}}} \mathbf{f} \, \frac{\partial \mathbf{v}(\mathbf{t})}{\partial \alpha} \, \mathrm{d}\mathbf{t} \tag{3-15}$$

expanding

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\tau} = \int_{0}^{t_{\mathrm{f}}} \mathbf{f} \, \frac{\partial \mathbf{v}(\mathbf{t})}{\partial \tau} \, \mathrm{d}\mathbf{t} \tag{3-16}$$

and

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}g} = \int_{0}^{t_{\mathrm{f}}} \mathbf{f} \, \frac{\partial \mathbf{v}(\mathbf{t})}{\partial g} \, \mathrm{d}\mathbf{t} \quad . \tag{3-17}$$



Figure 3-1 Speed Equation Solution and Sensitivity Coefficients

After some manipulation and evaluating Eq. 3-12 at  $t_{\mbox{\tiny f}}$ 

$$\frac{\tau}{R} \frac{dR}{d\tau} = \frac{\tau}{R} \left[ \frac{2fv(t_f)}{\tau^2} - \frac{t_f fg(1 + e^{-\tau t_f})}{\tau^2} \right]$$
(3-18)

and

$$\frac{g}{R} \frac{dR}{dg} = \frac{g}{R} \left[ \frac{ft_f}{\tau} - \frac{f(1 + e^{-\tau t_f})}{\tau^2} \right].$$
(3-19)

Equations 3-18 and 3-19 are analytical expressions for the sensitivity of the system response, R, to the changes in input or model parameters  $\alpha$ , given by g and  $\tau$ . The expression is based upon a solution to the forward differential equation for v(t). The  $\alpha_i/R$  multipliers are introduced as normalization factors.

Now the relationship between the forward and the adjoint methods can be demonstrated. The previous section has shown that it is possible to compute  $dR/d\alpha$  by solving the differentiated forward equations for each  $\alpha$  based on the expressions for  $\partial v/\partial \alpha$ . The alternative developed below is to solve a set of adjoint equations to obtain all of the  $dR/d\alpha$  for a given response.

Beginning with the initial forward equation, differentiate with respect to  $\alpha$ 

$$\frac{\mathrm{d}}{\mathrm{dt}} \left[ \frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}\alpha} \right] = \frac{\mathrm{d}\mathbf{g}}{\mathrm{d}\alpha} - \tau \left[ \frac{\mathrm{d}\mathbf{v}(t)}{\mathrm{d}\alpha} + \mathbf{v}\frac{\mathrm{d}\tau}{\mathrm{d}\alpha} \right]$$
(3-20)

define  $\phi$  as, <u>dv</u>

$$\frac{\mathrm{d}}{\mathrm{dt}} \left[ \phi \right] = \frac{\mathrm{dg}}{\mathrm{d\alpha}} - \tau \left[ \phi \right] + v \frac{\mathrm{d\tau}}{\mathrm{d\alpha}}$$
(3-21)

re-arranging,

$$\frac{\mathrm{d}\phi}{\mathrm{d}t} + \tau\phi = \mathrm{S} \tag{3-22}$$

where the source term, S is

dα

$$\mathbf{S} = \frac{\partial \mathbf{g}}{\partial \alpha} - \mathbf{v} \frac{\partial \tau}{\partial \alpha}$$
(3-23)

we write the adjoint equation to Eq. 3-22 as

$$-\frac{\mathrm{d}\phi^*}{\mathrm{d}t} + \tau\phi^* = \mathrm{S}^* \tag{3-24}$$

3-7

where  $\phi^*$  is the solution vector and  $S^*$  is a yet to be defined adjoint source.

Now from the previous section and from linear operator theory,

$$\int_{0}^{t_{f}} \phi(t) S^{*} dt = \int_{0}^{t_{f}} \phi^{*}(t) S dt + B.C.$$
(3-25)

where B.C. are the appropriate boundary conditions for the forward and adjoint equations

$$\varphi(0)=\frac{\mathrm{d} v}{\mathrm{d} \alpha}(0)=0$$

and

$$\Phi^*(t_f) = 0 \quad .$$

It is proposed to take advantage of the properties of the adjoint equations in the following manner. The desired term in Eq. 3-14 is

$$\int_{0}^{t_{\rm f}} \mathbf{f} \frac{\partial \mathbf{v}}{\partial \alpha} d\mathbf{t} \quad . \tag{3-26}$$

The desired equivalence between this term and Eq. 3-25 is found if we define

$$\mathbf{f} = \mathbf{S}^* \quad . \tag{3-27}$$

Thus,

$$\int_{0}^{t_{f}} \phi^{*}(t) S dt = \int_{0}^{t_{f}} f \frac{\partial v}{\partial \alpha} dt$$
(3-28)

using Eq. 3-14 and observing that  $\frac{\partial f}{\partial \alpha} = 0$ ,  $\frac{\partial \alpha}{\partial \alpha}$ 

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\alpha} = \int_{0}^{t_{\mathrm{f}}} \phi^{*}(t) \mathrm{f}\mathrm{d}t \quad . \tag{3-29}$$

At first it may seem that there is no significant advantage to adjoint formalism over the direct method. However, the properties of the adjoint method lead to some advantages which include

- the adjoint equation is linear by virtue of its properties,
- direct dependence on  $dv/d\alpha$  has been eliminated, and
- a single additional adjoint run is all that is required to generate the sensitivity coefficients for a given response.

In our example the equivalence between Eqs. 3-18, 3-19, and 3-29 can be demonstrated although in general this is difficult to do analytically.

Re-iterating the adjoint equation

$$\frac{-\mathrm{d}\phi^*}{\mathrm{d}t} = \tau \phi^* = \mathrm{S}^* \tag{3-30}$$

subject to  $\phi^*(t_f) = 0$ 

A solution is (using integrating factors)

$$\phi^{*}(t) = \frac{f}{\tau} \left[ 1 - e^{-\tau (t_{f} - t)} \right] .$$
(3-31)

We are interested in evaluating Eq. 3-29 analytically to show the equivalence.

$$\phi^* \mathbf{S} = \phi^* \left[ \frac{\partial \mathbf{g}}{\partial \alpha} - \mathbf{v}(\mathbf{t}) \ \frac{\partial \tau}{\partial \alpha} \right]$$
(3-32)

For  $\alpha = g$ 

$$\phi^* S = \phi^* \quad . \tag{3-33}$$

For  $\alpha = \tau$ 

$$\phi^* \mathbf{S} = -\phi^* \mathbf{v}(\mathbf{t}) \quad . \tag{3-34}$$

Evaluating Eq. 3-29 for each  $\alpha$ , then

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\mathbf{g}} = \int_{0}^{t_{\mathrm{f}}} \boldsymbol{\varphi}^{*} \mathrm{d}\mathbf{t} = \int_{0}^{t_{\mathrm{f}}} \frac{\mathrm{f}}{\tau} \left[ 1 - \mathrm{e}^{-\tau \left[ \mathbf{t}_{\mathrm{f}} - \mathbf{t} \right]} \right] \mathrm{d}\mathbf{t}$$
$$= \left[ \frac{\mathrm{f}\mathbf{t}_{\mathrm{f}}}{\tau} - \frac{\mathrm{f}^{\left( \mathbf{t} - \mathrm{e}^{-\tau \mathbf{t}_{\mathrm{f}}} \right)}}{\tau^{2}} \right]$$
(3-35)

and  $\alpha$ 

$$\frac{dR}{d\tau} = \int_{0}^{t_{f}} -\phi^{*}v(t)dt = \int_{0}^{t_{f}} \frac{fv(t)}{\tau} \left[1 - e^{-\tau(t_{f}-t)}\right] dt$$
(3-36)

where  $\mathbf{v}(t) = \frac{\mathbf{g}}{\tau} (-\mathbf{e}^{-\tau t}).$ 

Evaluating and rearranging the result is

$$\frac{\mathrm{dR}}{\mathrm{d\tau}} = \frac{2\mathrm{fv}(\mathrm{t}_{\mathrm{f}})}{\tau^2} - \frac{\mathrm{t}_{\mathrm{f}}\mathrm{fg}(1 + \mathrm{e}^{-\tau\mathrm{t}_{\mathrm{f}}})}{\tau^2}$$
(3-37)

which is the desired result.

Thus, it has been shown that the sensitivity response coefficients can be obtained from either the forward (direct) method or the adjoint method and equivalent results can be expected.

In this example,

$$\frac{g}{R} \frac{dR}{dg} = \frac{g}{R} \int_{0}^{t_{f}} \phi^{*}(t)dt = \frac{g}{R} \int_{0}^{t_{f}} f \frac{\partial v}{\partial g}(t) dt$$
(3-38)

$$\frac{\tau}{R} \frac{dR}{d\tau} = \frac{\tau}{R} \int_{0}^{t_{f}} -v(t)\phi^{*}(t)dt = \frac{\tau}{R} \int_{0}^{t_{f}} f \frac{\partial v}{\partial \tau} (t) dt .$$
(3-39)

The normalized sensitivity coefficients given in Eqs. 3-38 and 3-39 are integral quantities and they represent the percent change in R per percent change in  $\alpha$ .

Example calculations were performed to illustrate how the response functions compared with a direct calculation. Tables 3-1 and 3-2 show response function values at two different times for each of four perturbations about the base values of  $\tau$  and g.

Parameter	R <sub>dsa</sub>	R <sub>calculate</sub>
1.1 τ <sub>0</sub>	3.504	3.506
.9 τ <sub>0</sub>	3.707	3.709
1.1 g₀	3.966	3.966
.9 g <sub>o</sub>	3.245	3.245
$g_0 = 9.8$		
- 10		

# Table 3-1Response Values at 1.0 Second

$g_0$	=	9.8
$\tau_{0}$	=	1.0
R	=	3.605

# Table 3-2Response Times at 10.0 Seconds

Parameter	R <sub>dsa</sub>	R <sub>calculate</sub>
$\tau = 1.1 \tau_0$	80.360	80.992
$\tau = .9 \tau_0$	96.041	96.792
$g = 1.1 g_0$	97.02	97.02
$g = .9 g_0$	79.38	79.38

 $g_0 = 9.8$  $\tau_0 = 1.0$ 

 $R_{0}^{0} = 88.2$ 

Recall that the response is an effective distance that would be traveled at v(t) for the problem time  $t_{f}$ .

The base value,  $R_{o}$  is given in the tables. The values for  $R_{DSA}$  are those obtained from adjoint based response Eqs. 3-35 and 3-37, evaluated at  $t_{f}$ . The  $R_{CALCULATE}$  are values for R obtained from a direct integration of the forward equation solution, v(t). The comparisons are good and they illustrate the power of the method.

# 4 MODEL EQUATIONS

A simplified lumped parameter PWR core model was constructed to provide a vehicle for extending the adjoint DSA methodology to a thermal-hydraulic system with time-dependent power capability. This model consists of stacked, power producing heat conductors connected to a common coolant channel with a pressure driven mass flow. A one group point kinetics model provides a time-dependent energy source which can be coupled to the core system. The model geometry shown in Figure 4-1 contains two heated conductors, two fluid volumes, and three junctions.





#### Model Equations

The model equations are 'RETRAN-like' because the equations are based on a staggered mesh, with control volume centered energy and mass, and the momentum equation is solved at the volume boundaries.

Continuity:

$$\frac{\mathrm{d}}{\mathrm{dt}} \mathbf{M}_{1} = \mathbf{W}_{\mathrm{in}} - \mathbf{W}_{\mathrm{j}} \tag{4-1}$$

$$\frac{\mathrm{d}}{\mathrm{dt}} \mathbf{M}_2 = \mathbf{W}_{\mathrm{j}} - \mathbf{W}_{\mathrm{out}} \tag{4-2}$$

Energy:

$$\frac{d}{dt} E_{1} = W_{in}h_{in} - W_{j}h_{j} + h_{c}A_{w} (T_{M1} - T_{1})$$
(4-3)

$$\frac{\mathrm{d}}{\mathrm{dt}} E_2 = W_j h_j - W_{\mathrm{out}} h_{\mathrm{out}} + h_c A_w \left( T_{\mathrm{M2}} - T_2 \right)$$
(4-4)

Momentum:

$$I_{j} \frac{d}{dt} W_{in} = P_{in} - P_{1} - \frac{4}{D_{hy}} \frac{f_{w}}{8} L_{j} \frac{W_{in} |W_{in}|}{\rho_{in} A_{j}^{2}}$$
(4-5)

$$I_{j} \frac{d}{dt} W_{j} = P_{1} - P_{2} - \frac{4}{D_{hy}} \frac{f_{w}}{8} L_{j} \frac{W_{j} |W_{j}|}{\rho_{1} A_{j}^{2}}$$
(4-6)

$$I_{j} \frac{d}{dt} W_{out} = P_{2} - P_{out} - \frac{4}{D_{hy}} \frac{f_{w}}{8} L_{j} \frac{W_{out} |W_{out}|}{\rho_{2} A_{j}^{2}}$$
(4-7)

The temperature of the fuel rod is obtained from a lumped parameter conduction model in which the fuel and clad are combined into a single conduction node.

$$\left(\mathbf{M}_{\text{fuel}}\mathbf{C}_{\text{pfuel}} + \mathbf{M}_{\text{clad}}\mathbf{C}_{\text{pclad}}\right)_{\mathbf{M}1} \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{T}_{\mathbf{M}1} = \mathbf{U}\mathbf{A}\mathbf{w}_{\text{clad}} \left(\mathbf{T}_{1} - \mathbf{T}_{\mathbf{M}1}\right) + \mathbf{Pwr}(\mathbf{0})_{\mathbf{M}1}\mathbf{N}(t)$$
(4-8)

and

Model Equations

$$\left(\mathbf{M}_{\text{fuel}}\mathbf{C}_{\text{pfuel}} + \mathbf{M}_{\text{clad}}\mathbf{C}_{\text{pclad}}\right)_{M2} \frac{\mathrm{d}}{\mathrm{d}t} \mathbf{T}_{M2} = \mathbf{U}\mathbf{A}\mathbf{w}_{\text{clad}} \left(\mathbf{T}_{2} - \mathbf{T}_{M2}\right) + \mathbf{Pwr}(\mathbf{0})_{M2}\mathbf{N}(t)$$
(4-9)

where  $UAw_{clad}$  is an effective conductance for the combined fuel and clad. Accounting for the cylindrical geometry of the fuel and clad,  $UAw_{clad}$  is

$$UAw_{clad} = \frac{1.0}{R_{fuel} + R_{gap} + R_{clad} + R_{conv}} , \qquad (4-10)$$

where the resistances for each of the regions in the lumped model are for the fuel,

$$R_{\text{fuel}} = \frac{r_{\text{fuel}}}{2k_{\text{fuel}}Aw_{\text{fuel}}} , \qquad (4-11)$$

for the fuel-clad gap

$$R_{gap} = \frac{1.0}{H_g A w_{fuel}} , \qquad (4-12)$$

for the clad

$$R_{clad} = \frac{\left(r_{co} - r_{fuel}\right) \ln\left(\frac{Aw_{clad}}{Aw_{fuel}}\right)}{k_{clad} \left(Aw_{clad} - Aw_{fuel}\right)} , \qquad (4-13)$$

and for convection at the clad-fluid interface

$$\mathbf{R}_{\rm conv} = \frac{1}{\mathbf{h}_{\rm c} \mathbf{A} \mathbf{w}_{\rm clad}} \quad . \tag{4-14}$$

Equations 4-1 through 4-14 are closed by specifying an equation of state, a friction factor form, a reactivity function, and appropriate initial and boundary conditions. The equation of state used in the code is the same water property routines used in the RETRAN-3D code. Given the independent variables (M, E) all other fluid-state and transport properties are obtained along with derivatives of the state properties needed for the numerical solution method.

The equation of state is given by

$$P_i = P(E_i, M_i)$$

$$(4-15)$$

and

$$T_{i} = T(E_{i'}, M_{i})$$
 (4-16)

A single-phase friction factor is specified as

$$f_w = CRe^{-0.25}$$
 (4-17)

where

Re = Reynolds number = 
$$\frac{|W| D_e}{A_j \mu_j}$$
 (4-18)

 $\mu_i$  = fluid viscosity.

The neutron kinetics equations supply the normalized power, N(t), and precursor concentration, C(t). These equations are

$$\frac{d}{dt} N = \frac{\rho(t) - \beta}{\Lambda} N + \lambda C$$
(4-19)

and

$$\frac{\mathrm{d}}{\mathrm{dt}} \mathbf{C} = \frac{\beta}{\Lambda} \mathbf{N} - \lambda \mathbf{C} \quad . \tag{4-20}$$

The reactivity function is given as

$$\rho(t) = \rho_{exp} + \alpha_{mod} T_{mod} + \alpha_{dop} T_{M} - \rho_{bias}$$
(4-21)

where

 $\rho_{exp}$  = an explicit reactivity term,

- $\alpha_{mod}$  = moderator temperature coefficient,
- $\alpha_{dop}$  = metal temperature coefficient,
- $T_{mod}$  = average temperature of the coolant in the two nodes of the geometric model, and

$$T_{M}$$
 = average temperature of the two conduction regions.

The reactivity bias,  $\rho_{\text{bias}}$ , is determined from the state of the fuel rod and coolant at steady-state conditions. The explicit reactivity insertion,  $\rho_{\text{exp}}$ , is used as a forcing function during transient calculations. A constant value of  $\rho_{\text{exp}}$  is set at some time into

the transient and these values are reported along with the results of the calculations. At steady-state conditions,  $\rho_{_{exp}} = 0.0$ .

Initial and boundary conditions are

To complete the description, all of the model parameters are described below.

For volume i:

For junction j:

 $W_i = mass flow rate,$ 

 $h_i$  = enthalpy,

 $I_i = inertia = area/flow length,$ 

 $\dot{A}_{i}$  = flow area,

 $L_i^{\prime}$  = flow length,

 $f_w =$ friction factor, and

 $D_e$  = hydraulic diameter of channel.

For heat conductor k:

T <sub>m</sub>	=	temperature,
$(UA_W)_k$	=	heat transfer coefficient,
$\mathbf{h}_{\mathbf{C}^k}$	=	heat transfer coefficient,
$A_{\mathbf{W}^k}$	=	heat transfer area,
$PWR_{M_k}$	=	fraction of power deposited in conductor,
$(MC_p)_k$	=	heat capacity of conductor, and
$Q_k$	=	heat source to coolant.

For neutron equations:

 $\rho$  = reactivity

 $\beta$  = delayed neutron fraction,

 $\Lambda$  = prompt neutron fractions, and

 $\lambda$  = delayed neutron precursor decay constant.

In summary, the basic model equations have been developed for mass, energy, and momentum transfer; heat conduction; and neutron kinetics. The next step is to develop the adjoint equations, sources and sensitivity coefficients in a manner similar to that of the simple model developed in Section 3.

#### **Development of the Adjoint Equations and Sensitivity Coefficients**

As in Section 3, define

$$\Phi_{ij}(t) = \frac{\partial F_i}{\partial \alpha_j}$$
(4-22)

where the  $F_i$ 's are the dependent variables in the 11 coupled differential equations, Eqs. 4-1 through 4-9 and 4-19 and 4-20. The  $\alpha_j$  represents any parameter in the equation set which is summarized in the list in the last section. Differentiating with respect to the parameter  $\alpha_j$  leads, after some manipulation, to the set of equations

$$\frac{\partial \Phi_1}{\partial t} = \Phi_5 - \Phi_6 \quad , \tag{4-23}$$

$$\frac{\partial \Phi_2}{\partial t} = \Phi_6 - \Phi_7 \quad , \tag{4-24}$$

$$\frac{\partial \phi_3}{\partial t} + GG\phi_3 = - EE\phi_1 + h_{in}\phi_5 - FF\phi_6 - HH\phi_8 + S_3 , \qquad (4-25)$$

$$\frac{\partial \Phi_4}{\partial t} + PP \phi_3 = - KK \phi_2 + h_2 \phi_6 - LL \phi_7 - QQ \phi_9 + S_4 , \qquad (4-26)$$

$$B\frac{\partial \Phi_5}{\partial t} + C\phi_5 = -A\phi_1 - D\phi_3 + S_5 , \qquad (4-27)$$

$$G\frac{\partial \Phi_6}{\partial t} + H \Phi_6 = - E \Phi_1 - F \Phi_2 - I \Phi_3 - J \Phi_4 + S_6 , \qquad (4-28)$$

$$BB\frac{\partial \phi_7}{\partial t} + CC\phi_7 = -AA\phi_2 - DD\phi_4 + S_7 , \qquad (4-29)$$
$$N\frac{\partial \Phi_8}{\partial t} + P \Phi_8 = -L \Phi_1 - M \Phi_3 - S \Phi_6 - Q \Phi_{10} + S_8 , \qquad (4-30)$$

$$AD \frac{\partial \Phi_9}{\partial t} + AE \Phi_9 = -AB \Phi_2 - AC \Phi_4 - X \Phi_7 - AF \Phi_{10} + S_9 , \qquad (4-31)$$

$$\frac{\partial \phi_{10}}{\partial t} + BJ\phi_{10} = -BC\phi_1 - BD\phi_2 - BE\phi_3 - BF\phi_4$$
  
- BG\phi\_8 - BH\phi\_9 +  $\lambda \phi_{11} + S_{10}$ , (4-32)

and

$$\frac{\partial \phi_{11}}{\partial t} + \lambda \phi_{11} = -CD\phi_{10} + S_{11}$$
(4-33)

where

$$\Phi_1 = \frac{\partial \mathbf{M}_1}{\partial \alpha_j} = \text{Vol. 1 mass derivative,}$$
$$\Phi_2 = \frac{\partial \mathbf{M}_2}{\partial \alpha_j} = \text{Vol. 2 mass derivative,}$$

$$\phi_3 = \frac{\partial E_1}{\partial \alpha_j} = \text{Vol. 1 energy derivative,}$$

$$\phi_4 = \frac{\partial E_2}{\partial \alpha_j} = \text{Vol. 2 energy derivative,}$$

$$\phi_5 = \frac{\partial W_{in}}{\partial \alpha_j} = \text{Inlet flow derivative,}$$

$$\phi_6 = \frac{\partial \mathbf{W}}{\partial \alpha_j} = \text{Middle junction flow derivative,}$$

$$\begin{split} \varphi_7 &= \frac{\partial W_{out}}{\partial \alpha_j} &= \text{Exit junction flow derivative,} \\ \varphi_8 &= \frac{\partial T_{M1}}{\partial \alpha_j} &= \text{Conductor 1 temperature derivative,} \\ \varphi_9 &= \frac{\partial T_{M2}}{\partial \alpha_j} &= \text{Conductor 2 temperature derivative,} \\ \varphi_{10} &= \frac{\partial N}{\partial \alpha_j} &= \text{Normalized power derivative, and} \\ \varphi_{11} &= \frac{\partial C}{\partial \alpha_j} &= \text{Normalized precursor derivative,} \end{split}$$

where the coefficients contain derivatives with respect to the various forward dependent variables but do not contain any derivatives with respect to the parameter  $\alpha_j$ . The source terms,  $S_i$ , contain derivatives of the system parameters with respect to  $\alpha_j$ . The exact form of these expressions are given in Appendix B. Initial conditions are given by

$$\frac{\partial \mathbf{F}_{i}(\mathbf{0})}{\partial \boldsymbol{\alpha}_{j}}$$

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The set of equations adjoint to the left side of Eqs. 4-22 through 4-33 can be found by forming the bilinear product in a manner similar to the example problem.

$$\langle \phi^* L \phi \rangle = \langle \phi, M^* \phi^* \rangle + B.C.$$
 (4-34)

resulting in the set of equations

$$\frac{-\partial \phi_1^*}{\partial t} = \mathbf{S}_1^* \quad , \tag{4-35}$$

$$\frac{-\partial \phi_2^*}{\partial t} = S_2^* \quad , \tag{4-36}$$

$$\frac{-\partial \phi_3^*}{\partial t} + GG\phi_3^* = S_3^* , \qquad (4-37)$$

$$\frac{-\partial \phi_4^*}{\partial t} + PP \phi_4^* = S_4^* , \qquad (4-38)$$

$$\frac{-\partial \left[\mathbf{B}\boldsymbol{\phi}_{5}^{*}\right]}{\partial t} + \mathbf{C}\boldsymbol{\phi}_{5}^{*} = \mathbf{S}_{5}^{*} , \qquad (4-39)$$

$$\frac{-\partial \left[ \mathbf{G} \boldsymbol{\phi}_{6}^{*} \right]}{\partial \mathbf{t}} + \mathbf{H} \boldsymbol{\phi}_{6}^{*} = \mathbf{S}_{6}^{*} , \qquad (4-40)$$

$$\frac{-\partial \left[ \mathbf{B} \mathbf{B} \boldsymbol{\phi}_{7}^{*} \right]}{\partial t} + \mathbf{C} \mathbf{C} \boldsymbol{\phi}_{7}^{*} = \mathbf{S}_{7}^{*} , \qquad (4-41)$$

$$\frac{-\partial \left[N\varphi_{g}^{*}\right]}{\partial t} + P\varphi_{g}^{*} = S_{g}^{*} , \qquad (4-42)$$

$$\frac{-\partial \left[AD\varphi_{9}^{*}\right]}{\partial t} + AE\varphi_{9}^{*} = S_{9}^{*} , \qquad (4-43)$$

$$\frac{-\partial \phi_{10}^*}{\partial t} + BJ \phi_{10}^* = S_{10}^* , \qquad (4-44)$$

and

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$$\frac{-\partial \phi_{11}^{*}}{\partial t} + \lambda \phi_{11}^{*} = S_{11}^{*} .$$
 (4-45)

The adjoint source functions,  $S_i^*$ , depend upon the particular response function, E (F (s),  $\alpha_j$ ), specified in Eq. 3-2. The form of response function selected for testing this RETRAN-like model was

$$\mathbf{R} = \int_{\mathbf{t}} \sum_{i} \mathbf{f}_{i} \mathbf{F}_{i} d\mathbf{t}$$
(4-46)

where

 $f_i$  = weight function for variable  $F_i$ .

Thus, if  $f_{10} = 1.0$  and  $f_i = 0$ ,  $i \neq 10$ , the response function defines an integrated normalized power, or normalized energy. Using Eq. 4-46 with the transformation given in Eq. 3-10, the adjoint source functions are as follows

$$S_1^* = f_1 - EE\varphi_3^* - A\varphi_5^* - E\varphi_6^* - L\varphi_8^* - BC\varphi_{10}^*$$
, (4-47)

$$S_2^* = f_2 - KK\phi_4^* - F\phi_6^* - AA\phi_7^* - AB\phi_9^* - BD\phi_{10}^*$$
, (4-48)

$$S_3^* = f_3 - D\phi_5^* - I\phi_6^* - M\phi_8^* - BE\phi_{10}^*$$
, (4-49)

$$S_4^* = f_4 - J\phi_6^* - DD\phi_7^* - AC\phi_9^* - BF\phi_{10}^*$$
, (4-50)

$$S_5^* = f_5 + \phi_1^* + h_{in}\phi_3^*$$
, (4-51)

$$S_6^* = f_6 - \phi_1^* + \phi_2^* - FF\phi_3^* + h_2\phi_4^* - S\phi_8^* , \qquad (4-52)$$

$$S_7^* = f_7 - \phi_2^* - LL\phi_4^* - X\phi_9^*$$
, (4-53)

$$S_8^* = f_8 - HH\varphi_3^* - BG\varphi_{10}^*$$
, (4-54)

$$S_9^* = f_9 - QQ\phi_4^* - BH\phi_{10}^*$$
, (4-55)

$$S_{10}^{*} = f_{10} - Q\phi_{8}^{*} - AF\phi_{9}^{*} + \frac{\beta}{\Lambda}\phi_{11}^{*} , \qquad (4-56)$$

and

$$S_{11}^* = f_{11} + \lambda \phi_{10}^* \quad . \tag{4-57}$$

With the adjoint sources defined in Eqs. 4-47 through 4-57 the adjoint equations for the model become

$$\frac{\partial \phi_1^*}{\partial t} = -f_1 + EE\phi_3^* + A\phi_5^* + E\phi_6^* + L\phi_8^* + BC\phi_{10}^* , \qquad (4-58)$$

$$\frac{\partial \phi_2^*}{\partial t} = -f_2 + KK\phi_4^* + F\phi_6^* + AA\phi_7^* + AB\phi_9^* + BD\phi_{10}^* , \qquad (4-59)$$

$$\frac{\partial \phi_3^*}{\partial t} = -f_3 + GG\phi_3^* + D\phi_5^* + I\phi_6^* + M\phi_8^* + BE\phi_{10}^* , \qquad (4-60)$$

$$\frac{\partial \phi_4^*}{\partial t} = -f_4 + PP\phi_4^* + J\phi_6^* + DD\phi_7^* + AC\phi_9^* + BF\phi_{10}^* , \qquad (4-61)$$

$$\frac{\partial \Phi_5^*}{\partial t} = \frac{-f_5}{B} - \frac{1}{B} \Phi_1^* - \frac{h_{in}}{B} \Phi_3^* + \frac{1}{B} \left[ C - \frac{\partial B}{\partial t} \right] \Phi_5^* , \qquad (4-62)$$

$$\frac{\partial \phi_6^*}{\partial t} = \frac{-f_6}{G} + \frac{1}{G} \phi_1^* + \frac{1}{G} \phi_2^* + \frac{FF}{G} \phi_3^* - \frac{h_2}{G} \phi_4^* + \frac{1}{G} \left[ H - \frac{\partial G}{\partial t} \right] \phi_6^* + \frac{S}{G} \phi_8^* , \quad (4-63)$$

$$\frac{\partial \phi_7^*}{\partial t} = \frac{-\mathbf{f}_7}{\mathbf{BB}} + \frac{1}{\mathbf{BB}} \phi_2^* + \frac{\mathbf{LL}}{\mathbf{BB}} \phi_4^* + \frac{1}{\mathbf{BB}} \left[ \mathbf{CC} - \frac{\partial (\mathbf{BB})}{\partial t} \right] \phi_7^* + \frac{\mathbf{X}}{\mathbf{BB}} \phi_9^* \quad , \tag{4-64}$$

$$\frac{\partial \phi_8^*}{\partial t} = \frac{-f_8}{N} + \frac{HH}{N} \phi_3^* + \frac{1}{N} \left[ P - \frac{\partial N}{\partial t} \right] \phi_8^* + \frac{BG}{N} \phi_{10}^* , \qquad (4-65)$$

$$\frac{\partial \phi_{9}^{*}}{\partial t} = \frac{-f_{9}}{AD} + \frac{QQ}{AD} \phi_{4}^{*} + \frac{1}{AD} \left[ AE - \frac{\partial (AD)}{\partial t} \right] \phi_{9}^{*} + \frac{BH}{AD} \phi_{10}^{*} , \qquad (4-66)$$

$$\frac{\partial \phi_{10}^{*}}{\partial t} = -f_{10} + Q\phi_{8}^{*} + AF\phi_{9}^{*} + BJ\phi_{10}^{*} - \frac{\beta}{\Lambda}\phi_{11}^{*} , \qquad (4-67)$$

4-11

and

$$\frac{\partial \phi_{11}^{*}}{\partial t} = -f_{11} - \lambda \phi_{10}^{*} + \lambda \phi_{11}^{*} . \qquad (4-68)$$

The adjoint equations are a final value problem requiring  $\phi_i^*(t_{final})$  to be specified and are given as

$$\phi_i^*(t_{\text{final}}) = 0.0$$
  $i = 1,11$  . (4-69)

Once the weight functions,  $f_i$ , are specified which determine the response, Eq. 4-46, and the solution to the adjoint equations, Eqs. 4-58 through 4-68, are obtained, the sensitivity of the response to variation in the forward equation parameters may be determined through Eq. 3-10. For the 11-equation RETRAN-like model described in this section, the sensitivity of the response to a parameter,  $\alpha_i$ , is given by

$$\frac{\mathrm{dR}}{\mathrm{d}\alpha_{j}} = \left\langle \bar{\Phi}^{\mathrm{T}}, \bar{S}^{*} \right\rangle_{\mathrm{t}} = \left\langle \bar{\Phi}^{*\mathrm{T}}, \bar{S} \right\rangle_{\mathrm{t}} + \left[ \bar{\Phi}^{\mathrm{T}}, \mathbf{K} \bar{\Phi}^{*} \right] \Big|_{\mathrm{t=0}}$$
(4-70)

where K is a diagonal matrix.

Expanding Eq. 4-70 results in the following equation.

$$\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}\alpha_{j}} = \sum_{i=1}^{11} \left\langle \phi_{i}^{*} \mathbf{S}_{i} \right\rangle_{t} + \sum_{i=1}^{11} \phi_{i} \mathbf{K}_{ii} \phi_{i}^{*} \bigg|_{t=0}$$
(4-71)

where

$$\begin{split} S_{1} &= 0 , \\ K_{1,1} &= 1.0 , \\ S_{2} &= 0 , \\ K_{2,2} &= 1.0 , \end{split}$$
$$S_{3} &= W_{in} \frac{\partial h_{in}}{\partial \alpha_{j}} - W_{2} \frac{\partial h_{2}}{\partial \alpha_{j}} + W_{in} \left\{ \frac{\partial h_{in}}{\partial P_{in}} \frac{\partial P_{in}}{\partial \alpha_{j}} + \frac{\partial h_{in}}{\partial T_{in}} \frac{\partial T_{in}}{\partial \alpha_{j}} \right\}$$
$$+ (T_{M1} - T_{1}) \frac{\partial \{h_{e}A_{W}\}_{1}}{\partial \alpha_{j}} - (h_{c}A_{W})_{1} \frac{\partial T_{1}}{\partial \alpha_{j}} , \end{split}$$

 $K_{_{3,3}} = 1.0$  ,

$$\begin{split} \mathbf{S}_{4} &= \mathbf{W}_{2} \frac{\partial \mathbf{h}_{2}}{\partial \alpha_{j}} - \mathbf{W}_{\text{out}} \frac{\partial \mathbf{h}_{\text{out}}}{\partial \alpha_{j}} + \frac{\partial \{\mathbf{h}_{c} \mathbf{A}_{\mathbf{W}}\}_{2}}{\partial \alpha_{j}} \left(\mathbf{T}_{\text{M2}} - \mathbf{T}_{2}\right) \\ &- \left\{\mathbf{h}_{c} \mathbf{A}_{\mathbf{W}}\right\}_{2} \frac{\partial \mathbf{T}_{2}}{\partial \alpha_{j}} , \end{split}$$

 $K_{_{4,4}} = 1.0$  ,

$$\begin{split} \mathbf{S}_{5} &= \mathbf{P}_{in} \mathbf{A}_{1}^{2} \frac{\partial \mathbf{P}_{in}}{\partial \alpha_{j}} + (\mathbf{P}_{in} - \mathbf{P}_{1}) \mathbf{\rho}_{in} \frac{\partial \mathbf{A}_{j}^{2}}{\partial \alpha_{j}} + (\mathbf{P}_{in} - \mathbf{P}_{1}) \mathbf{A}_{1}^{2} \left\{ \frac{\partial \mathbf{\rho}_{in}}{\partial \mathbf{P}_{in}} \frac{\partial \mathbf{P}_{in}}{\partial \alpha_{j}} + \frac{\partial \mathbf{\rho}_{in}}{\partial \mathbf{T}_{in}} \frac{\partial \mathbf{T}_{in}}{\partial \alpha_{j}} \right\} \\ &- \frac{\partial \left\{ \frac{\mathbf{L}_{1}}{2\mathbf{D}_{e}} \right\}}{\partial \alpha_{j}} \mathbf{f}_{W} \mathbf{W}_{in} \left| \mathbf{W}_{in} \right| - \frac{\mathbf{L}_{1}}{2\mathbf{D}_{e}} \frac{\partial \mathbf{f}_{W}}{\partial \alpha_{j}} \mathbf{W}_{in} \left| \mathbf{W}_{in} \right| , \end{split}$$

$$\begin{split} \mathbf{K}_{5,5} &= \rho_{\mathrm{in}} \mathbf{A}_{1}^{2} \mathbf{I}_{1} ,\\ \mathbf{S}_{6} &= -\rho_{1} \dot{\mathbf{W}}_{2} \frac{\partial \left\{ \mathbf{A}_{2}^{2} \mathbf{I}_{2} \right\}}{\partial \alpha_{\mathrm{j}}} + \rho_{1} \mathbf{A}_{2}^{2} \frac{\partial \mathbf{P}_{1}}{\partial \alpha_{\mathrm{j}}} - \rho_{2} \mathbf{A}_{2}^{2} \frac{\partial \mathbf{P}_{2}}{\partial \alpha_{\mathrm{j}}} \\ &+ \left( \mathbf{P}_{1} - \mathbf{P}_{2} \right) \rho_{1} \frac{\partial \mathbf{A}_{2}^{2}}{\partial \alpha_{\mathrm{j}}} - \frac{\partial \left\{ \frac{\mathbf{L}_{1}}{2\mathbf{D}_{e}} \right\}}{\partial \alpha_{\mathrm{j}}} \mathbf{f}_{\mathrm{W}} \mathbf{W}_{2} \left| \mathbf{W}_{2} \right| - \frac{\mathbf{L}_{2}}{2\mathbf{D}_{e}} \frac{\partial \mathbf{f}_{\mathrm{W}}}{\partial \alpha_{\mathrm{j}}} \mathbf{W}_{2} \left| \mathbf{W}_{2} \right| , \end{split}$$

$$\begin{split} \mathbf{K}_{6,6} &= \rho_1 \mathbf{A}_2^2 \mathbf{I}_2 \ , \\ \mathbf{S}_7 &= - \frac{\partial \left\{ \mathbf{A}_3^2 \mathbf{I}_3 \right\}}{\partial \alpha_j} \rho_2 \dot{\mathbf{W}}_{out} + \rho_2 \mathbf{A}_3^2 \frac{\partial \mathbf{P}_2}{\partial \alpha_j} - \rho_2 \mathbf{A}_3^2 \frac{\partial \mathbf{P}_{out}}{\partial \alpha_j} \\ &+ \left( \mathbf{P}_2 - \mathbf{P}_{out} \right) \rho_2 \frac{\partial \mathbf{A}_3^2}{\partial \alpha_j} - \frac{\partial \left\{ \frac{\mathbf{L}_3}{2\mathbf{D}_e} \right\}}{\partial \alpha_j} \mathbf{f}_{\mathbf{W}} \mathbf{W}_{out} \left| \mathbf{W}_{out} \right| - \frac{\mathbf{L}_3}{2\mathbf{D}_e} \frac{\partial \mathbf{f}_{\mathbf{W}}}{\partial \alpha_j} \mathbf{W}_{out} \left| \mathbf{W}_{out} \right| \end{split}$$

4-13

,

$$\begin{split} \mathbf{K}_{7,7} &= \rho_2 \, \mathbf{A}_3^{\ 2} \, \mathbf{I}_3 \ , \\ \mathbf{S}_8 &= - \frac{\partial \{\mathbf{M} \mathbf{C}_p\}_{\mathbf{M}1}}{\partial \alpha_j} \, \dot{\mathbf{T}}_{\mathbf{M}1} + \frac{\partial \{\mathbf{U} \mathbf{A}_{\mathbf{W}}\}_{\mathbf{M}1}}{\partial \alpha_j} \left(\mathbf{T}_1 - \mathbf{T}_{\mathbf{M}1}\right) + \left(\mathbf{U} \mathbf{A}_{\mathbf{W}}\right)_{\mathbf{M}1} \, \frac{\partial \mathbf{T}_1}{\partial \alpha_j} \\ &+ \frac{\partial \{\mathbf{PWR}(\mathbf{0})\}_{\mathbf{M}1}}{\partial \alpha_j} \, \mathbf{N} \ , \end{split}$$

$$K_{8,8} = (MC_p)_{M1}$$
,

$$\begin{split} \mathbf{S}_{9} &= - \frac{\partial \left\{ \mathbf{M} \mathbf{C}_{p} \right\}_{M2}}{\partial \alpha_{j}} \ \dot{\mathbf{T}}_{M2} \, + \, \frac{\partial \left\{ \mathbf{U} \mathbf{A}_{W} \right\}_{M2}}{\partial \alpha_{j}} \left( \mathbf{T}_{2} \, - \, \mathbf{T}_{M2} \right) + \left( \mathbf{U} \mathbf{A}_{W} \right)_{M2} \, \frac{\partial \mathbf{T}_{2}}{\partial \alpha_{j}} \\ &+ \, \frac{\partial \left\{ \mathbf{PWR}(\mathbf{0}) \right\}_{M2}}{\partial \alpha_{j}} \ \mathbf{N} \ , \end{split}$$

$$\begin{split} \mathbf{K}_{9,9} &= (\mathbf{M}\mathbf{C}_{p})_{M2} ,\\ \mathbf{S}_{10} &= \frac{\mathbf{N}}{\Lambda} \frac{\partial \bar{p}}{\partial \alpha_{j}} - \frac{\mathbf{N}}{\Lambda} \frac{\partial \beta}{\partial \alpha_{j}} - \left\{ \frac{\bar{p} - \beta}{\Lambda} \right\} \frac{\mathbf{N}}{\Lambda} \frac{\partial \Lambda}{\partial \alpha_{j}} + \mathbf{C} \frac{\partial \lambda}{\partial \alpha_{j}} \\ \mathbf{K}_{10,10} &= 1.0,\\ \mathbf{S}_{10} &= \frac{\mathbf{N}}{\Lambda^{2}} \left\{ \Lambda \frac{\partial \beta}{\partial \alpha_{j}} - \beta \frac{\partial \Lambda}{\partial \alpha_{j}} \right\} - \mathbf{C} \frac{\partial \lambda}{\partial \alpha_{j}} , \end{split}$$

and

$$K_{11,11} = 1.0$$
 .

While the total response given by Eq. 4-71 appears quite complex, for any given  $\alpha_{j'}$  many terms in Eq. 4-71 will be zero resulting in a fairly simple calculation.

The remaining piece of information necessary to evaluate Eq. 4-71 are the initial values for the  $\phi_i$ 's, i.e.,

,

$$\varphi_{ij}(0) = \frac{\partial F_i(0)}{\partial \alpha_j} \quad .$$

These are obtained from the initial conditions for the forward equations given by

$$M_{1} = V_{1}\rho_{1}(T_{1}, P_{1}) , \qquad (4-72)$$

$$M_2 = V_2 \rho_2 (T_2, P_2) , \qquad (4-73)$$

$$\frac{1}{2D_{e}} \frac{f_{w}L_{1}}{\rho_{in}A_{1}^{2}} W |W| + \frac{1}{2D_{e}} \frac{f_{w}L_{2}}{\rho_{2}A_{2}^{2}} W |W| + \frac{1}{2D_{e}} \frac{f_{w}L_{3}}{\rho_{2}A_{3}^{2}} W |W| = P_{in} - P_{out}$$

$$W |W| = \frac{(P_{in} - P_{out}) 2D_{e}}{\sum_{j=1}^{3} \frac{\rho_{j}A_{j}^{2}}{f_{w}L_{j}}}, \qquad (4-74)$$

$$\mathbf{E}_{1} = \mathbf{M}_{1} \, \mathbf{e}_{1} \, (\mathbf{T}_{1}, \mathbf{P}_{1}) \,, \tag{4-75}$$

$$E_2 = M_2 e_2 (T_1, P_1) , \qquad (4-76)$$

$$T_{M1} = T_1 + \frac{PWR(0)_{M1}}{(UA_w)_{M1}} , \qquad (4-77)$$

$$T_{M2} = T_2 + \frac{PWR(0)_{M2}}{(UA_w)_{M2}}$$
, (4-78)

$$h_2 = h_{in} + \frac{(h_c A_W)_1}{W} (T_{M1} - T_1)$$
, (4-79)

$$h_{out} = h_2 + \frac{(h_c A_W)_2}{W} (T_{M2} - T_2) ,$$
 (4-80)

$$N(0) = 1.0$$
, (4-81)

$$C(0) = \frac{\beta \Lambda}{\lambda} , \qquad (4-82)$$

$$P_{1} = P_{in} - \frac{1}{2D_{e}} \frac{f_{W}L_{1}}{P_{in}A_{1}^{2}} W |W| , \qquad (4-82)$$

$$P_2 = P_2 - \frac{1}{2D_e} \frac{f_w L_2}{P_1 A_2^2} W |W| , \qquad (4-83)$$

$$\phi_{1}(0) = \frac{\partial \mathbf{M}_{1}(0)}{\partial \alpha_{j}} = \rho_{1} \frac{\partial \mathbf{V}_{1}}{\partial \alpha_{j}} + \mathbf{V}_{1} \left\{ \frac{\partial \rho_{1}}{\partial \mathbf{T}_{1}} \frac{\partial \mathbf{T}_{1}}{\partial \alpha_{j}} + \frac{\partial \rho_{1}}{\partial \mathbf{P}_{1}} \frac{\partial \mathbf{P}_{1}}{\partial \alpha_{j}} \right\},$$
(4-84)

$$\Phi_{2}(0) = \frac{\partial \mathbf{M}_{2}(0)}{\partial \alpha_{j}} = \rho_{2} \frac{\partial \mathbf{V}_{2}}{\partial \alpha_{j}} + \mathbf{V}_{2} \left\{ \frac{\partial \rho_{2}}{\partial \mathbf{T}_{2}} \frac{\partial \mathbf{T}_{2}}{\partial \alpha_{j}} + \frac{\partial \rho_{2}}{\partial \mathbf{P}_{2}} \frac{\partial \mathbf{P}_{2}}{\partial \alpha_{j}} \right\},$$
(4-85)

$$\phi_{3}(0) = \frac{\partial E_{1}(0)}{\partial \alpha_{j}} = e_{1} \left( T_{1}, P_{1} \right) \frac{\partial M_{1}(0)}{\partial \alpha_{j}} + M_{1} \left\{ \frac{\partial e_{1}}{\partial T_{1}} \frac{\partial T_{1}}{\partial \alpha_{j}} + \frac{\partial e_{1}}{\partial P_{1}} \frac{\partial P_{1}}{\partial \alpha_{j}} \right\}, \qquad (4-86)$$

$$\Phi_4(0) = \frac{\partial E_2(0)}{\partial \alpha_j} = e_2 \left( T_2, P_2 \right) \frac{\partial M_2(0)}{\partial \alpha_j} + M_2 \left\{ \frac{\partial e_2}{\partial T_2} \frac{\partial T_2}{\partial \alpha_j} + \frac{\partial e_2}{\partial P_2} \frac{\partial P_2}{\partial \alpha_j} \right\}, \quad (4-87)$$

$$\begin{split} \varphi_{5}(0) &= \varphi_{6}(0) = \varphi_{7}(0) = \frac{\partial W}{\partial \alpha_{j}} = 2D_{e} \sum_{j=1}^{3} \frac{\rho_{j}A_{j}^{2}}{f_{w}L_{j}} \left( \frac{\partial P_{in}}{\partial \alpha_{j}} - \frac{\partial P_{out}}{\partial \alpha_{j}} \right) \\ &+ 2 \left( P_{in} - P_{out} \right) \frac{\partial D_{e}}{\partial \alpha_{j}} \sum_{j=1}^{3} \frac{\rho_{j}A_{j}^{2}}{f_{w}L_{j}} \\ &+ 2D_{e} \left( P_{in} - P_{out} \right) \sum_{j=1}^{3} \rho_{j} \frac{\partial}{\partial \alpha_{j}} \left\{ \frac{A_{j}^{2}}{f_{w}L_{j}} \right\} \\ &+ 2D_{e} \left( P_{in} - P_{out} \right) \sum_{j=1}^{3} \frac{A_{j}^{2}}{f_{w}L_{j}} \left\{ \frac{\partial \rho_{j}}{\partial T_{j}} \frac{\partial T_{j}}{\partial \alpha_{j}} + \frac{\partial \rho_{j}}{\partial P_{j}} \frac{\partial P_{j}}{\partial \alpha_{j}} \right\} , \end{split}$$
(4-88)

$$\phi_{8}(0) = \frac{\partial T_{M1}(0)}{\partial \alpha_{j}} = \frac{\partial T_{1}}{\partial \alpha_{j}} + \frac{\partial \left\{ \frac{PWR(0)}{UA_{W}} \right\}_{M1}}{\partial \alpha_{j}} , \qquad (4-89)$$

$$\Phi_{9}(0) = \frac{\partial T_{M2}(0)}{\partial \alpha_{j}} = \frac{\partial T_{2}}{\partial \alpha_{j}} + \frac{\partial \left\{ \frac{PWR(0)}{UA_{W}} \right\}_{M2}}{\partial \alpha_{j}} , \qquad (4-90)$$

$$\phi_{10}(0) = \frac{\partial \mathbf{N}(0)}{\partial \alpha_{j}} = 0 \quad , \tag{4-91}$$

and

$$\Phi_{11}(0) = \frac{\partial \mathbf{C}(0)}{\partial \alpha_{j}} = \frac{\Lambda}{\lambda} \frac{\partial \beta}{\partial \alpha_{j}} + \frac{\beta}{\lambda} \frac{\partial \Lambda}{\partial \alpha_{j}} - \frac{\beta \Lambda}{\lambda^{2}} \frac{\partial \lambda}{\partial \alpha_{j}} .$$
(4-92)

The MINRET code was written to evaluate the equations given above. The program solves both the forward and adjoint model equations using the adjoint functions to evaluate the sensitivity of the specified response to parameters in the model.

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The time-dependent model equations are integrated using a fourth-order Runge-Kutta integration scheme with internal error control. The time-step size is adjusted within user-specified limits during the integration to keep the estimated relative error values within a specified value. The user specifies the number of time values at which to save the problem solution data which are written to external files.

The procedures for solving the adjoint equations are opposite of those which are used in the forward equations. In effect, the adjoint problem is started at the final time with the response as the source term. The adjoint model equations are integrated from the final time to the initial time using the same integration scheme as the forward equations except for negative time steps. The time-step size for the adjoint equations is internally controlled as for the forward solution scheme and additionally matches the forward solution edit time points.

The final step in a problem is to calculate the response and its sensitivity integrals. This calculation uses the derivatives of the model variables with respect to the specified parameter and is thus dependent upon the specified response and parameter. In the MINRET code, this step is done in a sensitivity routine tailored to these requirements.

A more detailed discussion of the code and the input requirements are provided in Appendix A.

## 5 RESULTS FROM THE ANALYSIS

The model equations developed in the previous section were programmed as a FORTRAN program called MINRET (<u>MIN</u>i-<u>RET</u>ran). A brief description of the program is supplied in Appendix A.

A problem was selected that would demonstrate the desired performance and provide an interesting transient within the limitations of the model. A PWR rod withdrawal with fuel temperature feedback was simulated by varying the explicit reactivity term initially and then following the model response for a period of about 4.0 seconds. The model will capture the significant trends of power rise and turn down due to Doppler. The channel dimensions for the PWR case is shown in Table 5-1.

Fuel and Clad	
Rod-to-Rod Pitch (square) (m)	0.01260
Fuel Radius (m)	0.00395
Clad Inside Radius (m)	0.00418
Clad Thickness (m)	0.00057
Clad Outside Radius (m)	0.00475
Gap Width (m)	0.00023
Flow Channel	
Flow Area (m <sup>2</sup> )	0.00008789
Heated and Wetted Perimeter (m)	0.02985
Equivalent Hydraulic Diameter (m)	0.011778
Equivalent Heated Diameter (m)	0.011778
Fluid Control Volumes	
Length (m)	0.500
Volume (m <sup>3</sup> )	0.000043945

## Table 5-1Typical Dimensions for PWR Fuel Rods and Flow Channels

For the calculations presented in this report, the pressure drop across the channel is user input via specification of  $P_{in}$  and  $P_{out}$  and the model equations determine the mass flow rate. The initial power is also set. The temperature of the fuel rod and the fluid is determined by the fluid flow rate and this power.

The thermophysical properties of the fuel, gap, and clad are assumed to be constant and have the following values for the fuel

 $\begin{array}{lll} k_{\rm fuel} &=& 3.60 \ (W/m \ K), \\ Cp_{\rm fuel} &=& 247.0 \ (J/kg \ K), \mbox{ and } \\ r_{\rm fuel} &=& 10970.0 \ (kg/m^3); \end{array}$ 

and for the clad

 $\begin{array}{rcl} k_{\rm clad} &=& 13.0 \ (W/m \ K), \\ Cp_{\rm clad} &=& 330.0 \ (J/kg \ K), \ and \\ r_{\rm clad} &=& 6500.0 \ (kg/m^3). \end{array}$ 

The nominal value for the gap conductance is

 $k_{_{gap}} ~=~ 5678.0 \, (W/m^2 \, K)$  ,

a value recommended by Lahey, and the gap conductance may be a parameter of interest that is varied as part of the sensitivity studies.

For the study, two representative response functions were defined

$$R_{\text{peak}} = \int_{0}^{t_{\text{f}}} n(t)\delta(t - tpk)dt$$
(5-1)

and

$$\mathbf{R}_{\mathbf{E}} = \int_{0}^{t_{\mathbf{r}}} \mathbf{n}(\mathbf{t}) \mathrm{d}\mathbf{t} \quad .$$
 (5-2)

Equation 5-1 represents a typical response of interest and effectively locates the point of maximum power. The properties of the direct delta function is such that the function is every where zero except at the time corresponding to the peak. The second integral is a simple integral and represents a response proportional to energy.

The response functions form the basis for the definition of the adjoint source terms for the model as discussed in the previous section.

Several different cases were studied during the course of this investigation, but two are presented in this report. The cases differed in the amount of reactivity added during the initial explicit insertion. The first transient was initiated using a \$1.50 ramp inserted at 0.1 seconds and fully inserted at .15 seconds.

Figures 5-1 and 5-2 indicate the typical response. Most of the interesting model changes are captured with the parameters shown. Figures 5-3 and 5-4 illustrate the same histories for the \$1.10 transient.

DSA results for those case studies are shown in Table 5-2. In the table, the base case response (peak power and energy at 4.0 seconds) are shown along with the sensitivity coefficients. For each case a set of coefficients are shown that indicate the sensitivity that a change in the parameter would have on the base case result. A small subset of all of the model parameter sensitivities is given.

The first set of results are from the \$1.50 case, indicating a peak power of 5.535 at .4904 seconds into the transient. The value for the BETA ( $\beta$ ) coefficient is -.9288 indicating that if all things were equal, a 1.0% change in the value of the input BETA will result in a corresponding 0.9288% inverse change in the value of R, or the peak power. A 10% change in Beta will correspond to a 9.288% change in R. Likewise, a 1.0% change in the value of the input Doppler coefficient (alphdop), all other things equal, will result in a 0.4655% inverse change in the peak power.

Using this information, the modeler can evaluate the relative impact of the individual parameters on the response by comparing the magnitude of the terms and can use the information to decide on the relative importance of these parameters for a given response. It is interesting to contrast the relative importance that the generation time ( $\Lambda$ ) has on the peak power compared with the delayed neutron decay constant ( $\lambda$ ) and observe that the delayed neutron lifetime plays a much smaller role in the determination of the peak power, in this instance.

The primary question at this point is how well does the DSA model predict changes in the response given perturbations in the input or model parameters.

A subset of all possible parameters were selected to illustrate. While in theory, all of the  $\alpha_i$  could be examined without penalty, only a few are chosen for clarity. The fuel temperature coefficient (alphdop), total  $\beta$ , and Mcp in Region 1 were chosen as representative of the type of information a typical modeler would be required to supply. These parameters were selected on the basis that they represent typical model input with some uncertainty due to exact fuel composition or point in the exposure cycle or those parameters that are known to have a significant influence on the proposed response from previous experience.

Figure 5-5 indicates the result from several variations upon the \$1.50 base case. Each curve shows the calculated power response from each of several cases. These results were produced by making the changes to the input parameters and reexecuting the forward cases.

Table 5-3 shows a comparison between the DSA results using selected coefficients from Table 5-1 and the results from direct calculations. The comparisons are good and give some confidence in the method. The information for the DSA calculation required no additional cases beyond the adjoint solution using the base case data.



Figure 5-1 RAMP Insertion Kinetics Response, \$1.5 Case



Figure 5-2 Conductor and Fluid Temperature Response, \$1.5 Case



Figure 5-3 RAMP Insertion Kinetics Response, \$1.10 Case



Figure 5-4 Conductor and Fluid Temperature Response, \$1.10 Case

Table	е	5-2		
Rod	Ej	ect	Sensitivity	Data

Case		Norm Pow (Max)	Time of Max Pow	Respon se Integral	alphdop	Beta	Λ	λ	(Mcp) <sub>1</sub>
\$1.5	rod eject	5.535x10⁰	0.4904	energy	-3.663x10 <sup>-1</sup>	-1.070x10 <sup>-4</sup>	7.045x10 <sup>-3</sup>	2.471x10 <sup>-2</sup>	1.898x10 <sup>-1</sup>
		5.535x10°	0.4904	peak power	-4.655x10 <sup>-1</sup>	-9.288x10 <sup>-1</sup>	-4.442x10 <sup>-1</sup>	9.698x10 <sup>-3</sup>	2.265x10 <sup>-1</sup>
\$1.1	rod eject	3.327x10°	0.5104	energy	-2.849x10 <sup>-1</sup>	-3.653x10 <sup>-1</sup>	4.823x10 <sup>-3</sup>	1.956x10 <sup>-2</sup>	1.477x10 <sup>-1</sup>
		3.327x10°	0.5104	peak power	-2.958x10 <sup>-1</sup>	-8.073x10 <sup>-1</sup>	-2.872x10 <sup>-1</sup>	9.856x10 <sup>-3</sup>	1.441x10 <sup>-1</sup>

Parameter	Perturbation	$R_{pred}E$	$R_{direct}E$	R <sub>pred</sub> Peak	R <sub>direct</sub> Peak
Doppler	$.9^*$ Doppler <sub>o</sub>	6.405	6.435	5.793	6.091
Beta	1.1*Beta₀	6.179	6.179	6.049	6.091
$M_{cp}$	1.1*Mcp <sub>0</sub>	6.296	6.408	5.66	5.79

Tab	le	5	5-3									
800	W	a	tt/C	haı	nnel	Ser	sitiv	vity	Co	mp	aris	sons



Figure 5-5 RAMP Insertion Kinetics Response, \$1.5 Insertion Direct Calculation

# **6** SUMMARY AND DISCUSSION

A simple 'proof-of-principle' model for sensitivity analysis methods studies has been developed. The basis for the work as been the adaptation of differential sensitivity analysis methods using adjoint equations and response functions based upon the adjoint solutions. The methods have been developed and discussed in the literature and have proven to be a reasonable and a theoretically justifiable alternative to the so-called 'forward' or direct methods in which many additional calculations are required.

The basic strength of the adjoint approach is that the resulting equations avoid the necessity of solving the equations that directly depend upon the parameters of interest (the dF/da) which is important if there are a large number. It would be of no advantage to re-solve the original basic forward equations over and over again to answer all of the sensitivity questions.

The adjoint equations are therefore linear and may in general be much easier and faster to solve.

The models and results that have been presented here are a first step in the area of differential sensitivity analysis for RETRAN-3D or other EPRI codes. The work is intended as a contribution to the body of work that already exists as well as a 'hands on' approach to adapt a new technique to gain insight and experience.

The various examples and test cases have provided a the 'proof-of-principle' criteria that were identified at the outset of the study. There now exists a test bed code to examine the theoretical basis for application of DSA to EPRI safety.

How does one proceed from here. There is a significant step between the relatively simple models studied in this work and the more complex, highly nonlinear models that are used in practice. The development and implementation of the adjoint field equations and the corresponding source terms may appear to be a formidable task.

There are reasonable ways to approach the problem and recent work reported in literature has shown some promise of automated methods and automatic differentiation codes[36,37,42] that have been used to both reduce the amount of work involved as well as improve the implementation accuracy by eliminating coding errors. Most of these

#### Summary and Discussion

applications have been using the forward or direct approach and little recent work has addressed the development of an automated adjoint sensitivity model.

On the other hand, work at CSA[43] involving methods for calculating the forward sensitivity derivatives in RETRAN-3D has shown promise and investigation into larger applications is worthwhile.

It is certain that the current trend in the development of advanced codes is to move to more predictive or first-order sensitivity models to aid the user in assessing the effect of model uncertainties on the response of interest. It is hoped the work presented here will help in the evaluation of such models for the EPRI codes.

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## A description of the minret code

The MINRET code was written to provide a vehicle for evaluating the theoretical development of the Adjoint DSA methods described in Sections 3 and 5 of this report. The program solves both the forward and adjoint model equations using the adjoint functions to evaluate the sensitivity of the specified response to parameters in the model.

The first step in a problem is to read and process the input data describing the time domain, core model characteristics, and reactivity perturbation parameters. These data are processed and edited on the output file.

The second step in a problem is to initialize the model equations to a steady-state condition. Initial values derived the steady-state form of the model equations using the input initial and boundary conditions. These values are iterated until a consistent steady state is achieved. Initial values specified for the code include inlet temperature, inlet pressure, and inlet enthalpy. The boundary condition for the code is the core exit pressure. RETRAN-3D equation-of-state routines are used to evaluate the thermodynamic water properties.

The time-dependent model equations are integrated using a fourth order Runge-Kutta integration scheme with internal error control. The time-step size is adjusted within user-specified limits during the integration to keep the estimated relative error values within a specified value. The user specifies the number of time values at which to save the problem solution data which are written to external files. The code edits the data at the time step following such a boundary but does not modify the time step to coincide precisely with the boundary.

The adjoint model equations are integrated from the final time to the initial time using the same integration scheme as the forward equations except for negative time steps. The time-step size for the adjoint equations is internally controlled as for the forward solution scheme and additionally matches the forward solution edit time points.

The final step in a problem is to calculate the response and its sensitivity integrals. This calculation uses the derivatives of the model variables with respect to the specified parameter and is thus dependent upon the specified response and parameter. In the MINRET code, this step is done in a sensitivity routine tailored to these requirements.

### **MINRET Code Input Data Description**

The input data records for the MINRET code are described below. All data records are in fixed format with an 80-character maximum length. The record number is listed with a description of its content followed by the format.

Record 1.	Title - A80					
Record 2.	IDs for Record 3 - A80					
Record 3.	Time-Step Contrtstart-dtout-tend-nout-siunts-iadj-scadj-	rol and General Data problem starting time (sec) not currently used problem end time (sec) number of edit points 0 => SI units, 1 => English 0 => forward solution, 1 => adjoint solution 0 => delete adjoint fcns 1 => save adjoint fcns	- F10.6 - F10.6 - F10.6 - I5 - I5 - I5 - I5			
Record 4.	IDs for Time Steps - A80					
Record 5.	Time-Step Values positive values f negative values h0 - hmax - hmin -	es for forward solution for adjoint solution initial time step (sec) maximum time-step size (sec) minimum time-step size (sec)	- F20.10 - F20.10 - F20.10			
Record 6.	IDs for Core Geo	ometry - A80				
Record 7.	Core Geometrynvol-njun-tlength-dia-	number of volumes number of junctions total channel length (M) channel diameter (M)	- I4 - I4 - F10.6 - F10.6			
Record 8.	IDs for Initial an	nd Boundary Conditions - A80				
Record 9.	Initial and Boun pin - tin - pinnew - pout -	dary Conditions inlet pressure (psia) inlet temperature (°F) not currently used outlet pressure (psia)	- F10.6 - F10.6 - F10.6 - F10.6			

### Description of the MINRET Code

Record 10.	IDs for Kinetics Parameters - A80				
Record 11.	Kinetics Model Reactivityrhoinit-initial reactivitybetan-one-groupbiglam-rkamda-pwr0-initial core	Parameters ctivity (ñ) > beta fetime (sec) > precursor decay constant (1/se e power (W)	- F10.6 - F10.6 - F10.6 ec) - F10.6 - F10.6		
Record 12.	IDs for Kinetics Parameters	s - A80			
Record 13.	Kinetics Model Explicit Rea (Routine RHOIN evaluates rhoa1 - explicit rea rhoa2 - explicit rea rhob1 - explicit rea const1 - explicit rea const2 - explicit rea	activity Parameters the reactivity expression.) activity parameter activity parameter activity parameter activity parameter activity parameter activity parameter	- F10.6 - F10.6 - F10.6 - F10.6 - F10.6		
Record 14.	IDs for Kinetics Parameters	s - A80			
Record 15.	Reactivity Feedback Coeffi alphmod - moderato alphdop - metal tem	cients r temperature coefficient (ñ/°F) perature coefficient (ñ/°F)	- F10.6 - F10.6		
Record 16.	IDs for Reactor Type - A80				
Record 17.	Reactor Type 'PWR' or 'BV	VR' - A3			
Record 18.	IDs for Material Conductiv	ities - A80			
Record 19.	Material Conductivitiestcfuel-fuel (W/mtcgap-gas gap (Vtcclad-cladding (V	n-°K) V/m**2-°K) (W/m-°K)	- F10.6 - F10.6 - F10.6		
Record 20.	IDs for Material Heat Capa	cities - A80			
Record 21.	Material Heat Capacities cpfuel - fuel (J/kg cpgap - gas gap (J cpclad - cladding (	-°K) /kg-°K) J/kg-°K)	- F10.6 - F10.6 - F10.6		
Record 22.	IDs for Material Densities -	A80			

Record 23.	Material Densities						
	rofuel	- fuel (kg/m**3)	- F10.6				
	rogap	- gas gap (kg/m**3)	- F10.6				
	roclad	- cladding (kg/m**3)	- F10.6				
Record 24.	IDs for Equation Solution Flags - A80						
Record 25.	Equation Sol	ition Flags					
	Select equation	Select equations for a particular model such as kinetics only.					
	1 => use equation						
	$0 \Rightarrow do not u$	se equation	- 11I5				
Record 26.	IDs for Respo	nse Weight fcn - A80					

Record 27-37.Weight fcns and Use Times

weight	-	value according to response	- E12.5
start time	-	starting time to use weight value (sec)	- E12.5
end time	-	ending time to use weight value (sec)	- E12.5
		weight value set to zero for time above	bounds.

Example of MINRET input data file.

1.	Test of Da	SA with PWF	R = 800 W;	dop feedb	ack only:	rod	eject	(1.50\$)
2.	tstart	dtout	tend	nout siun	ts iadj s	scadj		
з.	0.0	0.001	2.000	200 0	0 0	)		
4.	h0		hmax		hmin			
5.	0.00005		0.00005		0.0000	01		
6.	nvol njun	tlength	dia					
7.	2 3	1.0	0.01					
8.	pin	tin	pin new	pout				
9.	1000.0	300.0	1000.5	995.0				
10.	rhoinit	betan	biglam	xlamda	pwr0			
11.	0.00000	0.00750	0.0010	0.080	800.0			
12.	rhoal	rhoa2	rhob1	const1	const2	2		
13.	0.225	0.0225	0.0	0.1	0.15			
14.	alphmod	alphdop	alphmod	alphdo	P			
15.	0.0	-0.000659	-0.00659	-0.000	659			
16.	reactor ty	ype						
17.	pwr							
18.	tcfuel-UO2	2 tcgap	tcclad-ZI	Ric2				
19.	3.6	1000.0	13.0					
20.	cpfuel-UO2	2 cpgap	cpclad-ZI	Ric2				
21.	247.0	0.00	330.0					
22.	rofuel-UO2	2 rogap	roclad-ZI	Ric2				
23.	10970.0	0.00	6500.0					
24.	eq. solut:	ion flags		_		-	-	
25.	1 1	1 1 ]		. 1	1 1	1	1	
26.	sensitivi	ty weights	- adjoint	sources (	wt, start	tim,	end	tim)
27.	0.0	2.0	0.0					
28.	0.0	2.0	0.0					
29.	0.0	2.0	0.0					
30.	0.0	2.0	0.0					
31.	0.0	2.0	0.0					
32.	0.0	2.0	0.0					
33.	0.0	2.0	0.0					

Description of the MINRET Code

34.	0.0	2.0	0.0
35.	0.0	2.0	0.0
36.	1.0	2.0	0.0
37.	0.0	2.0	0.0

## ${old B}$ sensitivity model equation coefficients

Equations 4-23 through 4-33 in Section 4 are obtained by differentiating Eqs. 4-1 through 4-9, 4-17, and 4-20 with respect to the parameter  $\alpha_{j}$ . As stated in Section 5, the coefficients contain a number of derivatives with respect to the various dependent variables in the forward equation set. The complete specification of these coefficients is as follows

$$\begin{split} & GG = W_2 \ \frac{\partial h_2}{\partial E_1} + \left(h_c A_W\right)_1 \ \frac{\partial T_1}{\partial E_1} - \left(T_{M1} - T_1\right) \ \frac{\partial T_1}{\partial E_1} \ \frac{\partial \left(h_c A_W\right)_1}{\partial T_1} \\ & EE = W_2 \ \frac{\partial h_2}{\partial M_1} + \left(h_c A_W\right)_1 \ \frac{\partial T_1}{\partial M_1} - \left(T_{M1} - T_1\right) \ \frac{\partial T_1}{\partial M_1} \ \frac{\partial \left(h_c A_W\right)_1}{\partial T_1} \\ & FF = h_2 + W_2 \ \frac{\partial h_2}{\partial \tilde{W}_1} \ \frac{\partial \tilde{W}_1}{\partial W_2} - \left(T_{M1} - T_1\right) \ \frac{\partial \left(h_c A_W\right)_1}{\partial W_2} \\ & EH = -h_2 + W_2 \ \frac{\partial h_2}{\partial \tilde{W}_1} \ \frac{\partial \tilde{W}_1}{\partial W_{in}} \\ & HH = - \ \frac{\partial \left(h_c A_W\right)_1}{\partial T_{M1}} \ \left(T_{M1} - T_1\right) - \left(h_c A_W\right)_1 \\ & PP = W_{out} \ \frac{\partial h_{out}}{\partial E_2} + \left(h_c A_W\right)_2 \ \frac{\partial T_2}{\partial E_2} - \left(T_{M2} - T_2\right) \ \frac{\partial T_2}{\partial E_2} \ \frac{\partial \left(h_c A_W\right)_2}{\partial T_2} \\ & KK = W_{out} \ \frac{\partial h_{out}}{\partial M_2} + \left(h_c A_W\right)_2 \ \frac{\partial T_2}{\partial M_2} - \left(T_{M2} - T_2\right) \ \frac{\partial T_2}{\partial M_2} \ \frac{\partial \left(h_c A_W\right)_2}{\partial T_2} \\ & KS = -W_2 \ \frac{\partial h_2}{\partial E_1} \end{split}$$

$$\begin{aligned} H6 &= -h_2 - W_2 \frac{\partial h_2}{\partial \bar{W}_1} \frac{\partial \bar{W}_1}{\partial W_2} + W_{out} \frac{\partial h_{out}}{\partial \bar{W}_2} \frac{\partial \bar{W}_2}{\partial W_2} \\ LL &= h_{out} + W_{out} \frac{\partial h_{out}}{\partial \bar{W}_2} \frac{\partial \bar{W}_2}{\partial W_{out}} - (\Gamma_{M2} - T_2) \frac{\partial [h_c A_W]_2}{\partial W_{out}} \\ K5 &= -W_2 \frac{\partial h_2}{\partial \bar{W}_1} \frac{\partial \bar{W}_1}{\partial W_{in}} \\ QQ &= -(\Gamma_{M2} - T_2) \frac{\partial [h_c A_W]_2}{\partial T_{M2}} - (h_c A_W)_2 \\ B &= P_{in} A_1^2 I_1 \\ C &= \frac{L_1}{2D_e} \frac{\partial f_W}{\partial W_{in}} W_{in} |W_{in}| + \frac{L_1}{2D_e} 2f_W |W_{in}| \\ A &= P_{in} A_1^2 \frac{\partial P_1}{\partial E_1} \\ G &= P_1 A_2^2 I_2 \\ H &= \frac{L_2}{2D_e} \frac{\partial f_W}{\partial W_2} W_2 |W_2| + \frac{L_2}{2D_e} 2f_W |W_2| \\ E &= A_2^2 I_2 \frac{\partial P_1}{\partial M_1} \dot{W}_2 - P_1 A_2^2 \frac{\partial P_1}{\partial M_1} - (P_1 - P_2) A_2^2 \frac{\partial P_1}{\partial M_1} \\ F &= P_1 A_2^2 \frac{\partial P_2}{\partial M_2} \\ I &= A_2^2 I_2 \frac{\partial P_1}{\partial H_1} \dot{W}_2 - P_1 A_2^2 \frac{\partial P_1}{\partial E_1} - (P_1 - P_2) A_2^2 \frac{\partial P_1}{\partial E_1} \\ J &= P_1 A_2^2 \frac{\partial P_2}{\partial E_2} \end{aligned}$$

B-2

$$\begin{split} \mathbf{BB} &= \mathbf{P}_{2}\mathbf{A}_{3}^{2}\mathbf{I}_{3} \\ \mathbf{CC} &= \frac{\mathbf{L}_{3}}{2\mathbf{D}_{e}} \frac{\partial \mathbf{f}_{W}}{\partial \mathbf{W}_{out}} |\mathbf{W}_{out}| + \frac{\mathbf{L}_{3}}{2\mathbf{D}_{e}} 2\mathbf{f}_{W} |\mathbf{W}_{out}| \\ \mathbf{AA} &= \mathbf{A}_{3}^{2}\mathbf{I}_{3} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{M}_{2}} \dot{\mathbf{W}}_{out} - \mathbf{P}_{2}\mathbf{A}_{3}^{2} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{M}_{2}} - \left(\mathbf{P}_{2} - \mathbf{P}_{out}\right) \mathbf{A}_{3}^{2} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{M}_{2}} \\ \mathbf{DD} &= \mathbf{A}_{3}^{2}\mathbf{I}_{3} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{E}_{2}} \dot{\mathbf{W}}_{out} - \mathbf{P}_{2}\mathbf{A}_{3}^{2} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{E}_{2}} - \left(\mathbf{P}_{2} - \mathbf{P}_{out}\right) \mathbf{A}_{3}^{2} \frac{\partial \mathbf{P}_{2}}{\partial \mathbf{E}_{2}} \\ \mathbf{N} &= \left(\mathbf{MC}_{p}\right)_{M1} \\ \mathbf{P} &= \frac{\partial \left(\mathbf{MC}_{p}\right)_{M1}}{\partial \mathbf{T}_{M1}} \dot{\mathbf{T}}_{M1} + \left(\mathbf{UA}_{w}\right)_{M1} - \left(\mathbf{T}_{1} - \mathbf{T}_{M1}\right) \frac{\partial \left(\mathbf{UA}_{w}\right)_{M1}}{\partial \mathbf{T}_{1}} \\ \mathbf{L} &= -\left(\mathbf{UA}_{w}\right)_{M1} \frac{\partial \mathbf{T}_{1}}{\partial \mathbf{M}_{1}} - \left(\mathbf{T}_{1} - \mathbf{T}_{M1}\right) \frac{\partial \mathbf{T}_{1}}{\partial \mathbf{H}_{1}} \frac{\partial \left(\mathbf{UA}_{w}\right)_{M1}}{\partial \mathbf{T}_{1}} \\ \mathbf{M} &= -\left(\mathbf{UA}_{w}\right)_{M1} \frac{\partial \mathbf{T}_{1}}{\partial \mathbf{E}_{1}} - \left(\mathbf{T}_{1} - \mathbf{T}_{M1}\right) \frac{\partial \mathbf{T}_{1}}{\partial \mathbf{E}_{1}} \frac{\partial \left(\mathbf{UA}_{w}\right)_{M1}}{\partial \mathbf{T}_{1}} \\ \mathbf{S} &= -\left(\mathbf{T}_{1} - \mathbf{T}_{M1}\right) \frac{\partial \left(\mathbf{UA}_{w}\right)_{M1}}{\partial \mathbf{W}_{2}} \\ \mathbf{Q} &= -\mathbf{PWR0}_{M1} \\ \mathbf{AD} &= \left(\mathbf{MC}_{p}\right)_{M2} \\ \mathbf{AE} &= \frac{\partial \left(\mathbf{MC}_{p}\right)_{M2}}{\partial \mathbf{T}_{M2}} \dot{\mathbf{T}}_{M2} + \left(\mathbf{UA}_{w}\right)_{M2} - \left(\mathbf{T}_{2} - \mathbf{T}_{M2}\right) \frac{\partial \left(\mathbf{UA}_{w}\right)_{M2}}{\partial \mathbf{T}_{2}} \\ \mathbf{AB} &= -\left(\mathbf{UA}_{w}\right)_{M2} \frac{\partial \mathbf{T}_{2}}{\partial \mathbf{M}_{2}} - \left(\mathbf{T}_{2} - \mathbf{T}_{M2}\right) \frac{\partial \mathbf{T}_{2}}{\partial \mathbf{T}_{2}} \frac{\partial \left(\mathbf{UA}_{w}\right)_{M2}}{\partial \mathbf{T}_{2}} \\ \mathbf{AC} &= -\left(\mathbf{UA}_{w}\right)_{M2} \frac{\partial \mathbf{T}_{2}}{\partial \mathbf{T}_{2}} - \left(\mathbf{T}_{2} - \mathbf{T}_{M2}\right) \frac{\partial \mathbf{T}_{2}}{\partial \mathbf{T}_{2}} \frac{\partial \left(\mathbf{UA}_{w}\right)_{M2}}{\partial \mathbf{T}_{2}} \\ \end{array}$$

$$X = -(T_2 - T_{M2}) \frac{\partial \{UA_w\}_{M2}}{\partial W_{out}}$$

$$AF = -PWR0_{M2}$$

$$BJ = -\{\frac{\bar{p} - \beta}{\Lambda}\}$$

$$BC = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_1} \frac{\partial T_1}{\partial M_1}$$

$$BD = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_2} \frac{\partial T_2}{\partial M_2}$$

$$BE = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_1} \frac{\partial T_1}{\partial E_1}$$

$$BF = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_2} \frac{\partial T_2}{\partial E_2}$$

$$BG = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_{M1}}$$

$$BH = -\frac{N}{\Lambda} \frac{\partial \bar{p}}{\partial T_{M2}}$$

$$CD = -\frac{\beta}{\Lambda}$$