280
10/9/79

DR. 130

ORNL/TM-6900

MASTER

**Sensitivity Theory Applied to a
Transient Thermal-Hydraulics Problem**

C. F. Weber
E. M. Oblow

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

OAK RIDGE NATIONAL LABORATORY
OPERATED BY UNION CARBIDE CORPORATION · FOR THE DEPARTMENT OF ENERGY

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Printed in the United States of America. Available from
National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road, Springfield, Virginia 22161
NTIS price codes—Printed Copy: A06 Microfiche A01

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for any third party's use or the results of such use of any information, apparatus, product or process disclosed in this report, or represents that its use by such third party would not infringe privately owned rights.

ORNL/TM-6900
Distribution Category UC-79p
Breeder Reactor Safety

Contract W-7405-eng-26
Engineering Physics Division

SENSITIVITY THEORY APPLIED TO A TRANSIENT THERMAL-HYDRAULICS PROBLEM

C. F. Weber[†] and E. M. Oblow

Date Published: October 1979

NOTICE

This report was prepared as an account of work sponsored by the United States Government. Neither the United States nor the United States Department of Energy, nor any of their employees, nor any of their contractors, subcontractors, or their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness or usefulness of any information, apparatus, product or process disclosed, or represents that its use would not infringe privately owned rights.

[†]UCND Computer Sciences Division.

OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37830
operated by
UNION CARBIDE CORPORATION
for the
DEPARTMENT OF ENERGY

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

ACKNOWLEDGEMENTS

The authors are indebted to D. G. Cacuci, E. T. Tomlinson, and C. V. Parks for suggestions concerning the problem formulation and particular applications of interest. H. L. Dodds gave much encouragement and helped explain confusing terminology. Appreciation is also directed to Professors J. S. Bradley and P. F. Pasqua of The University of Tennessee for arranging the research assistantship that made this work possible. Finally, many thanks go to LaWanda Klobe for her diligent efforts in preparing and editing the manuscript.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

TABLE OF CONTENTS

ABSTRACT	v
I. INTRODUCTION	1
II. APPLICATION OF DIFFERENTIAL SENSITIVITY THEORY	4
III. DISCRETIZATION AND NOTATION	18
IV. DIFFERENCE APPROXIMATION TO THE FORWARD SYSTEM	22
V. DIFFERENCE APPROXIMATION TO THE ADJOINT SYSTEM	32
VI. ASSESSING THE VALIDITY OF THE NUMERICAL SOLUTION	37
VII. RESULTS AND CONCLUSIONS	47
REFERENCES	55
APPENDICES	
A. DERIVATION OF THE GOVERNING EQUATIONS	57
B. TYPICAL PROBLEM PARAMETERS	63
C. DERIVATION OF THE SYSTEM OF EQUATIONS SATISFIED BY SENSITIVITY VARIABLES ϕ AND χ	65
D. DERIVATION OF THE ADJOINT RESPONSE REPRESENTATION	71
E. DERIVATION OF THE FORWARD CONDUCTION DIFFERENCE EQUATIONS	75
F. DIFFERENCE APPROXIMATION TO THE ADJOINT FUEL CONDUCTION EQUATION	85
G. PROOF OF DIAGONAL DOMINANCE OF DISCRETE SOLUTION MATRICES	93
H. COMPUTATION OF SENSITIVITY INTEGRALS	97

LIST OF FIGURES

FIGURE	PAGE
1. Reactor Fuel Pin	3
2. Fuel Pin Radial Mesh	18

LIST OF TABLES

TABLE	
I. Parameter Limitations for Adjoint Coolant Stability	49
II. Peak Fuel Temperature	51
III. Peak Clad Temperature	52
IV. Outlet Coolant Temperature	53
H-I. Integration Methods for Sensitivity Integrals	101

ABSTRACT

A new method for sensitivity analysis of transient nonlinear problems is developed and applied to a reactor thermal-hydraulics problem. The method resembles the differential sensitivity methods currently used in the linear problems of reactor physics, but it is applicable to nonlinear systems as well. The equations governing heat transfer and fluid flow in a fuel pin and surrounding coolant are given and used to derive a second set of equations (commonly known as the "adjoint equations") used in the sensitivity analysis.

Both systems contain one second-order parabolic and one first-order hyperbolic partial differential equation. Difference equations are derived to approximate both systems and the convergence properties of these discrete systems are evaluated, yielding a useful analysis of the numerical solution. The solution functions are used to derive sensitivity coefficients for any desired integral response. These sensitivity coefficients are used in a first-order perturbation theory to predict changes in a response resulting from changes in parameter values. The results of a test problem are shown, verifying that this procedure is indeed useful for a wide variety of sensitivity calculations.

CHAPTER I

INTRODUCTION

The use of nuclear power has become an extremely controversial subject in the U.S. and abroad. Both the general public and the scientific community hold diverse viewpoints concerning all aspects of the issue — political, economic, environmental, etc. Although most scientists are convinced that fission reactors can provide answers to our energy needs without endangering human health and safety, some doubts still remain. As a result, stringent regulations have been imposed in licensing and operating reactors. These regulations deal with many accident situations which, though their probability of occurring is small, might have disastrous consequences.

In devising accident regulations, the U.S. Nuclear Regulatory Commission relies heavily on computer codes that simulate reactor transient behavior. Of great importance is the determination of which reactor system parameters have significant influence on the safe operation of the reactor. For example, if coolant stops flowing or slows down sufficiently, the reactor core could melt, and harmful radiation may be released to the atmosphere. Thus, reactor safety depends heavily on the coolant flow rate. In practice, thousands of such parameters affect the system integrity in varying degrees; hence, it is necessary to quantify their effects upon important safety factors.

The safety factors of primary interest are generally related to physical quantities such as temperature and pressure at different points in the reactor. Accordingly, a *response* is specified to represent each safety factor. Responses of particular importance are the maximum (or peak) temperatures occurring in each material (fuel, coolant, etc.).

Sensitivity analysis in reactor safety seeks to determine the effect of each system parameter on a particular response. That is, if a parameter should change by a specified amount, what changes in each response can be expected? To answer this question, a number of sensitivity studies have been performed using response surface methodology.⁷ The reactor system is modeled (by computer code

simulation) and a response computed for given accident conditions. A parameter is then perturbed and a new response computed, thus revealing the response dependence upon the parameter. Because this procedure requires many expensive computations, it is advantageous to develop a new method of sensitivity analysis.

A differential sensitivity method has been used successfully in several areas of physics and engineering, with extensive applications in solving radiation transport problems.⁷ E. M. Obloy of Oak Ridge National Laboratory has applied this technique to a simple, steady-state problem in reactor safety.⁷ As a continuation of his work, it is the intent of this paper to apply this differential sensitivity theory to a transient thermal hydraulics problem that represents a simplified portion of a reactor system.

The problem to be investigated is the development and application of this new sensitivity methodology to a particular problem in nuclear reactor analysis — heat transfer and fluid flow in a reactor fuel subassembly. Briefly, the subassembly contains fuel pins which are surrounded by coolant. Each fuel pin (see Fig. 1) consists of *fuel* (some fissile substance mixed with a nonfissile diluent material) and *cladding* (a protective sheath of noncorrosive material, usually zirconium or stainless steel). The pins are often pressurized with helium, which collects between the fuel and cladding, forming a small *gap*. During operation, fission gases (chiefly xenon) also accumulate in the gap. The fuel rods (i.e., fuel, gap, and cladding) are grouped in symmetric bundles, or subassemblies. Among the fuel rods within a subassembly, physical quantities such as temperature, pressure, and neutron density do not vary appreciably; hence, this subsystem can be modeled by considering only one fuel rod and its surrounding coolant. To further simplify this problem, pressure variations are neglected, single phase coolant flow is assumed, and the nuclear heat generation is given by a simple power distribution, making temperature the only unknown physical quantity.

To implement this program, it is necessary to (1) model the temperature distribution in the fuel rod and coolant; (2) specify certain key temperatures as responses; (3) apply differential sensitivity

Figure 1. Reactor Fuel Pin.

theory to predict response variation due to parameter changes; and (4) apply numerical methods to obtain approximate solutions. In Chapter II, the governing differential equations of the system are stated and the differential sensitivity theory is developed, yielding a second set of differential equations and a number of integrals. Chapter III begins the process of discrete approximation, which is continued in Chapters IV and V with the derivation of difference equations for each differential system. Chapter VI contains some numerical analysis results of interest, while Chapter VII outlines the implementation and results of the computer solution procedures.

CHAPTER II

APPLICATION OF DIFFERENTIAL SENSITIVITY THEORY

As a prerequisite to any sensitivity study, it is necessary to model the properties of the physical system and identify the parameters that influence the system. The heat distribution in a fuel rod and surrounding coolant can be approximated by two coupled partial differential equations, one to model heat conduction in the fuel pin, the other to simulate convection heat transfer in the coolant. These equations, with appropriate boundary and initial conditions, are based on the following assumptions:

- a. The problem has angular symmetry.
- b. Heat conduction is negligible in the coolant and negligible axially in the fuel rod.
- c. Heat transfer by convection is negligible in the fuel pin and occurs in the coolant only in the axial direction. (2.1)
- d. All materials present (fuel, clad, and coolant) are homogeneous.
- e. Heat flux and temperature are differentiable in each material region.

The resulting formulation has three independent variables — r , z , and t , representing radial, axial, and time dimensions, respectively. The two dependent variables are $T = T(r, z, t)$ and $T_c = T_c(z, t)$, the unknown fuel rod and coolant temperatures. Under the assumptions (2.1), T and T_c satisfy the following system of coupled equations (see Appendix A):

$$\rho C_p \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) = Q, \quad \left\{ \begin{array}{l} 0 < r < R_f \\ R_g < r < R \end{array} \right\}, \quad 0 < z < L, \quad 0 < t < t_f \quad (2.2)$$

$$T(r, z, 0) = T_0(r, z), \quad 0 < r < R, \quad 0 < z < L \quad (2.3)$$

$$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0 \quad (2.4)$$

$$\left. \left(rk \frac{\partial T}{\partial r} \right) \right|_{r=R_f^-} = \left. \left(rk \frac{\partial T}{\partial r} \right) \right|_{r=R_g^+} \quad (2.5)$$

$$\left. \left(k \frac{\partial T}{\partial r} + h_g T \right) \right|_{r=R_f^-} = \left. (h_g T) \right|_{r=R_g^+} \quad (2.6)$$

$$\left. \left(k \frac{\partial T}{\partial r} + h_c T \right) \right|_{r=R} = h_c T_c \quad (2.7)$$

$$0 < z < L, 0 < t < t_f$$

$$\frac{\partial}{\partial t}(A\rho C_p T_c) + \frac{\partial}{\partial z}(wC_p T_c) + 2\pi R h_c T_c = 2\pi R h_c T(R, z, t),$$

$$0 < z < L, 0 < t < t_f \quad (2.8)$$

$$T_c(z, 0) = T_{c0}(z), \quad 0 < z < L \quad (2.9)$$

$$T_c(0, t) = T_{c1}(t), \quad 0 < t < t_f \quad (2.10)$$

where R_f , R_g , R = outer radii of fuel, gap, and clad, respectively (cm)

L = fuel rod height (cm)

t_f = final time (sec)

ρ = density (gm/cm³)

C_p = heat capacity (j/gm-°C)

k = thermal conductivity (w/cm-°C)

Q = nuclear heat source density (w/cm³-sec)

h_g = gap conductance (w/cm²-°C)

h_c = coolant-clad heat transfer coefficient (w/cm²-°C)

A = cross-sectional flow area of coolant channel (cm²)

w = coolant mass flow rate (gm/sec).

Past results indicate a large temperature drop (> 1500°C) in the quarter-centimeter distance between the fuel center and the coolant.⁷

The coolant temperature itself increases significantly in traveling the length of the fuel rod. For these reasons, temperature dependence is significant for the physical data k , C_p , h_g , h_c , and ρ . Thus, Eqs. (2.2)-(2.10) represent a coupled system of *nonlinear* partial differential equations.

Often the greatest interest is not in the entire temperature distribution, but rather averages or specific temperature values at certain points. For this reason, the system response P is defined as an integral over all dependent variables

$$P = 2\pi \iiint f(r,z,t) T(r,z,t) r \, dr \, dz \, dt + \iint g(z,t) T_c(z,t) dz \, dt . \quad (2.11)$$

The functions f and g are arbitrary weight functions which can be chosen so that P will represent such useful results as average central fuel, peak clad or outlet coolant temperature.

The purpose of sensitivity analysis is to determine the effect on a particular response of small changes in any system parameter. Letting α denote an arbitrary parameter, the current procedure seeks to determine $dP/d\alpha$, an estimate of the change in P for small changes in α . For a discussion of the particular parameters that may be represented by α , see Appendix B.

For the sake of generality, assume that all physical quantities depend on either the fuel pin or coolant temperature. Also note that all data (except the independent variable limits R_f , R_g , R , L , and t_f) may depend explicitly on α and that the unknown temperatures will depend implicitly on α . The following relationships illustrate the general dependence of each function in the fuel pin: $T = T(r,z,t;\alpha)$,

$(\rho C_p) = (\rho C_p)[T(r,z,t;\alpha);\alpha]$, $k = k[\lambda(r,z,t;\alpha);\alpha]$, $Q = Q(r,z,t;\alpha)$, $h_g = h_g[T(r,z,t;\alpha);\alpha]$, and $T_0 = T_0(r,z;\alpha)$. Similarly, functional dependences in the coolant are $T_c = T_c(z,t;\alpha)$, $h_c = h_c[T_c(z,t;\alpha);\alpha]$, $(A\rho C_p) = (A\rho C_p)[T_c(z,t;\alpha);\alpha]$, $(wC_p) = (wC_p)[T_c(z,t;\alpha);\alpha]$,

$T_{c0} = T_{c0}(z;\alpha)$, and $T_{c1} = T_{c1}(t;\alpha)$. Response functional dependences are $P = P(\alpha)$, $f = f(r,z,t;\alpha)$, and $g = g(z,t;\alpha)$.

In order to calculate $dP/d\alpha$, assume that the system of Eqs. (2.2)-(2.10) has a known, unique solution for certain values of all input data. In particular, assume the solution is known for the specific value $\alpha = \alpha_0$ (the design point solution), and that a unique solution exists for α in some neighborhood of α_0 . The present sensitivity methodology requires more than the well-posedness condition of continuous solution dependence on the data. It is, in fact, a necessary assumption that the solution functions, their first axial and time derivatives, and second radial derivative (fuel pin) are *differentiable* with respect to α in a neighborhood of α_0 .

Differentiating Eq. (2.11) and evaluating at $\alpha = \alpha_0$ gives

$$\left. \frac{dP}{d\alpha} \right|_{\alpha=\alpha_0} = \left. \frac{\partial P}{\partial \alpha} \right|_{\alpha=\alpha_0} + 2\pi \iiint \left(f \frac{\partial T}{\partial \alpha} \right) \Big|_{\alpha=\alpha_0} r dr dz dt + \iint g \left(\frac{\partial T_c}{\partial \alpha} \right) \Big|_{\alpha=\alpha_0} dz dt \quad (2.12)$$

where $\partial P/\partial \alpha$ is the "direct effect" term representing an explicit change in the response,

$$\frac{\partial P}{\partial \alpha} = 2\pi \iiint \frac{\partial f}{\partial \alpha} T r dr dz dt + \iint \frac{\partial g}{\partial \alpha} T_c dz dt \quad (2.13)$$

Once the system of Eqs. (2.2)-(2.10) has been solved, computation of $\partial P/\partial \alpha$ is straightforward. However, the two remaining terms in Eq. (2.12) are not immediately known, since T and T_c depend implicitly on α . It is possible to compute $\partial T/\partial \alpha|_{\alpha=\alpha_0}$ and $\partial T_c/\partial \alpha|_{\alpha=\alpha_0}$; however, for reasons to be shown later, it is advantageous to eliminate these quantities from Eq. (2.12).

To simplify notation, define the dependent variables

$$\phi = \phi(r, z, t) \equiv \frac{\partial T}{\partial \alpha}(r, z, t; \alpha_0), \quad \chi = \chi(z, t) \equiv \frac{\partial T_c}{\partial \alpha}(z, t; \alpha_0).$$

Using these definitions, Eq. (2.12) becomes

$$\begin{aligned}
\left. \frac{dP}{d\alpha} \right|_{\alpha=\alpha_0} &= \left. \frac{\partial P}{\partial \alpha} \right|_{\alpha=\alpha_0} + 2\pi \iiint f(r,z,t;\alpha_0) \phi(r,z,t) r dr dz dt \\
&+ \iint g(z,t;\alpha_0) \chi(z,t) dz dt
\end{aligned} \tag{2.14}$$

Observe that ϕ and χ must satisfy the system of equations that results if each Eq. (2.2)-(2.10) is differentiated with respect to α and evaluated at $\alpha = \alpha_0$. It can be shown (see Appendix C for details) that this results in the following system of equations:

$$\begin{aligned}
\frac{\partial}{\partial t} (\rho C_p \phi) - \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} (k\phi) \right] &= S_\phi, \quad \left\{ \begin{array}{l} U < r < R_f \\ R_g < r < R \end{array} \right\}, \quad 0 < z < L, \quad 0 < t < t_f \\
\phi(r,z,0) &= \phi_0(r,z), \quad 0 < r < R, \quad 0 < z < L \\
\left. \frac{\partial}{\partial r} (k\phi) \right|_{r=0} &= 0 \\
\left[r \frac{\partial}{\partial r} (k\phi) \right]_{r=R_f^-} &= \left[r \frac{\partial}{\partial r} (k\phi) \right]_{r=R_g^+} + a \\
\left[\frac{\partial}{\partial r} (k\phi) + h_g^- \phi \right]_{r=R_f^-} &= \left[h_g^- \phi \right]_{r=R_g^+} + b \\
\left[\frac{\partial}{\partial r} (k\phi) + h_c \phi \right]_{r=R} &= h_c^- \chi + c
\end{aligned} \quad \left. \begin{array}{l} \\ \\ \\ \\ \end{array} \right\} \quad 0 < z < L, \quad 0 < t < t_f \tag{2.15}$$

$$\begin{aligned}
\frac{\partial}{\partial t} [(A\rho C_p)^- \chi] + \frac{\partial}{\partial z} [(wC_p)^- \chi] + 2\pi R h_c^- \chi &= 2\pi R h_c \phi(R,z,t) + S_\chi, \quad 0 < z < L, \quad 0 < t < t_f \\
\chi(z,0) &= \chi_0(z), \quad 0 < z < L \\
\chi(0,t) &= \chi_1(t), \quad 0 < t < t_f,
\end{aligned}$$

where

$$S_\phi = S_\phi(r,z,t) \equiv \left[\frac{\partial Q}{\partial \alpha} - \frac{\partial T}{\partial t} \frac{\partial}{\partial \alpha} (\rho C_p) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \right]_{\alpha=\alpha_0}$$

$$\phi_0 = \frac{\partial T_0}{\partial \alpha}$$

$$a = a(z,t) \equiv \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_g^+} - \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_f^-}$$

$$b = b(z, t) \equiv \left(\frac{\partial h_g}{\partial \alpha} T \right) \Big|_{r=R_g^+} - \left(\frac{\partial h_g}{\partial \alpha} T + \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_f^-}$$

$$c = c(z, t) = \left[- \frac{\partial h_c}{\partial \alpha} (T - T_c) - \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right]_{r=R}$$

$$S_X = S_X(z, t) \equiv 2\pi R \frac{\partial h_c}{\partial \alpha} (T - T_c) \Big|_{r=R} - \frac{\partial}{\partial t} \left[T_c \frac{\partial}{\partial \alpha} (A\rho C_p) \right] - \frac{\partial}{\partial z} \left[T_c \frac{\partial}{\partial \alpha} (wC_p) \right]$$

$$h_c' = h_c'(z, t) = h_c - \frac{\partial h_c}{\partial T_c} (T - T_c) \Big|_{r=R}$$

$$(A\rho C_p)' = (A\rho C_p)'(z, t) \equiv T_c \frac{\partial}{\partial T_c} (A\rho C_p) + (A\rho C_p)$$

$$(wC_p)' = (wC_p)'(z, t) \equiv T_c \frac{\partial}{\partial T_c} (wC_p) + (wC_p)$$

$$X_0 = \frac{\partial T_{c0}}{\partial \alpha}$$

$$X_1 = \frac{\partial T_{c1}}{\partial \alpha} .$$

The system (2.15) could be solved and the results used in Eq. (2.14) to calculate $dP/d\alpha|_{\alpha=\alpha_0}$. Because several of the coefficient functions depend on derivatives of α , system (2.15) must be solved for each individual α . An alternative is to re-solve the original system of Eqs. (2.2)-(2.10) with slightly perturbed data and compare the two responses. This is the technique used by response surface methods (discussed in Chapter I). Both of these procedures require repeated solution of an entire system in order to obtain sensitivity results for several parameters. This impracticality motivates consideration of an alternate sensitivity methodology.

For simplicity, let L and M denote the differential operators that appear in system (2.15), i.e.,

$$L\phi \equiv \frac{\partial}{\partial t} (\rho C_p \phi) - \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} (k\phi) \right]$$

and

$$M\chi \equiv \frac{\partial}{\partial t} [(A\rho C_p)\chi] + \frac{\partial}{\partial z} [(wC_p)\chi] + 2\pi R h_c \chi$$

A third system will now be defined whose differential operators are mathematically adjoint to the operators L and M above. By proper choice of source functions and auxiliary conditions, this "adjoint system" will be independent of differential changes in any parameter α , and will provide for replacement of ϕ and χ in Eq. (2.14).

Let ϕ^* and χ^* be arbitrary functions, with $\phi^* = \phi^*(r, z, t)$ defined for $0 < r < R$, $0 < z < L$, $0 < t < t_f$ and $\chi^* = \chi^*(z, t)$ defined for $0 < z < L$, $0 < t < t_f$. In addition, it is necessary that ϕ^* be twice differentiable in r and once differentiable in t for $0 < r < R_f$ and $R_g < r < R$; χ^* must be once differentiable in each variable throughout its domain.

Defining the adjoint operators L^* and M^* by

$$L^*\phi^* = -(\rho C_p) \frac{\partial \phi^*}{\partial t} - \frac{1}{r} k \frac{\partial}{\partial r} \left(r \frac{\partial \phi^*}{\partial r} \right)$$

$$M^*\chi^* = -(A\rho C_p) \frac{\partial \chi^*}{\partial t} - (wC_p) \frac{\partial \chi^*}{\partial z} + 2\pi R h_c \chi^* ,$$

and integrating by parts yields

$$\begin{aligned} \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* L\phi \, r \, dr \, dz \, dt &= \int_0^{t_f} \int_0^L \int_0^{R_f} \phi L^*\phi^* \, r \, dr \, dz \, dt \\ &+ \int_0^L \int_0^{R_f} (\rho C_p \phi \phi^*) \Big|_0^{t_f} r \, dr \, dz \\ &+ \int_0^{t_f} \int_0^L \left[r k \phi \frac{\partial \phi^*}{\partial r} - r \phi^* \frac{\partial}{\partial r} (k\phi) \right] \Big|_0^{R_f} dz \, dt , \end{aligned} \quad (2.16)$$

$$\begin{aligned}
\int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* L \phi \, r \, dr \, dz \, dt &= \int_0^{t_f} \int_0^L \int_{R_g}^R \phi L^* \phi^* \, r \, dr \, dz \, dt \\
&+ \int_0^L \int_{R_g}^R (\rho C_p \phi \phi^*) \Big|_0^{t_f} r \, dr \, dz \\
&+ \int_0^{t_f} \int_0^L \left[r k \phi \frac{\partial \phi^*}{\partial r} - r \phi^* \frac{\partial}{\partial r} (k \phi) \right]_{R_g}^R dz \, dt, \quad (2.17)
\end{aligned}$$

$$\begin{aligned}
\int_0^{t_f} \int_0^L \chi^* M \chi \, dz \, dt &= \int_0^{t_f} \int_0^L \chi M^* \chi^* \, dz \, dt + \int_0^L [\chi^* \chi (A \rho C_p)]_0^{t_f} dz \\
&+ \int_0^{t_f} [\chi^* \chi (w C_p)]_0^L dt. \quad (2.18)
\end{aligned}$$

Until now, ϕ^* and χ^* have been arbitrary functions satisfying certain differentiability requirements. Consistent with the ultimate purpose of finding replacement terms for ϕ and χ in Eq. (2.14), let ϕ^* and χ^* now denote specific functions, namely the solutions of the following differential system:

$$L^*\phi^* = f, \quad \left\{ \begin{array}{l} 0 < r < R_f \\ R_g < r < R \end{array} \right\}, \quad 0 < z < L, \quad 0 < t < t_f$$

$$\phi^*|_{t=t_f} = 0, \quad 0 < r < R, \quad 0 < z < L$$

$$\left. \begin{array}{l} \frac{\partial \phi^*}{\partial r} \Big|_{r=0} = 0 \\ \left(rk \frac{\partial \phi^*}{\partial r} \right) \Big|_{r=R_f^-} = \left(rk \frac{\partial \phi^*}{\partial r} \right) \Big|_{r=R_g^+} \\ \left(k \frac{\partial \phi^*}{\partial r} + h_g^* \phi^* \right) \Big|_{r=R_f^-} = h_g^* \psi^* \Big|_{r=R_g^+} \\ \left(k \frac{\partial \phi^*}{\partial r} + h_c \phi^* \right) \Big|_{r=R} = h_c \chi^* \end{array} \right\} \quad 0 < z < L, \quad 0 < t < t_f$$

$$M^*\chi^* = g + 2\pi h_c^*(r\phi^*) \Big|_{r=R}, \quad 0 < z < L, \quad 0 < t < t_f$$

$$\chi^*|_{t=t_f} = 0, \quad 0 < z < L$$

$$\chi^*|_{z=L} = 0, \quad 0 < t < t_f. \quad (2.19)$$

(Recall that f and g are the weight functions in Eqs. (2.11)-(2.14).)

Note that system (2.19) is independent of any parameter α . Also, observe that once the temperature distribution is known from Eqs. (2.2)-(2.10), (2.19) is a *linear* system of equations.

Multiplying Eqs. (2.16) and (2.17) by 2π , then adding both to Eq. (2.18) and rearranging (see Appendix D for details) gives

$$\begin{aligned}
& 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} f \phi r dr dz dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R f \phi r dr dz dt + \int_0^{t_f} \int_0^L g \chi dz dt \\
& = 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* S_\phi r dr dz dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* S_\phi r dr dz dt \\
& + \int_0^{t_f} \int_0^L \chi^* S_\chi dz dt + 2\pi \int_0^L \int_0^{R_f} (\rho C_P \phi \phi^*) \Big|_{t=0} r dr dz \\
& + 2\pi \int_0^L \int_{R_g}^R (\rho C_P \phi \phi^*) \Big|_{t=0} r dr dz + \int_0^L [\chi^* \chi (A \rho C_P)']_{t=0} dz \\
& + 2\pi \int_0^{t_f} \int_0^L \left[(a - R_f b) \phi^* \Big|_{R_g^+} + R_f b \phi^* \Big|_{R_f^-} + c (r \phi^*) \Big|_R \right] dz dt \\
& + \int_0^{t_f} [\chi^* \chi (w C_P)']_{z=0} dt . \tag{2.20}
\end{aligned}$$

Careful observation reveals that the left-hand side of Eq. (2.20) corresponds exactly with the integral terms on the right-hand side of Eq. (2.14)! Furthermore, no term on the right-hand side of Eq. (2.20) contains a reference to any value of ϕ or χ except the known initial and boundary values $\phi(r, z, 0)$, $\chi(z, 0)$, and $\chi(0, t)$. Thus, substitution of Eq. (2.20) into Eq. (2.14) will provide a representation of $dP/d\alpha$ that can be obtained by solving system (2.19) rather than system (2.15). Because system (2.19) is independent of any specific α , this representation can be used to evaluate response sensitivity for many parameters. Performing this substitution and showing the quantities S_ϕ , S_χ , a , b , and c explicitly, the following equation is obtained:

$$\begin{aligned}
\left. \frac{dP}{d\alpha} \right|_{\alpha=\alpha_0} &= \left. \frac{\partial P}{\partial \alpha} \right|_{\alpha=\alpha_0} + 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* \frac{\partial Q}{\partial \alpha} r \, dr \, dz \, dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* \frac{\partial Q}{\partial \alpha} r \, dr \, dz \, dt \\
&- 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* \frac{\partial T}{\partial t} \frac{\partial}{\partial \alpha} (\rho C_p) r \, dr \, dz \, dt - 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* \frac{\partial T}{\partial t} \frac{\partial}{\partial \alpha} (\rho C_p) r \, dr \, dz \, dt \\
&- 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \frac{\partial \phi^*}{\partial r} r \, dr \, dz \, dt - 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \frac{\partial \phi^*}{\partial r} r \, dr \, dz \, dt \\
&- 2\pi \int_0^{t_f} \int_0^L \frac{\partial h_g}{\partial \alpha} R_f \left[T \Big|_{R_f^-} - T \Big|_{R_g^+} \right] \left[\phi^* \Big|_{R_f^-} - \phi^* \Big|_{R_g^+} \right] dz \, dt \\
&- 2\pi \int_0^{t_f} \int_0^L \frac{\partial h_c}{\partial \alpha} [r(T - T_c)(\phi^* - \chi^*)]_{r=R} dz \, dt \\
&+ 2\pi \int_0^L \int_0^{R_f} \frac{\partial T_0}{\partial \alpha} (\rho C_p \phi^*) \Big|_{t=0} r \, dr \, dz + 2\pi \int_0^L \int_{R_g}^R \frac{\partial T_0}{\partial \alpha} (\rho C_p \phi^*) \Big|_{t=0} r \, dr \, dz \\
&- \int_0^{t_f} \int_0^L \chi^* \frac{\partial}{\partial t} \left[T_c \frac{\partial}{\partial \alpha} (A \rho C_p) \right] dz \, dt - \int_0^{t_f} \int_0^L \chi^* \frac{\partial}{\partial z} \left[T_c \frac{\partial}{\partial \alpha} (w C_p) \right] dz \, dt \\
&+ \int_0^L \frac{\partial T_{c0}}{\partial \alpha} [\chi^* (A \rho C_p)]_{t=0} dz + \int_0^{t_f} \frac{\partial T_{c1}}{\partial \alpha} [\chi^* (w C_p)]_{z=0} dt . \tag{2.21}
\end{aligned}$$

At first glance, Eq. (2.21) seems extremely complicated and it appears that a great deal of work remains. However, each term is independent of the others and represents a specific sensitivity calculation. For instance, if the fuel thermal conductivity is expressed as $k_f(T) = \bar{k}_f \cdot u(T)$ and $\alpha = \bar{k}_f$, then all terms in Eq. (2.21) would vanish except the one involving thermal conductivity in the fuel region, i.e.,

$$\frac{dP}{d\bar{k}_f} = -2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \frac{\partial T}{\partial r} \frac{\partial \phi^*}{\partial r} u(T) r \, dr \, dz \, dt .$$

Thus, after T , T_c , ϕ^* , and χ^* have been determined, each term in Eq. (2.21) could be computed and regarded as a distinct sensitivity quantity.

In practice, an important quantity is $\frac{dP/P}{d\alpha/\alpha} = \frac{dP}{d\alpha} \cdot \frac{\alpha}{P}$, which is commonly referred to as the sensitivity of P to α . For the "scale factor" type of parameter (discussed in Appendix B), computation of this quantity is straightforward. In the above example, this sensitivity coefficient is

$$\begin{aligned} \frac{dP/P}{dk_f/k_f} &= - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_0^{R_f} \frac{\partial T}{\partial r} \frac{\partial \phi^*}{\partial r} \bar{k}_f u(T) r \, dr \, dz \, dt \\ &= - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_0^{R_f} \frac{\partial T}{\partial r} \frac{\partial \phi^*}{\partial r} k_f(T) r \, dr \, dz \, dt . \end{aligned}$$

(To limit the scope of the present work, the actual sensitivity integral computations done here will consider only this scale factor type of parameter.)

For computational purposes, it is expedient to introduce the following changes in both the dependent and independent variables of system (2.19):

$$\xi = L - z, \quad \tau = t_f - t ,$$

$$T^*(r, \xi, \tau) \equiv \phi^*(r, L - \xi, t_f - \tau) = \phi^*(r, z, t) ,$$

$$T_c^*(\xi, \tau) \equiv \chi^*(L - \xi, t_f - \tau) = \chi^*(z, t) .$$

In addition, the functions $(\rho C_p)^*$, k^* , h_g^* , h_c^* , f^* , $(A\rho C_p)^*$, $(wC_p)^*$, h_c' , and g^* are defined as the transformations of their unstarred counterparts,

$$k^*(r, \xi, \tau) \equiv k(r, L-\xi, t_f-\tau) = k(r, z, t) = k[T(r, z, t)] ,$$

$$h'^*(\xi, \tau) \equiv h'(L-\xi, t_f-\tau) = h'(z, t) = h'[T_c(z, t)] ,$$

etc.

Note also these new derivatives,

$$\frac{\partial \phi^*}{\partial t} = \frac{\partial T^*}{\partial \tau} \frac{d\tau}{dt} = - \frac{\partial T^*}{\partial \tau}, \quad \frac{\partial \phi^*}{\partial r} = \frac{\partial T^*}{\partial r},$$

$$\frac{\partial \chi^*}{\partial t} = \frac{\partial T_c^*}{\partial \tau} \frac{d\tau}{dt} = - \frac{\partial T_c^*}{\partial \tau}, \quad \frac{\partial \chi^*}{\partial z} = \frac{\partial T_c^*}{\partial \xi} \frac{d\xi}{dz} = - \frac{\partial T_c^*}{\partial \xi} .$$

Substitution of these expressions into system (2.19) produces the following system of partial differential equations in the transformed variables:

$$(\rho C_p)^* \frac{\partial T^*}{\partial \tau} - \frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) = f^*, \quad \left\{ \begin{array}{l} 0 < r < R_f \\ R_g < r < R \end{array} \right\}, \quad 0 < z < L, \quad 0 < t < t_f$$

$$T^*(r, \xi, 0) = 0, \quad 0 < r < R, \quad 0 < \xi < L.$$

$$\left. \begin{array}{l} \frac{\partial T^*}{\partial r} \Big|_{r=0} = 0, \\ \left(r k^* \frac{\partial T^*}{\partial r} \right) \Big|_{r=R_f^-} = \left(r k^* \frac{\partial T^*}{\partial r} \right) \Big|_{r=R_g^+} \\ \left(k^* \frac{\partial T^*}{\partial r} + h_g'^* T^* \right) \Big|_{r=R_f^-} = h_g'^* T^* \Big|_{r=R_g^+} \\ \left(k^* \frac{\partial T^*}{\partial r} + h_c^* T^* \right) \Big|_{r=R} = h_c^* T_c^* \end{array} \right\} \quad 0 < \xi < L, \quad 0 < t < t_f$$

$$(A \rho C_p)^* \frac{\partial T_c^*}{\partial \tau} + (w C_p)^* \frac{\partial T_c^*}{\partial \xi} + 2\pi R h_c'^* T_c^* = g^* + 2\pi R h_c'^* T^* \Big|_{r=R}, \quad 0 < \xi < L, \quad 0 < \tau < t_f$$

$$T_c^*(\xi, 0) = 0, \quad 0 < \xi < L$$

$$T_c^*(0, \tau) = 0, \quad 0 < \tau < t_f. \quad (2.22)$$

There are several advantages in using system (2.22). All auxiliary conditions are of the same form as those in the original problem, Eqs. (2.2)-(2.10). Also, the differential equations more closely resemble the original conduction and convection equations. Because of these similarities between systems (2.22) and (2.2)-(2.10), one solution method could handle both problems. Thus, system (2.22) is solved rather than system (2.19), after which the adjoint solutions are converted back to ϕ^* and χ^* to perform the integrations of Eq. (2.21).

One final word concerning terminology is needed. It appears that a convention has developed which labels the system of Eqs. (2.2)-(2.10) as the "forward" system and system (2.19) as the "adjoint" system. This terminology is also adopted here. However, note that system (2.19) is *not* mathematically adjoint to the forward system, but rather to system (2.15), whose usefulness has now been exhausted. In addition, system (2.22) is referred to as the "transformed adjoint" system.

CHAPTER III

DISCRETIZATION AND NOTATION

Calculation of sensitivity coefficients involves a three-step procedure, (i) solution of the heat balance Eqs. (2.2)-(2.10), (ii) determination of the functions T^* and T_c^* from system (2.22), and (iii) computation of the integrals in Eq. (2.21). Equations (2.2)-(2.10) form a system of coupled, nonlinear, partial differential equations. Upon their solution, system (2.22) is linear, but still involves two coupled equations with variable coefficients. Possibilities of analytical solution are remote, thus motivating consideration of numerical methods.

To approximate both the forward and adjoint systems with difference equations, introduce the discrete mesh (r_i, z_j, t_k) , $i=1,2,\dots,I$; $j=1,2,\dots,J$; $k=0,1,\dots,K$. Mesh spacing is uniform in the axial and time dimensions; hence, $z_j = (j-1)\Delta z$, $t_k = k \Delta t$, $z_1 = 0$, $z_J = (J-1)\Delta z = L$, $t_0 = 0$, and $t_K = K \Delta t = t_f$. The radial nodes span two distinct regions (fuel and cladding) and thus are in general *not* uniformly spaced. In addition, past results reveal a large temperature drop in the outer part of the fuel,⁷ suggesting a smaller mesh spacing than is needed in the interior. Consider then the following radial mesh structure in the fuel region of the fuel rod: r_i , $i=1,2,\dots,I_f$, are radial node points at which temperature values are determined; each r_i is embedded in a radial mesh element whose boundaries are delineated by intermediate radial points $\hat{r}_i$, $i=1,2,\dots,I_f-1$ (see Fig. 2). The two node points r_1 and r_{I_f} are located at the material region boundaries, i.e., $r_1 = 0$ and $r_{I_f} = R_f$.

Figure 2. Fuel Pin Radial Mesh.

In view of earlier arguments (and also to follow the precedents set by major production codes^{5,12}), the node points r_i and the intermediate points $\hat{r}_i$ should satisfy the relations

$$\text{a. } \hat{r}_i^2 = \frac{1}{2} (r_i^2 + r_{i+1}^2) \quad \text{b. } r_i^2 = \frac{1}{2} (\hat{r}_{i-1}^2 + \hat{r}_i^2) . \quad (3.1)$$

Assuming that the number of nodes I_f and the fuel region boundaries r_1 and r_{I_f} are given, Eq. (3.1) implies the following:

$$\hat{r}_1^2 = r_{I_f}^2 / (2I_f - 2)$$

$$r_i^2 = (2i - 2)\hat{r}_1^2, \quad i=1,2,\dots,I_f$$

$$\hat{r}_i^2 = (2i - 1)\hat{r}_1^2, \quad i=1,2,\dots,I_f-1.$$

In the cladding region of the fuel rod, temperatures are lower and do not change as rapidly as in the fuel region.⁷ For this reason (and again following the precedent of current production codes^{5,12}), radial nodes and intermediate points are equally spaced. Thus, given the number of cladding nodes I_c and the region boundary nodes $r_{I_f+1} = R_g$ and $r_{I_f+I_c} = r_I = R$, the uniform stepsize is

$$\Delta r = (R - R_g) / (I_c - 1)$$

and the radial mesh points are

$$r_{I_f+i} = R_g + (i-1)\Delta r, \quad i=1,2,\dots,I_c$$

$$\hat{r}_{I_f+i} = R_g + \left(i - \frac{1}{2}\right)\Delta r, \quad i=1,2,\dots,I_c-1.$$

In both the fuel and cladding the radial stepsizes are defined as

$$\Delta r_i = r_{i+1} - r_i, \quad i=1,2,\dots,I-1.$$

For convenience, define the radial intervals

$$v_i = \left\{ r: \hat{r}_{i-1} < r \leq \hat{r}_i \right\}, \quad i=2,3,\dots,I_f-1, I_f+2,\dots,I-1$$

$$v_1 = \left\{ r: r_1 = 0 \leq r \leq \hat{r}_1 \right\}$$

$$v_{I_f} = \left\{ r: \hat{r}_{I_f-1} < r \leq r_{I_f} = R_f \right\}$$

$$v_{I_f+1} = \left\{ r: r_{I_f+1} = R_g \leq r \leq \hat{r}_{I_f+1} \right\}$$

$$v_I = \left\{ r: \hat{r}_{I-1} < r \leq r_I = R \right\}$$

and the "volume" of each interval,

$$v_i = \hat{r}_i^2 - \hat{r}_{i-1}^2, \quad i=2,3,\dots,I_f-1, I_f+2,\dots,I-1$$

$$v_1 = \hat{r}_1^2$$

$$v_{I_f} = r_{I_f}^2 - \hat{r}_{I_f-1}^2$$

$$v_{I_f+1} = \hat{r}_{I_f+1}^2 - r_{I_f+1}^2$$

$$v_I = r_I^2 - \hat{r}_{I-1}^2.$$

Note also the compact notation for functions evaluated at points of the discrete mesh,

$$\begin{aligned} T_{i,j}^k &\equiv T(r_i, z_j, t_k), \quad T_{c,j}^k \equiv T_c(z_j, t_k), \quad (\rho C_p)_{i,j}^{k+1} \equiv (\rho C_p)(T_{i,j}^{k+1}), \\ k_{i,j+\frac{1}{2}}^k &\equiv k\left[T(\hat{r}_i, z_{j+\frac{1}{2}}, t_k)\right], \quad h_{c,j+1}^{k+1} \equiv h_c\left[T_{c,j+1}^{k+1}\right], \text{ etc.} \end{aligned}$$

Consider now the transformed adjoint system (2.22). The independent variables are discretized as (r_i, ξ_j, τ_k) , where the r_i , $i=1,2,\dots,I$, are identical with the forward radial variables, and

$$\xi_j \equiv L - z_j = (J-1)\Delta z - (j-1)\Delta z = (J-j)\Delta z = z_{J-j+1}$$

$$\tau_k \equiv t_f - t_k = K \Delta t - k \Delta t = (K-k)\Delta t = t_{K-k}.$$

Also adopt the other notation used in the forward problem, $\hat{r}_i$, Δr_i , $i=1,2,\dots,I$, and the discretized function notation,

$$T_{i,j}^{*k} \equiv T^*(r_i, \xi_j, \tau_k), \quad h_{c,j}^{*k} \equiv h_c^*(\xi_j, \tau_k), \quad \text{etc.}$$

CHAPTER IV

DIFFERENCE APPROXIMATION TO THE FORWARD SYSTEM

Consider the heat conduction equation (2.2) of the forward system and its associated boundary and initial conditions (2.3)-(2.7). The problem spans both the fuel and clad regions [it is actually two different problems coupled by the interface conditions (2.5) and (2.6)], with nonuniform mesh spacing in the fuel region. The system contains the nonlinear coefficient functions ρ , C_p , k , h_g , and h_c , and linear (but nonconstant) terms $1/r$, r , and Q . The transient nature of the problem indicates that rapid temperature variations may occur. For these reasons, a solution method must be tailored to this specific problem.

Several numerical methods were considered, among them a predictor-corrector for nonlinear problems² and direct differencing of derivatives. The predictor-corrector was not especially suited for iteration, since it required two different computations at each time step. Because of the irregular radial mesh, direct differencing was also discarded. Finally, a third procedure was adopted that overcame these difficulties.

Equation (2.2) is integrated over the spatial volume element $r dr d\theta dz$ and over the time element dt , with $r \in v_i$, $0 < \theta < 2\pi$, $z_j < z < z_{j+1}$, and $t_k < t < t_{k+1}$. The result is analogous to the integral form of the energy balance equation [see Eq. (A.4) in Appendix A],

$$\int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_0^{2\pi} \int_{v_i} \left[(\rho C_p) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(rk \frac{\partial T}{\partial r} \right) - Q \right] r dr d\theta dz dt = 0, \quad (4.1)$$

$$i = 1, 2, \dots, I; \quad j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1.$$

Simplifying and approximating each term in Eq. (4.1) results in a difference approximation for the unknown function $T(r,z,t)$.

Obviously, an approximation to the integral form of the energy balance equation is as valid as an approximation to the differential form, Eq. (2.2). The two major production codes that solve the system (2.2)-(2.10) for fast reactor safety analysis both use this method.^{5,12} The discrete ordinates method of solving neutron density problems also follows the same procedure by integrating the Boltzmann transport equation and approximating each term thus obtained.¹⁰ A final justification for this method is that of practicality — boundary conditions, iteration and the irregular mesh are all handled easily.

Taylor's Theorem and simple averaging are used extensively in approximating each term of the integrated conduction equation (see Appendix E for details). For integrals over interior radial regions of the fuel and cladding, the following equation is obtained:

$$\begin{aligned}
 & T_{i-1,j+\frac{1}{2}}^{k+1} \left[-P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1} \right] + T_{i,j+\frac{1}{2}}^{k+1} \left[V_i (\rho C_P)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1} \right. \\
 & \quad \left. + P_i k_{i,j+\frac{1}{2}}^{k+1} \right] + T_{i+1,j+\frac{1}{2}}^{k+1} \left[-P_i k_{i,j+\frac{1}{2}}^{k+1} \right] = V_i (\rho C_P)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} T_{i,j+\frac{1}{2}}^k \\
 & \quad - P_{i-1} k_{i-1,j+\frac{1}{2}}^k \left(T_{i,j+\frac{1}{2}}^k - T_{i-1,j+\frac{1}{2}}^k \right) + P_i k_{i,j+\frac{1}{2}}^k \left(T_{i+1,j+\frac{1}{2}}^k - T_{i,j+\frac{1}{2}}^k \right) \\
 & \quad + \tilde{Q}_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t(\Delta r_i + \Delta r_{i-1}) + \Delta t(\hat{r}_i - \hat{r}_{i-1})^2 + \Delta t(\Delta z)^2] ,
 \end{aligned} \tag{4.2}$$

$$i = 2, 3, \dots, I_f - 1, I_f + 2, \dots, I - 1; j = 1, 2, \dots, J - 1; k = 0, 1, \dots, K - 1,$$

where

$$P_i = \frac{\Delta t \hat{r}_i}{\Delta r_i} . \tag{4.3}$$

Equation (4.2) represents a nonlinear, implicit method for calculating the unknown discrete temperatures at time step t_{k+1} , assuming all

temperatures are known at the previous time step t_k . Since the coefficient functions k and ρC_p depend on the temperature, they cannot be immediately evaluated at the new time step; hence, they must be approximated by iteration or extrapolation.

To simplify notation, define the following quantities:

$$A_{i,j}^{k+1} \equiv -P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1}$$

$$B_{i,j}^{k+1} \equiv V_i (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1} + P_i k_{i,j+\frac{1}{2}}^{k+1}$$

$$C_{i,j}^{k+1} \equiv -P_i k_{i,j+\frac{1}{2}}^{k+1}$$

$$D_{i,j}^k \equiv V_i (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} T_{i,j+\frac{1}{2}}^k - P_{i-1} k_{i-1,j+\frac{1}{2}}^k (T_{i,j+\frac{1}{2}}^k - T_{i-1,j+\frac{1}{2}}^k) \\ + P_i k_{i,j+\frac{1}{2}}^k (T_{i+1,j+\frac{1}{2}}^k - T_{i,j+\frac{1}{2}}^k) + \tilde{Q}_{i,j+\frac{1}{2}}^{k+\frac{1}{2}}.$$

Using these quantities and ignoring the error terms, Eq. (4.2) reduces to the difference equation

$$A_{ij}^{k+1} T_{i-1,j+\frac{1}{2}}^{k+1} + B_{ij}^{k+1} T_{i,j+\frac{1}{2}}^{k+1} + C_{ij}^{k+1} T_{i+1,j+\frac{1}{2}}^{k+1} = D_{ij}^k. \quad (4.4)$$

$$i = 2, 3, \dots, I_f - 1, I_f + 2, \dots, I - 1; j = 1, 2, \dots, J - 1; k = 0, 1, \dots, K - 1,$$

which is a discrete approximation to Eq. (4.1) for all axial and time steps and for radial intervals interior to each region.

For the radial volume immediately surrounding $r = 0$, Eq. (4.1) is equivalent to

$$T_{1,j+\frac{1}{2}}^{k+1} \left[V_1 (\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_1 k_{1,j+\frac{1}{2}}^{k+1} \right] + T_{2,j+\frac{1}{2}}^{k+1} \left[-P_1 k_{1,j+\frac{1}{2}}^{k+1} \right] \\ = V_1 (\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} T_{1,j+\frac{1}{2}}^k + P_1 k_{1,j+\frac{1}{2}}^k (T_{2,j+\frac{1}{2}}^k - T_{1,j+\frac{1}{2}}^k) \\ + \tilde{Q}_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^2 + \Delta t (\Delta r_1 + \hat{r}_1^2) + \Delta t (\Delta z)^2], \quad (4.5)$$

Defining

$$B_{1,j}^{k+1} \equiv V_1(\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_1 k_{1,j+\frac{1}{2}}^{k+1}$$

$$C_{1,j}^{k+1} \equiv -P_1 k_{1,j+\frac{1}{2}}^{k+1}$$

$$D_{1,j}^k \equiv V_1(\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} T_{1,j+\frac{1}{2}}^k + P_1 k_{1,j+\frac{1}{2}}^k (T_{2,j+\frac{1}{2}}^k - T_{1,j+\frac{1}{2}}^k) + \tilde{Q}_{1,j+\frac{1}{2}}^{k+\frac{1}{2}}$$

and substituting into Eq. (4.5) gives the difference equation

$$B_{1,j}^{k+1} T_{1,j+\frac{1}{2}}^{k+1} + C_{1,j}^{k+1} T_{2,j+\frac{1}{2}}^{k+1} = D_{1,j}^k, \quad j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1. \quad (4.6)$$

Difference equations at the radial mesh regions bounding the fuel and clad ($i = I_f, I_f+1, I$) are obtained by identical term-by-term approximations and use of the interface and boundary conditions (2.5)-(2.7). Considerable simplification results in the following discrete approximations to Eq. (4.1) (see Appendix E for details), which can be rearranged as

$$A_{I_f,j}^{k+1} T_{I_f-1,j+\frac{1}{2}}^{k+1} + B_{I_f,j}^{k+1} T_{I_f,j+\frac{1}{2}}^{k+1} + C_{I_f,j}^{k+1} T_{I_f+1,j+\frac{1}{2}}^{k+1} = D_{I_f,j}^k, \quad (4.7)$$

$$j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1,$$

where

$$A_{I_f,j}^{k+1} \equiv -P_{I_f-1} k_{I_f-1,j+\frac{1}{2}}^{k+1}$$

$$B_{I_f, j}^{k+1} \equiv V_{I_f} (\rho C_p)_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I_f-1} k_{I_f-1, j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^{k+1}$$

$$C_{I_f, j}^{k+1} \equiv -r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^{k+1}$$

$$\begin{aligned} D_{I_f, j}^k &\equiv V_{I_f} (\rho C_p)_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} T_{I_f, j+\frac{1}{2}}^k \\ &\quad - P_{I_f-1} k_{I_f-1, j+\frac{1}{2}}^k \left(T_{I_f, j+\frac{1}{2}}^k - T_{I_f-1, j+\frac{1}{2}}^k \right) \\ &\quad + r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^k \left(T_{I_f+1, j+\frac{1}{2}}^k - T_{I_f, j+\frac{1}{2}}^k \right) + \tilde{Q}_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}}, \end{aligned}$$

$$A_{I_f+1, j}^{k+1} T_{I_f, j+\frac{1}{2}}^{k+1} + B_{I_f+1, j}^{k+1} T_{I_f+1, j+\frac{1}{2}}^{k+1} + C_{I_f+1, j}^{k+1} T_{I_f+2, j+\frac{1}{2}}^{k+1} = D_{I_f+1, j+\frac{1}{2}}^k,$$

$$j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1, \quad (4.8)$$

where

$$A_{I_f+1, j}^{k+1} \equiv -r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^{k+1}$$

$$B_{I_f+1, j}^{k+1} \equiv V_{I_f+1} (\rho C_p)_{I_f+1, j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I_f+1} k_{I_f+1, j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^{k+1}$$

$$C_{I_f+1, j}^{k+1} \equiv -P_{I_f+1} k_{I_f+1, j+\frac{1}{2}}^{k+1}$$

$$\begin{aligned} D_{I_f+1, j}^k &\equiv V_{I_f+1} (\rho C_p)_{I_f+1, j+\frac{1}{2}}^{k+\frac{1}{2}} T_{I_f+1, j+\frac{1}{2}}^k \\ &\quad + P_{I_f+1} k_{I_f+1, j+\frac{1}{2}}^k \left(T_{I_f+2, j+\frac{1}{2}}^k - T_{I_f+1, j+\frac{1}{2}}^k \right) \\ &\quad - r_{I_f} \Delta t h_{g, j+\frac{1}{2}}^k \left(T_{I_f+1, j+\frac{1}{2}}^k - T_{I_f, j+\frac{1}{2}}^k \right) + \tilde{Q}_{I_f+1, j+\frac{1}{2}}^{k+\frac{1}{2}}, \end{aligned}$$

$$A_{I,j}^{k+1} T_{I-1,j+\frac{1}{2}}^{k+1} + B_{I,j}^{k+1} T_{I,j+\frac{1}{2}}^{k+1} + 2C_{I,j}^{k+1} T_{c,j+\frac{1}{2}}^{k+1} = D_{I,j}^k, \quad (4.9)$$

$$j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1,$$

where

$$A_{I,j}^{k+1} \equiv -P_{I-1} k_{I-1,j+\frac{1}{2}}^{k+1}$$

$$B_{I,j}^{k+1} \equiv V_I (\rho C_p)_{I,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I-1} k_{I-1,j+\frac{1}{2}}^{k+1} + r_I \Delta t h_{c,j+\frac{1}{2}}^{k+1}$$

$$C_{I,j}^{k+1} \equiv -\frac{1}{2} r_I \Delta t h_{c,j+\frac{1}{2}}^{k+1}$$

$$D_{I,j}^k \equiv V_I (\rho C_p)_{I,j+\frac{1}{2}}^{k+\frac{1}{2}} T_{I,j+\frac{1}{2}}^k - P_{I-1} k_{I-1,j+\frac{1}{2}}^k (T_{I,j+\frac{1}{2}}^k - T_{I-1,j+\frac{1}{2}}^k) \\ - r_I \Delta t h_{c,j+\frac{1}{2}}^k (T_{I,j+\frac{1}{2}}^k - T_{c,j+\frac{1}{2}}^k) + \tilde{Q}_{I,j+\frac{1}{2}}^{k+\frac{1}{2}}.$$

The half-step coolant temperature in Eq. (4.9) is approximated by a simple average

$$T_{c,j+\frac{1}{2}}^{k+1} \sim \frac{1}{2} (T_{c,j}^{k+1} + T_{c,j+1}^{k+1}),$$

which allows Eq. (4.9) to be rewritten

$$A_{I,j}^{k+1} T_{I-1,j+\frac{1}{2}}^{k+1} + B_{I,j}^{k+1} T_{I,j+\frac{1}{2}}^{k+1} + C_{I,j}^{k+1} T_{c,j+1}^{k+1} = D_{I,j}^k - C_{I,j}^{k+1} T_{c,j}^{k+1}, \quad (4.10)$$

$$j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1.$$

Equations (4.4), (4.6), (4.7), (4.8), and (4.10) represent the final forms of the discrete approximation to the forward conduction equation for each radial interval and each axial and time step. Noting the appearance of coolant temperatures in Eq. (4.10), it is necessary now to approximate the forward convection equation.

Consider then the discretization of Eq. (2.8) describing heat convection in the coolant. There is no radial dependence; hence, the discrete mesh is reduced to the points $(z_j, t_k) = ((j-1)\Delta z, k\Delta t)$. The uniform mesh spacing and presence of only first derivatives make this problem simpler than that posed by the fuel conduction, although Eq. (2.8) is still nonlinear. For convenience, define the following functions for temporary usage:

$$u = u(T_c) \equiv (\rho C_p)(T_c)$$

$$v = v(T_c) \equiv (w C_p)(T_c)$$

$$x = x(T_c) \equiv 2\pi R h_c(T_c).$$

Using these definitions, Eq. (2.8) can be rewritten

$$\frac{\partial}{\partial t} (uT_c) + \frac{\partial}{\partial z} (vT_c) + xT_c = xT(R, z, t), \quad 0 < z < L, \quad 0 < t < t_f. \quad (4.11)$$

Evaluating Eq. (4.11) at the mesh point $(z_{j+\frac{1}{2}}, t_{k+\frac{1}{2}})$, and using Taylor's Theorem produces the following equivalent form:

$$\begin{aligned} & \frac{\alpha_1}{\Delta t} \left[(uT_c)_{j+1}^{k+1} - (uT_c)_{j+1}^k \right] + \frac{(1 - \alpha_1)}{\Delta t} \left[(uT_c)_j^{k+1} - (uT_c)_j^k \right] \\ & + \frac{\alpha_2}{\Delta z} \left[(vT_c)_{j+1}^{k+1} - (vT_c)_j^{k+1} \right] + \frac{(1 - \alpha_2)}{\Delta z} \left[(vT_c)_{j+1}^k - (vT_c)_j^k \right] \\ & + \alpha_1 \alpha_2 (xT_c)_{j+1}^{k+1} + \alpha_1 (1 - \alpha_2) (xT_c)_{j+1}^k + (1 - \alpha_1) \alpha_2 (xT_c)_j^{k+1} \\ & + (1 - \alpha_1)(1 - \alpha_2) (xT_c)_j^k - \alpha_2 T_{I, j+\frac{1}{2}}^{k+1} \left[\alpha_1 x_{j+1}^{k+1} + (1 - \alpha_1) x_j^{k+1} \right] \\ & + (1 - \alpha_2) T_{I, j+\frac{1}{2}}^k \left[\alpha_1 x_{j+1}^k + (1 - \alpha_1) x_j^k \right] \\ & = \frac{\Delta z}{2} (2\alpha_1 - 1) \left[\frac{\partial^2 (uT_c)}{\partial z \partial t} + \frac{\partial (xT_c)}{\partial z} - T_I \frac{\partial x}{\partial z} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} + \end{aligned}$$

$$\begin{aligned}
& + \frac{\Delta t}{2} (2\alpha_2 - 1) \left[\frac{\partial^2 (vT_c)}{\partial t \partial z} + \frac{\partial (xT_c)}{\partial t} - \frac{\partial}{\partial t} (xT_I) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
& + \frac{\Delta t \cdot \Delta z}{4} (2\alpha_1 - 1)(2\alpha_2 - 1) \left[\frac{\partial^2 (xT_c)}{\partial z \partial t} - \frac{\partial}{\partial t} \left(T_I \frac{\partial x}{\partial z} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
& + O[(\Delta z)^2 + (\Delta t)^2] , \tag{4.12}
\end{aligned}$$

where α_1 and α_2 are weighting parameters, $0 \leq \alpha_1, \alpha_2 \leq 1$. (The method is explicit if $\alpha_2 = 0$ and fully implicit if $\alpha_2 = 1$.)

To approximate, all terms of order Δz or Δt (the entire right-hand side) are ignored. Defining

$$\begin{aligned}
A_{I+1,j}^{k+1} & \equiv -\alpha_2 \alpha_1 \Delta t x_{j+1}^{k+1} - \alpha_2 (1-\alpha_1) \Delta t x_j^{k+1} \\
B_{I+1,j}^{k+1} & \equiv \alpha_1 u_{j+1}^{k+1} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+1}^{k+1} + \alpha_1 \alpha_2 \Delta t x_{j+1}^{k+1} \\
E_j^{k+1} & \equiv (1-\alpha_2) u_j^{k+1} - \alpha_2 \frac{\Delta t}{\Delta z} v_j^{k+1} + (1-\alpha_1) \alpha_2 \Delta t x_j^{k+1} \\
D_{I+1,j}^k & \equiv T_{c,j}^k \left[(1-\alpha_1) u_j^k + (1-\alpha_2) \frac{\Delta t}{\Delta z} v_j^k - (1-\alpha_1)(1-\alpha_2) \Delta t x_j^k \right] \\
& + T_{c,j+1}^k \left[\alpha_1 u_{j+1}^k - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+1}^k - \alpha_1 (1-\alpha_2) \Delta t x_{j+1}^k \right] \\
& + \Delta t (1-\alpha_2) T_{I,j+\frac{1}{2}}^k \left[\alpha_1 x_{j+1}^k + (1-\alpha_1) x_j^k \right]
\end{aligned}$$

substituting into Eq. (4.12) and rearranging then gives the difference equation

$$\begin{aligned}
A_{I+1,j}^{k+1} T_{I,j+\frac{1}{2}}^{k+1} + B_{I+1,j}^{k+1} T_{c,j+1}^{k+1} & = D_{I+1,j}^k - E_j^{k+1} T_{c,j}^{k+1} , \\
j & = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1. \tag{4.13}
\end{aligned}$$

The inlet coolant temperature is given by boundary condition (2.10). Computation at each axial level results in a radial profile of fuel temperatures at the half-step, $T_{i,j+\frac{1}{2}}^{k+1}$, $i = 1, 2, \dots, I$, and the nodal outlet coolant temperature at the full step $T_{c,j+1}^{k+1}$; hence, in calculating these quantities, the nodal inlet coolant temperature $T_{c,j}^{k+1}$ is known either from the boundary condition (2.10) or from computations at the previous axial level. Thus, the right-hand sides of Eqs. (4.10) and (4.13) are known completely.

Eqs. (4.4), (4.6), (4.7), (4.8), (4.10), and (4.13) define a system of nonlinear difference equations in the unknown temperatures at each axial level. This system can be rewritten in matrix notation

$$H_j^{k+1} T_j^{k+1} = D_j^k, \quad j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1, \quad (4.14)$$

where T_j^{k+1} is the vector of unknowns

$$T_j^{k+1} = \left(T_{1,j+\frac{1}{2}}^{k+1}, T_{2,j+\frac{1}{2}}^{k+1}, \dots, T_{I,j+\frac{1}{2}}^{k+1}, T_{c,j+1}^{k+1} \right)^T,$$

D_j^k is the vector composed of known quantities,

$$D_j^k = \left(D_{1,j}^k, D_{2,j}^k, \dots, D_{I-1,j}^k, D_{I,j}^k - C_{I,j}^{k+1} T_{c,j}^{k+1}, D_{1+1,j}^k - E_j^{k+1} T_{c,j}^{k+1} \right)^T,$$

and the matrix H_j^{k+1} has the elements $h_{m,n}$, with

$$h_{m,n} = \begin{cases} B_{m,j}^{k+1} & m = n \\ A_{m,j}^{k+1} & m = n + 1 \\ C_{m,j}^{k+1} & m = n - 1 \\ 0 & \text{otherwise} \end{cases}$$

Each element of the matrix H_j^{k+1} depends on unknown fuel and coolant temperatures, and must be determined by iteration. All nonlinear terms are first approximated by their values at the previous time step t_k , and Eq. (4.14) is solved as a linear system to obtain an approximation for the vector T_j^{k+1} . These temperatures can then be used to reevaluate the elements of H_j^{k+1} and D_j^k , resulting in an updated matrix equation. Solving this version of Eq. (4.14) will hopefully produce an even better approximation to the difference solution. By continuing this process, an iteration procedure is defined. If it converges (in practice, it converges easily to 3 significant digits in 4-6 iterations), the unknown vector T_j^{k+1} can be estimated very accurately.

CHAPTER V

DIFFERENCE APPROXIMATION TO THE ADJOINT SYSTEM

Consider the transformed adjoint system (2.22). The coefficient functions $(\rho C_p)^*$, k^* , h_g^* , $h_g'^*$, h_c^* , $h_c'^*$, $(A\rho C_p)^{*-}$, and $(wC_p)^{*-}$ are dependent on local temperatures; hence, if the temperature distribution is known, these quantities are known functions of the independent variables. Because temperatures are known only at the discrete mesh points (r_i, z_j, t_k) [and thus at (r_i, ξ_j, τ_k)], it is necessary for the adjoint calculations to follow the same mesh arrangement. In addition, it would be expedient for the same computer code to solve both the forward and adjoint problems. For convenience, then, the adjoint system will be discretized by the same procedure as was used in the forward case.

The conduction equation of system (2.22) is integrated over each volume element and each time interval,

$$\int_{\tau_k}^{\tau_{k+1}} \int_{\xi_j}^{\xi_{j+1}} \int_0^{2\pi} \int_{V_i} \left[(\rho C_p)^* \frac{\partial T^*}{\partial \tau} - \frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) - f^* \right] r dr d\theta d\xi d\tau = 0, \quad (5.1)$$

$i = 1, 2, \dots, I; j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1.$

Each term of Eq. (5.1) is approximated using procedures identical to those used for the forward equations in the previous chapter. This results in the following set of difference equations (details of their derivation can be found in Appendix F):

$$\left. \begin{aligned} A_{i,j}^{*k+1} T_{i-1,j+\frac{1}{2}}^{*k+1} + B_{i,j}^{*k+1} T_{i,j+\frac{1}{2}}^{*k+1} + C_{i,j}^{*k+1} T_{i+1,j+\frac{1}{2}}^{*k+1} &= D_{i,j}^{*k}, \quad i = 1, 2, \dots, I-1 \\ A_{I,j}^{*k+1} T_{I-1,j+\frac{1}{2}}^{*k+1} + B_{I,j}^{*k+1} T_{I,j+\frac{1}{2}}^{*k+1} + C_{I,j}^{*k+1} T_{c,j+1}^{*k+1} &= D_{I,j}^{*k} - C_{I,j}^{*k+1} T_{c,j}^{*k+1}, \end{aligned} \right\} \quad (5.2)$$

where

$$\begin{aligned}
 A_{i,j}^{*k+1} &= \begin{cases} 0, & i = 1 \\ -P_{i-1} k_{i,j+\frac{1}{2}}^{*k+1}, & i = 2, 3, \dots, I_f, I_f+2, \dots, I \\ -\Delta t r_{I_f} h_{g,j+\frac{1}{2}}^{*k+1}, & i = I_f+1 \end{cases} \\
 C_{i,j}^{*k+1} &= \begin{cases} -P_i k_{i,j+\frac{1}{2}}^{*k+1}, & i = 1, 2, \dots, I_f-1, I_f+1, \dots, I-1 \\ -\Delta t r_{I_f} h_{g,j+\frac{1}{2}}^{*k+1}, & i = I_f \\ -\frac{1}{2} \Delta t r_I h_{c,j+\frac{1}{2}}^{*k+1}, & i = I \end{cases} \\
 B_{i,j}^{*k+1} &= \begin{cases} V_i (\rho C_p)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} - A_{i,j}^{*k+1} - C_{i,j}^{*k+1}, & i = 1, 2, \dots, I-1 \\ V_I (\rho C_p)_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}} - A_{I,j}^{*k+1} - 2C_{I,j}^{*k+1}, & i = I \end{cases} \\
 D_{i,j}^{*k} &= \begin{cases} V_i (\rho C_p)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{i,j+\frac{1}{2}}^{*k} + A_{i,j}^{*k} (T_{i,j+\frac{1}{2}}^{*k} - T_{i-1,j+\frac{1}{2}}^{*k}) \\ \quad - C_{i,j}^{*k} (T_{i+1,j+\frac{1}{2}}^{*k} - T_{i,j+\frac{1}{2}}^{*k}) + \frac{2}{\Delta z} F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}}, & i = 1, 2, \dots, I-1 \\ V_I (\rho C_p)_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{I,j+\frac{1}{2}}^{*k} + A_{I,j}^{*k} (T_{I,j+\frac{1}{2}}^{*k} - T_{I-1,j+\frac{1}{2}}^{*k}) \\ \quad + 2C_{I,j}^{*k} (T_{I,j+\frac{1}{2}}^{*k} - T_{c,j+\frac{1}{2}}^{*k}) + \frac{2}{\Delta z} F_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}}, & i = I \end{cases}
 \end{aligned}$$

The adjoint source term $F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}}$ appearing in the quantities $D_{i,j}^{*k}$ represents the integral

$$F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} \equiv \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} f(r,z,t) r dr dz dt$$

and is discussed further in Appendix F.

Turning now to the convection equation of the transformed adjoint system (2.22), again introduce simplifying notation

$$u^* = u^*(\xi, \tau) \equiv (A\rho C_p)^{-*}$$

$$v^* = v^*(\xi, \tau) \equiv (w C_p)^{-*}$$

$$x^* = x^*(\xi, \tau) \equiv 2\pi R h^{-*},$$

which allows the differential equation to be written

$$u^* \frac{\partial T_c^*}{\partial \tau} + v^* \frac{\partial T_c^*}{\partial \xi} + x^* T_c^* = g^* + x^* T^*(R, \xi, \tau),$$

$$0 < \xi < L, \quad 0 < \tau < t_f.$$

Individual terms are approximated in a manner analogous to the forward convection approximation (4.12), yielding a similar difference equation,

$$\begin{aligned} & u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\frac{\alpha_1}{\Delta t} (T_{c,j+1}^{*k+1} - T_{c,j+1}^{*k}) + \frac{(1-\alpha_1)}{\Delta t} (T_{c,j}^{*k+1} - T_{c,j}^{*k}) \right] \\ & + v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\frac{\alpha_2}{\Delta z} (T_{c,j+1}^{*k+1} - T_{c,j}^{*k+1}) + \frac{(1-\alpha_2)}{\Delta z} (T_{c,j+1}^{*k} - T_{c,j}^{*k}) \right] \\ & + x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\alpha_1 \alpha_2 T_{c,j+1}^{*k+1} + \alpha_1 (1-\alpha_2) T_{c,j+1}^{*k} + (1-\alpha_1) \alpha_2 T_{c,j}^{*k+1} + (1-\alpha_1)(1-\alpha_2) T_{c,j}^{*k} \right] \\ & = g_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\alpha_2 T_{I,j+\frac{1}{2}}^{*k+1} + (1-\alpha_2) T_{I,j+\frac{1}{2}}^{*k} \right], \end{aligned} \quad (5.3)$$

where, as before, the weighting parameters α_1 and α_2 are restricted by $0 \leq \alpha_1, \alpha_2 \leq 1$. Evaluation of the coefficient functions u^* , v^* , and x^* is done by simple averaging; for example,

$$\begin{aligned} u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} &= (A\rho C_p)^{-*} (\xi_{j+\frac{1}{2}}, \tau_{k+\frac{1}{2}}) = (A\rho C_p)^{-*} (z_{J-j+\frac{1}{2}}, t_{K-k-\frac{1}{2}}) \\ &= (A\rho C_p)^{-*} \left(T_{c, J-j+\frac{1}{2}}^{K-k-\frac{1}{2}} \right) \\ &= (A\rho C_p)^{-*} \left[\frac{1}{2} T_{c, J-j+\frac{1}{2}}^{K-k} + \frac{1}{2} T_{c, J-j+\frac{1}{2}}^{K-k-1} \right] + O[(\Delta t)^2]. \end{aligned}$$

Eq. (5.3) can be rearranged in the form

$$\begin{aligned} A_{I+1,j}^{*k+1} T_{I,j+\frac{1}{2}}^{*k+1} + B_{I+1,j}^{*k+1} T_{c,j+1}^{*k+1} &= D_{I+1,j}^{*k} - E_j^{*k+1} T_{c,j}^{*k+1}, \\ j &= 1, 2, \dots, J-1; k = 0, 1, \dots, K-1, \end{aligned} \quad (5.4)$$

where

$$\begin{aligned} A_{I+1,j}^{*k+1} &\equiv -\alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \\ B_{I+1,j}^{*k+1} &\equiv \alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_1 \alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \\ E_j^{*k+1} &\equiv (1-\alpha_1) u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + (1-\alpha_1) \alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \\ D_{I+1,j}^{*k+1} &\equiv T_{c,j}^{*k} \left[(1-\alpha_1) u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_1)(1-\alpha_2) \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \right] \\ &\quad + T_{c,j+1}^{*k} \left[\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_1(1-\alpha_2) \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \right] \\ &\quad + \Delta t g_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + (1-\alpha_2) \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{I,j+\frac{1}{2}}^{*k}. \end{aligned}$$

As in the forward problem, Eqs. (5.2) and (5.4) are combined to form the matrix equation

$$H_j^{*k+1} T_j^{*k+1} = D_j^{*k}, \quad j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1, \quad (5.5)$$

where T_j^{*k+1} is the vector of adjoint function unknowns

$$T_j^{*k+1} = (T_{1,j+\frac{1}{2}}^{*k+1}, T_{2,j+\frac{1}{2}}^{*k+1}, \dots, T_{I,j+\frac{1}{2}}^{*k+1}, T_{c,j+1}^{*k+1})^T,$$

and D_j^{*k} is the data vector of known quantities,

$$D_j^{*k} = (D_{1,j}^{*k}, D_{2,j}^{*k}, \dots, D_{I-1,j}^{*k}, D_{I,j}^{*k} - C_{I,j}^{*k+1} T_{c,j}^{*k+1}, D_{I+1,j}^{*k} - E_j^{*k+1} T_{c,j}^{*k+1})^T.$$

The matrix H_j^{*k+1} has elements $h_{m,n}^*$, with

$$h_{m,n}^* = \begin{cases} B_{m,j}^{*k+1} & m = n \\ A_{m,j}^{*k+1} & m = n + 1 \\ C_{m,j}^{*k+1} & m = n - 1 \\ 0 & \text{otherwise} \end{cases}$$

Unlike the forward problem, all elements of the matrix H_j^{*k+1} and the vector D_j^{*k} are known, since the coefficient functions are determined by the forward problem solution. Thus, Eq. (5.5) is a true *linear* system and can be solved without iteration.

CHAPTER VI

ASSESSING THE VALIDITY OF THE NUMERICAL SOLUTION

In Chapters IV and V, the systems of governing equations for both forward and adjoint problems were approximated by matrix systems of difference equations. This chapter is concerned with the validity of the difference solutions — do they adequately approximate the differential systems? Topics of concern include *existence* and *uniqueness* of the solution and the *convergence* of the difference solution to the actual differential equations. This last topic covers the two important subjects of *consistency* and *stability*.

Study of partial differential equations has centered around linear problems with constant coefficients. A number of existence and uniqueness results are known for this type of problem with various auxiliary conditions. However, very little is known in general about nonlinear differential equations, and even less about coupled systems of such equations; hence, hope that the forward system of equations [(2.2)-(2.10)] has a unique solution is motivated not by analytic proof, but by an understanding of the physical nature of the problem. In like manner, the assumption of uniqueness for the adjoint solution is based on similarities between the forward and adjoint systems, not on rigorous proof. However, in spite of this incomplete understanding of the actual solutions, it is possible to show existence and uniqueness of the approximating difference solutions!

The numerical solutions are obtained by solving either Eq. (4.14) for the forward case or Eq. (5.5) for the adjoint problem. Because the matrices and the data vectors are unique quantities, the solution vectors T_j^{k+1} and T_j^{*k+1} exist and are unique if and only if the matrices H_j^{k+1} and H_j^{*k+1} are nonsingular. It is a straightforward exercise to demonstrate that both matrices are strictly diagonally dominant, and this is a sufficient condition for nonsingularity.⁸ (Diagonal dominance also implies that no pivoting is necessary in performing the Gaussian elimination procedures for solving both systems.¹¹) Appendix G contains

the details of this exercise; however, it is important to note several points here.

In both the forward and adjoint cases, the diagonal dominance requirements hold unconditionally for rows $i = 1, 2, \dots, I$ (nodes in the fuel rod). The coolant rows $i = I+1$ require slight restrictions on certain discretization parameters (stated in detail in Appendix G), although these restrictions are easily met in practice.

It is also significant that although a unique solution exists, the forward matrix equation (4.14) cannot be determined exactly, but must be solved by iteration. However, it is certain that at each iteration the matrix H_j^{k+1} is diagonally dominant, since the proof in Appendix G is based on the common occurrence of data functions in the coefficients $A_{i,j}^{k+1}$, $B_{i,j}^{k+1}$ and $C_{i,j}^{k+1}$, and not on any particular time level or temperature; hence, the same proof can be applied to each iteration of H_j^{k+1} .

In order to be considered an appropriate approximation, a difference equation must be *consistent* with its differential equation. That is, as all stepsizes approach zero, the difference equation must approach (pointwise) the exact differential equation it supposedly approximates. Because Eq. (4.2) is a rearrangement of Eq. (4.1), it is easily seen that subtracting the differential equation (4.2) from the difference approximation (4.4) gives this result for interior radial regions of the fuel and clad ($i = 2, 3, \dots, I_f - 1, I_f + 2, \dots, I - 1$):

(Difference Equation) - (Differential Equation)

$$= 0[(\Delta t)^3 + \Delta t(\Delta r_i + \Delta r_{i-1}) + \Delta t(\hat{r}_i - \hat{r}_{i-1})^2 + \Delta t(\Delta z)^2] \quad (6.1)$$

Clearly, the right-hand side of Eq. (6.1) vanishes as stepsizes approach zero, showing that the difference approximation (4.4) is consistent with the integrated differential equation (4.1), or its equivalent form (4.2). Referring to Appendices E and F, it can also be seen that analogous consistency results hold for the forward equation approximations at the material boundaries and for all adjoint conduction equation approximations.

Consider now the consistency of the forward convection approximation. Since Eq. (4.12) is equivalent to Eq. (4.11), then subtracting this differential equation from the difference approximation (4.13) yields

$$\begin{aligned}
 & (\text{Difference Equation}) - (\text{Differential Equation}) \\
 &= \frac{\Delta z}{2} (2\alpha_1 - 1) \left[\frac{\partial^2 (uT_c)}{\partial z \partial t} + \frac{\partial (xT_c)}{\partial z} - T_I \frac{\partial x}{\partial z} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
 &+ \frac{\Delta t}{2} (2\alpha_2 - 1) \left[\frac{\partial^2 (vT_c)}{\partial t \partial z} + \frac{\partial (xT_c)}{\partial t} - \frac{\partial}{\partial t} (xT_I) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
 &+ \frac{\Delta t \cdot \Delta z}{4} (2\alpha_1 - 1)(2\alpha_2 - 1) \left[\frac{\partial^2 (xT_c)}{\partial t \partial z} - \frac{\partial}{\partial t} \left(T_I \frac{\partial x}{\partial z} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
 &+ O[(\Delta z)^2 + (\Delta t)^2] . \tag{6.2}
 \end{aligned}$$

It is clear that as $\Delta t, \Delta z \rightarrow 0$, the right-hand side of Eq. (6.2) vanishes, proving that the difference approximation is consistent. In addition, the right-hand side of Eq. (6.2) also reveals that if $\alpha_1 = \alpha_2 = \frac{1}{2}$, the method has second order accuracy in both variables, whereas $\alpha_1 \neq \frac{1}{2}$ or $\alpha_2 \neq \frac{1}{2}$ results in a first-order approximation. Analogous results also hold for the adjoint convection equation.

Stability analysis is concerned with the effect of small round-off errors due to lack of infinite precision in computational capability. It is important that errors arising at one time step should not be amplified at subsequent time steps. Stability generally depends on the type of difference approximation, the magnitude of coefficient functions, and the values of parameters used in the numerical approximation. Once a particular difference scheme has been selected, it is imperative to choose step-sizes and other parameters so as to ensure stability.

It is well known that for the heat conduction equation with constant coefficients, the Crank-Nicolson methodology results in a stable difference scheme.² Because the coefficient functions used in the forward and adjoint fuel equations are slowly varying functions of temperature, it is reasonable to suppose that the Crank-Nicolson approximation will result in stable difference equations for both cases.

It is possible to be more definite in the stability analysis of the forward convection equation. Equation (4.13) can be written as the matrix equation

$$P T_C^{k+1} = Q T_C^k + b, \quad k = 0, 1, \dots, K-1 \quad (6.3)$$

where

$$P = \begin{bmatrix} B_{I+1,1}^{k+1} & & & \\ E_2^{k+1} & B_{I+1,2}^{k+1} & & \\ & E_3^{k+1} & B_{I+1,3}^{k+1} & \\ & & \ddots & \ddots \\ & & & E_{J-1}^{k+1} & B_{I+1,J-1}^{k+1} \end{bmatrix}, \quad Q = \begin{bmatrix} m_1^k & & & \\ n_2^k & m_2^k & & \\ & n_3^k & m_3^k & \\ & & \ddots & \ddots \\ & & & n_{J-1}^k & m_{J-1}^k \end{bmatrix},$$

$$b = \begin{bmatrix} -A_{I+1,1}^{k+1} T_{I,1+\frac{1}{2}}^{k+1} + (1-\alpha_2) T_{I,1+\frac{1}{2}}^k [\alpha_1 x_2^k + (1-\alpha_1) x_1^k] - E_1^{k+1} (T_{c1})^{k+1} + n_1^k (T_{c1})^k \\ -A_{I+1,2}^{k+1} T_{I,2+\frac{1}{2}}^{k+1} + (1-\alpha_2) T_{I,2+\frac{1}{2}}^k [\alpha_1 x_3^k + (1-\alpha_1) x_2^k] \\ \vdots \\ -A_{I+1,J-1}^{k+1} T_{I,J-\frac{1}{2}}^{k+1} + (1-\alpha_2) T_{I,J-\frac{1}{2}}^k [\alpha_1 x_J^k + (1-\alpha_1) x_{J-1}^k] \end{bmatrix},$$

$$T_C^k = (T_{c,2}^k, T_{c,3}^k, \dots, T_{c,J}^k)^T,$$

and the elements m_j^k, n_j^k are defined as

$$m_j^k \equiv \alpha_1 u_{j+1}^k - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+1}^k - \alpha_1(1-\alpha_2)\Delta t x_{j+1}^k$$

$$n_j^k \equiv (1-\alpha_1)u_j^k + (1-\alpha_2) \frac{\Delta t}{\Delta z} v_j^k - (1-\alpha_1)(1-\alpha_2)\Delta t x_j^k .$$

Examination of the quantities E_j^{k+1} and $B_{I+1,j}^{k+1}$ reveals that for $\alpha_1 \geq \frac{1}{2}$, $\alpha_2 > 0$, the matrix P is strictly diagonally dominant and therefore invertible. If T_c^k represents the exact solution to Eq. (6.3) and $\bar{T}_c^k$ the vector actually computed, the round-off error can be expressed as $\bar{e}^k = T_c^k - \bar{T}_c^k$, with $\bar{e}^k = (e_1^k, e_2^k, \dots, e_{J-1}^k)^T$. For simplicity, assume the vector b is insignificant in propagating error to the calculation at the next time step. Letting $\bar{e}^{k+1}$ denote the *effect* of the round-off error from time step k on the computation of temperature at time step $k+1$, the following matrix equation must be satisfied:

$$P \bar{e}^{k+1} = Q \bar{e}^k, \quad k = 0, 1, \dots, K-1 . \quad (6.4)$$

If the eigenvalues of $P^{-1}Q$ are distinct, then $\bar{e}^k$ can be expressed as a linear combination of the corresponding eigenvectors, which yields

$$\bar{e}^{k+1} = P^{-1}Q \bar{e}^k = P^{-1}Q \sum_{j=1}^{J-1} \alpha_j \bar{x}_j = \sum_{j=1}^{J-1} \alpha_j \lambda_j \bar{x}_j , \quad (6.5)$$

where α_j are constants and λ_j are eigenvalues of $P^{-1}Q$, $j = 1, 2, \dots, J-1$. Now, $P^{-1}Qx = \lambda x$ implies $(Q-\lambda P)x = 0$; hence, for nonzero x , $\det(Q-\lambda P) = 0$. Since both P and Q are lower triangular, the determinant of $(Q-\lambda P)$ is simply the product of the diagonal elements

$$\det(Q-\lambda P) = \prod_{j=1}^{J-1} \left(m_j^k - \lambda B_{I+1,j}^{k+1} \right) = 0 ,$$

giving the eigenvalues $\lambda_j = m_j^k / B_{I+1,j}^{k+1}$ (in practice, these are generally distinct, due to nonconstant terms in m_j^k and $B_{I+1,j}^{k+1}$). It follows that the corresponding normalized eigenvectors are the $J-1$ unit vectors $\bar{x}_j = (0, \dots, 0, 1, 0, \dots, 0)^T$, with the "1" in the j th position. Stability requires that $|e_j^{k+1}| \leq |e_j^k|$, $j = 1, 2, \dots, J-1$, and from Eq. (6.5), this happens if and only if $|\lambda_j| \leq 1$, $j = 1, 2, \dots, J-1$. Imposing this restriction produces

$$-1 \leq \frac{\alpha_1 u_{j+1}^k - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+1}^k - \alpha_1(1-\alpha_2)\Delta t x_{j+1}^k}{\alpha_1 u_{j+1}^{k+1} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+1}^{k+1} + \alpha_1\alpha_2 \Delta t x_{j+1}^{k+1}} \leq 1, \quad j = 1, 2, \dots, J-1,$$

which yields the two inequalities

$$\begin{aligned} \alpha_1 \left(u_{j+1}^k - u_{j+1}^{k+1} \right) - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+1}^k - \alpha_2 \frac{\Delta t}{\Delta z} v_{j+1}^{k+1} \\ - \alpha_1(1-\alpha_2)\Delta t x_{j+1}^k - \alpha_1\alpha_2\Delta t x_{j+1}^{k+1} \leq 0, \\ \alpha_1 \left(u_{j+1}^k + u_{j+1}^{k+1} \right) + \alpha_2 \frac{\Delta t}{\Delta z} \left(v_{j+1}^k + v_{j+1}^{k+1} \right) - \frac{\Delta t}{\Delta z} v_{j+1}^k \\ + \alpha_1\alpha_2\Delta t \left(x_{j+1}^k + x_{j+1}^{k+1} \right) - \alpha_1\Delta t x_{j+1}^k \geq 0. \end{aligned}$$

Examination of the functions u , v , and x reveals that both inequalities are satisfied for $\frac{1}{2} \leq \alpha_2 \leq 1$. Thus, stability for the forward convection approximation is guaranteed if $\frac{1}{2} \leq \alpha_1$, $\alpha_2 \leq 1$, with no constraints imposed on the stepsizes.

The stability analysis of the adjoint convection equation follows the same basic procedure as the forward case. Defining $\vec{e}^k$ as the vector of round-off errors occurring at time step k , and neglecting error propagation through the fuel terms in Eq. (5.4), the effect $\vec{e}^{k+1}$ of these errors on the computations at time step $k+1$ satisfies the matrix equation

$$P^* \bar{e}^{*k+1} = Q^* \bar{e}^{*k}, \quad (6.6)$$

where

$$P^* = \begin{bmatrix} B_{I+1,1}^{*k+1} & & & \\ E_2^{*k+1} & B_{I+1,2}^{*k+1} & & \\ & \ddots & \ddots & \\ & & E_{J-1}^{*k+1} & B_{I+1,J-1}^{*k+1} \end{bmatrix}, \quad Q^* = \begin{bmatrix} m_1^{*k} & & & \\ n_2^{*k} & m_2^{*k} & & \\ & \ddots & \ddots & \\ & & n_{J-1}^{*k} & m_{J-1}^{*k} \end{bmatrix}$$

$$\bar{e}^{*k} = (e_1^{*k}, e_2^{*k}, \dots, e_{J-1}^{*k})^T$$

$$m_j^{*k} \equiv \alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_1(1-\alpha_2)\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}}$$

$$n_j^{*k} \equiv (1-\alpha_1)u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_1)(1-\alpha_2)\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}}.$$

Imposing the restriction $\frac{1}{2} \leq \alpha_1 \leq 1$ provides strict diagonal dominance in P^* , thus permitting its inversion. As in the forward problem, $\bar{e}^{*k}$ is represented as a linear combination of the eigenvectors $\bar{y}_j$ of $P^{*-1}Q^*$,

$$\bar{e}^{*k+1} = P^{*-1}Q^* \bar{e}^{*k} = P^{*-1}Q^* \sum_{j=1}^{J-1} \beta_j \bar{y}_j = \sum_{j=1}^{J-1} \beta_j \gamma_j \bar{y}_j, \quad (6.7)$$

where β_j are constants and γ_j are eigenvalues of $P^{*-1}Q^*$. Proceeding as before yields eigenvalues $\gamma_j = m_j^{*k}/B_{I+1,j}^{*k+1}$ (distinct), and corresponding eigenvectors $y_j = (0, \dots, 0, 1, 0, \dots, 0)^T$, the $J-1$ unit vectors. The difference scheme is stable if $|\gamma_j| \leq 1$, $j = 1, 2, \dots, J-1$, or

$$-1 \leq \frac{\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_1(1-\alpha_2)\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}}}{\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_1\alpha_2\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}}} \leq 1,$$

$$j = 1, 2, \dots, J-1.$$

It can be shown that u^* , v^* , and x^* are positive functions; hence, the only useful inequality is the left-hand one. Simplification leads to

$$2\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + (2\alpha_2-1) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_1(2\alpha_2-1)\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \geq 0,$$

which obviously holds for $\frac{1}{2} \leq \alpha_2 \leq 1$. Thus, stability of the adjoint difference approximation also follows if $\frac{1}{2} \leq \alpha_1$, $\alpha_2 \leq 1$.

In addition to its use in stability analysis, Eq. (6.7) lends itself to another important observation. The stability requirement of $-1 \leq \gamma_j \leq 1$ ensures that e_j^{*k+1} will not exceed e_j^{*k} in magnitude. Further examination of Eq. (6.7) reveals that the effect e_j^{*k+1} of e_j^{*k} will change signs if $-1 \leq \gamma_j \leq 0$. In order to prevent such "oscillation," it is necessary to impose the additional restriction

$$\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - (1-\alpha_2) \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_1(1-\alpha_2)\Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} \geq 0. \quad (6.8)$$

Obviously $\alpha_2 = 1$ satisfies this condition (creating a fully implicit method), and, in practice, other variations of problem parameters also satisfy Eq. (6.8). Further discussion of the relevance and applicability of this restriction occurs in Chapter VII.

Consider now a second important stability problem in the adjoint coolant computations. If an error is introduced at a particular axial step, it is essential that its effect should not increase in computations at the next axial step. From Eq. (5.4), a forward substitution algorithm can be formed to determine the unknown adjoint coolant values,

$$T_{c,j+1}^{*k+1} = \left[-E_j^{*k+1} T_{c,j}^{*k+1} - A_{I+1,j}^{*k+1} T_{I,j+\frac{1}{2}}^{*k+1} - D_{I+1,j}^{*k} \right] / B_{I+1,j}^{*k+1},$$

$$j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1.$$

Assuming no error propagates through the adjoint fuel values, the round-off error is propagated axially as

$$e_{j+1}^{*k+1} = -\frac{E_j^{*k+1}}{B_{I+1,j}^{*k+1}} e_j^{*k+1}, \quad j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1. \quad (6.9)$$

The method is stable for $|e_{j+1}^{*k+1}| \leq |e_j^{*k+1}|$ or $|E_j^{*k+1}/B_{I+1,j}^{*k+1}| \leq 1$. This restriction gives the inequalities

$$-1 \leq \frac{(1-\alpha_1)u_{j+\frac{1}{2}}^{*k+1} - \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+1} + (1-\alpha_1)\alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+1}}{\alpha_1 u_{j+\frac{1}{2}}^{*k+1} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+1} + \alpha_1 \alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+1}} \leq 1,$$

which yield, upon rearranging,

$$(1-2\alpha_1)u_{j+\frac{1}{2}}^{*k+1} - 2\alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+1} + (1-2\alpha_1)\alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+1} \leq 0$$

$$u_{j+\frac{1}{2}}^{*k+1} + \alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+1} \geq 0.$$

The second inequality always holds, while the first is easily satisfied if $\alpha_1 \geq \frac{1}{2}$, making this a sufficient condition for axial stability.

Again regarding Eq. (6.9), prevention of axial oscillation requires $E_j^{*k+1} \leq 0$, or

$$(1-\alpha_1)u_{j+\frac{1}{2}}^{*k+1} - \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+1} + (1-\alpha_1)\alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+1} \leq 0,$$

$$j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1, \quad (6.10)$$

which is clearly satisfied for $\alpha_1 = 1$. Other combinations of problem parameters also satisfy Eq. (6.10), and will be discussed further in the next chapter.

CHAPTER VII

RESULTS AND CONCLUSIONS

The preceding chapters have been concerned with the theoretical development of a particular sensitivity problem. A computer code was written to solve the difference equations of Chapters IV and V, and to perform the sensitivity integrals of Eq. (2.21), which are discretized in Appendix H. Information concerning the physical data functions and initial conditions was obtained from a steady-state code written by E. M. Oblow of Oak Ridge National Laboratory, the safety analysis code MELT-III,¹² and the publication "MATPRO-VERSION 09."¹³

The stability analysis of Chapter VI is very useful in understanding many of the problems encountered in debugging and running the code. Of particular importance is the oscillation analysis pertaining to the adjoint coolant function. Because the adjoint initial and boundary values are zero, any oscillation due to round-off error results in negative adjoint coolant values that propagate immediately into the fuel adjoints. These negative values are disturbing, although in many calculations they are not important. However, in certain cases they cause significant damage; hence, it is necessary to control their effects. This is most easily accomplished by varying the parameters α_1 , α_2 , and Δt so as to satisfy Eqs. (6.8) and (6.10).

Equation (6.8) can be rewritten as

$$\Delta t(1-\alpha_2)(M_1/\Delta z + M_2\alpha_1) \leq \alpha_1, \quad (7.1)$$

where

$$M_1 = \max_{(z,t)} \left\{ \frac{(wC_p)^-}{(A\rho C_p)^-} \right\} \quad \text{and} \quad M_2 = \max_{(z,t)} \left\{ \frac{2\pi Rh^-}{(A\rho C_p)^-} \right\},$$

and Eq. (6.10) can be expressed as

$$\alpha_2 \Delta t \, m_1(\alpha_1) \geq (1 - \alpha_1), \quad (7.2)$$

where

$$m_1(\alpha_1) = \min_{(z,t)} \left\{ \frac{1}{\Delta z} \frac{(wC_p)^-}{(A\rho C_p)^-} - (1 - \alpha_1) \frac{2\pi R h^-}{(A\rho C_p)^-} \right\}.$$

For given values of Δt and α_1 , Eqs. (7.1) and (7.2) give minimum values for α_2 which satisfy Eqs. (6.8) and (6.10). Certain choices of these parameters appear in Table I, where B_1 and B_2 are the lower bounds for α_2 as determined from Eqs. (7.1) and (7.2), respectively. It is important to note that even if Eqs. (6.8) and (6.10) are violated, the resulting oscillation may be negligible. That is, unless an oscillation is of the same order of magnitude as the solution itself, it will not affect the solution adversely (provided the stability conditions are met). For this reason the forward solution (with coolant temperatures ranging from 390°C-570°C) is largely immune to any oscillatory problem, while the adjoint solution (seldom greater than one) is much more susceptible.

Complications also arise from other sources that restrict problem parameters even more than Eqs. (7.1) and (7.2). For instance, many applications require point sources (resembling Dirac delta functions) as the adjoint source functions. Because of the zero initial conditions, these positive sources propagate in the coolant as wave fronts, thus posing further restrictions on the time step.

In practice, runs with $\Delta t \leq 0.05$ sec. were successful (provided weighting parameters α_1 and α_2 were chosen correctly), whereas larger stepsizes resulted in totally spurious results. Primary calculations were done with parameter values of $\Delta t = 0.02$ sec., $\alpha_1 = 0.5$, and $\alpha_2 = 1.0$, which, although in slight violation of Eq. (7.1), showed no negative oscillations. Other runs with the parameters Δt and α_2 chosen in accordance with or in slight violation of Eqs. (7.1) and (7.2) yielded sensitivity coefficients *almost identical* to the original calculations! Thus, certain variations of Δt , α_1 , and α_2 , and even the

Table I. Parameter Limitations for Adjoint Coolant Stability

Time Step (sec)	Bound ^a	Value of α_1 ^b					
		0.5	0.6	0.7	0.8	0.9	1.0
0.005	B ₁	0.49	0.43	0.39	0.35	0.32	0.29
	B ₂	5.71	2.27	1.13	0.57	0.23	0
0.01	B ₁	0.74	0.72	0.70	0.68	0.66	0.65
	B ₂	2.86	1.14	0.57	0.28	0.11	0
0.02	B ₁	0.87	0.86	0.85	0.84	0.83	0.82
	B ₂	1.43	0.57	0.28	0.14	0.06	0
0.03	B ₁	0.91	0.91	0.90	0.89	0.89	0.88
	B ₂	0.95	0.38	0.19	0.09	0.04	0
0.04	B ₁	0.94	0.93	0.92	0.92	0.92	0.91
	B ₂	0.71	0.28	0.14	0.07	0.03	0
0.05	B ₁	0.95	0.94	0.94	0.94	0.93	0.93
	B ₂	0.57	0.23	0.11	0.06	0.03	0

^aB₁ = bound from Eq. (7.1); B₂ = bound from Eq. (7.2).

^bFor $\alpha_1 = 0.5, 0.6, 0.7, 0.8, 0.9, 1.0$, table entries are corresponding minimum values for α_2 , as determined from Eqs. (7.1) and (7.2).

presence of slight negative oscillations, had only small effects on the sensitivity results (provided that the numerical stability was maintained).

The topic of greatest interest is, of course, the successful computation of the sensitivity coefficients. Three particular responses were studied (peak fuel, clad, and coolant temperatures), and a set of sensitivity coefficients $\left(\frac{dP/P}{d\alpha/\alpha}, \text{ for each } \alpha\right)$ was computed for each. Using this data, predictions were made of the new responses that would result if perturbed values of each α were used in place of the original values. For instance, the peak fuel temperature response (2059°C) had a fuel heat source sensitivity coefficient of $\frac{dP/P}{d\bar{Q}_f/\bar{Q}_f} = 0.1343$. For a 10% change in $\bar{Q}_f$, i.e., $\Delta\bar{Q}_f/\bar{Q}_f = 0.1$, the predicted new response is

$$\begin{aligned}\tilde{P} &= P + \Delta P = P + \frac{dP}{d\bar{Q}_f} \cdot \Delta\bar{Q}_f = P \left[1 + \frac{dP/P}{d\bar{Q}_f/\bar{Q}_f} \cdot \frac{\Delta\bar{Q}_f}{\bar{Q}_f} \right] \\ &= 2059^{\circ}\text{C} [1 + (0.1343)(0.1)] = 2087^{\circ}\text{C} . \quad (7.3)\end{aligned}$$

Note that all predictions formulated as in Eq. (7.3) are linearized approximations to the actual perturbed responses.

For each of the original responses, the sensitivity coefficients for relevant α 's are shown in Tables II, III, and IV. In addition, predicted responses, computed as in Eq. (7.3), are given for certain perturbations of each parameter α . In order to verify these results, a shortened version of the computer code recalculated the forward temperatures using perturbed physical data. The new responses thus obtained appear in the last columns of Tables II, III, and IV.

From these tables, it is obvious that the linearized predictions using the sensitivity coefficients as in Eq. (7.3) agree very well with the actual perturbed responses, even for parameter perturbations of 25%! Observe also that the method uses very practical computational procedures, and thus conclude that the differential sensitivity theory applied to transient reactor safety problems is feasible and promising.

Table II. Peak Fuel Temperature
(Original Response = 2059°C)

Parameter α	$\frac{dP/P}{d\alpha/\alpha}$	$\frac{\Delta\alpha}{\alpha}$	Predicted Response	Actual Perturbed Response
$(\bar{T}_0)_f$ (initial fuel temperature)	0.8763	.05 .10 .25	2149 2239 2510	2149 2237 2500
$\bar{Q}_f$ (fuel heat source)	0.1343	.05 .10 .25	2073 2087 2128	2073 2087 2128
$\bar{k}_f$ (fuel thermal conductivity)	-0.1153	.05 .10 .25	2047 2035 2000	2047 2036 2002
$(\bar{\rho C}_p)_f$ (fuel density-specific heat)	-0.01275	.25	2052	2054
$\bar{h}_g$ (gap conductance)	-0.00558	.25	2056	2056
$(\bar{T}_0)_c$ (init. clad temp.)	0.00206	.25	2060	2060
$\bar{T}_{c0}$ (init. coolant temp.)	0.00113	.25	2060	2060
$\bar{T}_{c1}$ (coolant inlet temp.)	0.00066	.25	2059	2059
$(\bar{wC}_p)$ (coolant mass flow rate-spec. heat)	-0.00045	-.25	2059	2059
$\bar{k}_c$ (clad thermal cond.)	-0.00018	.25	2059	2059
$\bar{h}_c$ (heat trans. coeff.)	-0.00005	.25	2059	2059
$(\bar{\rho C}_p)_c$ (clad density-spec. heat)	$-5 \cdot 10^{-7}$	.25	2059	2059
$(\bar{A\rho C}_p)$ (coolant area-density-spec. heat)	$-2 \cdot 10^{-7}$	.25	2059	2059

Table III. Peak Clad Temperature
(Original Response = 568.6°C)

Parameter α		$\frac{dP/P}{d\alpha/\alpha}$	$\frac{\Delta\alpha}{\alpha}$	Predicted Response	Actual Perturbed Response
$\bar{T}_{cl}$	(coolant inlet temperature)	0.5244	.05	583.5	583.4
			.10	598.4	598.4
			.25	643.1	643.0
$(\bar{T}_0)_f$	(initial fuel temperature)	0.3547	.05	578.7	578.7
			.10	588.8	588.9
			.25	619.0	619.5
$(\overline{wC_p})$	(coolant mass flow rate-specific heat)	-0.2604	-.05	576.0	576.3
			-.10	583.4	584.8
			-.25	605.6	616.1
$\bar{h}_g$	(gap conductance)	0.1415	.05	572.6	572.5
			.10	576.6	576.2
			.25	588.7	586.2
$\bar{k}_f$	(fuel thermal conductivity)	0.0756	.10	572.9	572.7
			.25	579.3	578.0
$\bar{Q}_f$	(fuel heat source)	0.0639	.10	572.2	572.3
			.25	577.7	577.7
$(\bar{T}_0)_c$	(initial clad temp.)	0.0168	.25	571.0	571.2
$\bar{k}_c$	(clad thermal cond.)	-0.0105	.25	567.1	567.4
$\bar{T}_{c0}$	(initial coolant temp.)	0.0097	.25	570.0	570.3
$\bar{h}_c$	(heat trans. coeff.)	-0.0033	.25	568.1	568.2
$(\overline{\rho C_p})_f$	(fuel density-spec. heat)	-0.0039	.25	568.0	568.2
$(\overline{\rho C_p})_c$	(clad density-spec. heat)	-0.0017	.25	568.4	568.4
$(\overline{A\rho C_p})$	(coolant density-area-spec. heat)	-0.0009	.25	568.5	568.5

Table IV. Outlet Coolant Temperature
(Original Response = 562.3°C)

Parameter α	$\frac{dP/P}{d\alpha/\alpha}$	$\frac{\Delta\alpha}{\alpha}$	Predicted Response	Actual Perturbed Response
$\bar{T}_{cl}$ (coolant inlet temperature)	0.5378	.05 .10 .25	577.4 592.5 637.9	577.6 592.6 637.3
$(\bar{T}_0)_f$ (initial fuel temperature)	0.3449	.05 .10 .25	572.0 581.7 610.8	572.6 582.5 612.4
$(\overline{wC_p})$ (coolant mass flow rate-specific heat)	-0.2766	-.05 -.10 -.25	570.1 577.9 601.2	570.8 579.7 611.8
$\bar{k}_f$ (fuel thermal conductivity)	0.0741	.10 .25	566.5 572.7	566.7 571.8
$\bar{Q}_f$ (fuel heat source)	0.0642	.10 .25	565.9 571.3	566.3 571.6
$\bar{h}_g$ (gap conductance)	0.1364	.05 .10 .25	566.1 570.0 581.5	566.5 570.1 579.6
$(\bar{T}_0)_c$ (initial clad temp.)	0.0157	.25	564.5	565.3
$\bar{T}_{c0}$ (initial coolant temp.)	0.0079	.25	563.4	564.4
$\bar{k}_c$ (clad thermal cond.)	0.0059	.25	563.1	563.4
$(\overline{\rho C_p})_f$ (fuel density-spec. heat)	-0.0038	.25	561.8	562.3
$(\overline{\rho C_p})_c$ (clad density-spec. heat)	-0.0014	.25	562.1	562.5
$\bar{h}_c$ (heat trans. coeff.)	0.0021	.25	562.6	563.0
$(\overline{A\rho C_p})$ (coolant area-density-spec. heat)	-0.0007	.25	562.2	562.6

Because of the preliminary nature of this work, many topics have been covered in general or even skipped entirely. It would definitely be advantageous to review the differencing schemes and perhaps devise more accurate, efficient approximations. Further work would be useful in studying the wave propagation of the adjoint coolant source. More efficient computer coding could be developed and several other areas of numerical analysis could be explored. Future plans already call for more detailed modeling of the physical system and more practical sensitivity calculations. In short, this project has yielded encouraging preliminary results, but has also uncovered new problems and presented many new areas for study.

REFERENCES

1. Agrawal, A. K., Guppy, J. G., Madni, I. K., Quan, V., Weaver, W. L. III, and Yang, J. W. *Nucl. Sci. Eng.*, 64, 480-491 (1977).
2. Ames, W. F. *Numerical Methods for Partial Differential Equations*, Academic Press, New York (1977).
3. Apostol, T. M. *Mathematical Analysis*, Addison-Wesley Publishing Company, Reading, Mass. (1975).
4. Conte, S. D. and de Boor, C. *Elementary Numerical Analysis: An Algorithmic Approach*, McGraw-Hill, Inc., New York (1972).
5. Dunn, F. E., et al. "The SAS2A LMFBR Accident Analysis Computer Code," ANL-8138, Argonne National Laboratory (1974).
6. Lin, C. C. and Segal, L. A. *Mathematics Applied to Deterministic Problems in the Natural Sciences*, Macmillan Publishing Co., Inc., New York (1974).
7. Oblow, E. M. "Sensitivity Theory for Reactor Thermal-Hydraulics Problems," ORNL/TM-6303, Oak Ridge National Laboratory (1978).
8. Ortega, J. M. *Numerical Analysis*, Academic Press, New York (1972).
9. Ozisik, M. N. *Boundary Value Problems of Heat Conduction*, International Textbook Company, Scranton, Pa. (1968).
10. Stevens, P. N. and Trubey, D. K. "Weapons Radiation Shielding Handbook, Chapter 3/Methods for Calculating Neutron and Gamma-Ray Attenuation," DNA-1892-3, Rev. 1, Defense Nuclear Agency (1972).
11. Stewart, G. W. *Introduction to Matrix Computations*, Academic Press, New York (1973).
12. Waltar, A. E., et al. "MELT-III, a Neutronics, Thermal-Hydraulics Computer Program for Fast Reactor Safety Analysis," Vol. I, HEDL-TME 74-47, UC-79p, e, d, b, Hanford Engineering Development Laboratory (1974).
13. "MATPRO-VERSION 09, A Handbook of Material Properties for Use in the Analysis of Light Water Reactor Fuel Rod Behavior," TREE-NUREG-1005, U.S. Nuclear Regulatory Commission (1976).

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX A

DERIVATION OF THE GOVERNING EQUATIONS

For any homogeneous medium, consider the arbitrary material region $R(t)$, bounded by the surface $S(t)$. Let $\vec{x} = (x, y, z) = (r, \theta, z)$ be an arbitrary point and $d\vec{x} = dx dy dz = r dr d\theta dz$ an arbitrary volume element in $R(t)$; let $d\sigma$ be an arbitrary surface element of $S(t)$. At $t = 0$, $R(0)$ is the region bounded by $S(0)$. The total heat in $R(t)$ at time t is given by

$$Q_1(t) = \iiint_{R(t)} \rho H d\vec{x}, \quad (A.1)$$

where

$T = T(\vec{x}, t)$ = temperature

$H = H(T) = \int C_p dT$ = enthalpy

$C_p = C_p(T)$ = specific heat

$\rho = \rho(T)$ = density.

The total change in the amount of heat in $R(t)$ between times t and $t + \Delta t$ is then $Q_1(t + \Delta t) - Q_1(t)$. Also at time t , the net heat flow per unit time into $R(t)$ through the surface $S(t)$ is

$$\dot{Q}_2(t) = - \iint_{S(t)} \vec{q} \cdot \vec{n} d\sigma, \quad (A.2)$$

where

$\vec{q} = -k \nabla T$ = heat flux

$k = k(T)$ = thermal conductivity

$\vec{n}$ = unit exterior normal to $S(t)$.

The total heat generated internally in $R(t)$ between times t and $t + \Delta t$ is

$$Q_3 = \int_t^{t+\Delta t} \iiint_{R(t)} Q \, d\vec{x} \, dt, \quad (\text{A.3})$$

where $Q = Q(\vec{x}, t)$ is the heat source density function, i.e., the amount of heat generated per volume per unit time.

The energy balance for the time interval $(t, t + \Delta t)$ is

net increase of heat in $R(t)$

= net flow into $R(t)$ + total heat generated internally in $R(t)$,

which is expressed quantitatively by combining Eqs. (A.1), (A.2), and (A.3),

$$Q_1(t + \Delta t) - Q_1(t) = \int_t^{t+\Delta t} \dot{Q}_2(t) \, dt + Q_3.$$

Substituting for Q_1 , $\dot{Q}_2$, and Q_3 produces

$$\left[\iiint_{R(t)} \rho H \, d\vec{x} \right]_t^{t+\Delta t} = \int_t^{t+\Delta t} \left[- \oiint_{S(t)} \vec{q} \cdot \vec{n} \, d\sigma + \iiint_{R(t)} Q \, d\vec{x} \right] dt.$$

The Differential Mean Value Theorem is used on the left-hand side and the Integral Mean Value Theorem on the right; hence, the balance equation becomes

$$\Delta t \left[\frac{d}{dt} \iiint_{R(t)} \rho H \, d\vec{x} \right]_{t=t^*} = \Delta t \left[- \oiint_{S(t)} \vec{q} \cdot \vec{n} \, d\sigma + \iiint_{R(t)} Q \, d\vec{x} \right]_{t=t^{**}},$$

$$t < t^* < t + \Delta t, \quad t \leq t^{**} \leq t + \Delta t.$$

Dividing by Δt and letting $\Delta t \rightarrow 0$ (so that $t^* \rightarrow t$ and $t^{**} \rightarrow t$) yields

$$\frac{d}{dt} \iiint_{R(t)} \rho H \, d\vec{x} = - \oint_{S(t)} \vec{q} \cdot \vec{n} \, d\sigma + \iiint_{R(t)} Q \, d\vec{x}, \quad (\text{A.4})$$

which is the *integral form* of the energy balance equation.

Using the Reynolds Transport Theorem, a result from continuum mechanics,⁶ the left-hand side of Eq. (A.4) becomes

$$\frac{d}{dt} \iiint_{R(t)} \rho H \, d\vec{x} = \iiint_{R(t)} \frac{\partial}{\partial t} (\rho H) \, d\vec{x} + \oint_{S(t)} (\rho H \vec{v}) \cdot \vec{n} \, d\sigma, \quad (\text{A.5})$$

where $\vec{v} = \vec{v}(\vec{x}, t)$ is the velocity of the medium. Substituting Eq. (A.5) into Eq. (A.4) gives

$$\iiint_{R(t)} \left[\frac{\partial}{\partial t} (\rho H) - Q \right] d\vec{x} = - \oint_{S(t)} [\vec{q} + \rho H \vec{v}] \cdot \vec{n} \, d\sigma,$$

which is transformed by applying the Divergence Theorem to the surface integral, yielding

$$\iiint_{R(t)} \left[\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\vec{q} + \rho H \vec{v}) - Q \right] d\vec{x} = 0. \quad (\text{A.6})$$

Because $R(t)$ is an arbitrary region, application of the Dubois-Reymond Lemma⁶ to Eq. (A.6) implies that for each point $(\vec{x}, t)$,

$$\frac{\partial}{\partial t} (\rho H) + \nabla \cdot (\vec{q} + \rho H \vec{v}) - Q = 0, \quad (\text{A.7})$$

which is the *differential form* of the energy balance equation.

Equation (A.7) can be simplified using assumptions (2.1) for this particular application; use of (2.1 a) produces

$$\frac{\partial}{\partial t} (\rho H) + \frac{1}{r} \frac{\partial}{\partial r} (r q_1 + r \rho H v_1) + \frac{\partial}{\partial z} (q_3 + \rho H v_3) - Q = 0, \quad (\text{A.8})$$

where $q_1 = -k \partial T / \partial r$, $q_3 = -k \partial T / \partial z$, and v_1 , v_3 are the radial and axial velocity components, respectively. Since conduction is negligible axially and convection is negligible radially in both fuel and coolant, Eq. (A.8) reduces to

$$\frac{\partial}{\partial t} (\rho H) + \frac{1}{r} \frac{\partial}{\partial r} (r q_1) + \frac{\partial}{\partial z} (\rho H v_3) - Q = 0. \quad (\text{A.9})$$

To define a specific domain, let $0 \leq r \leq R$, $0 \leq z \leq L$, $0 \leq t \leq t_f$ in the fuel pin and $R \leq r \leq R_{\text{MAX}}$, $0 \leq z \leq L$, $0 \leq t \leq t_f$ in the coolant. Specify also the material interface boundaries $r = R_f$ (outer radius of fuel) and $r = R_g$ (outer radius of gap).

For the fuel and cladding regions of the fuel rod, no axial convection occurs and density is constant; hence, Eq. (A.9) reduces to

$$\rho \frac{\partial H}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r q_1) = Q.$$

From the definition of H ,

$$\frac{\partial H}{\partial t} = \frac{\partial}{\partial t} \int_0^T C_p(T') dT' = C_p \frac{\partial T}{\partial t},$$

and thus the final form is obtained for the energy balance equation in the fuel rod,

$$\rho C_p \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) = Q, \quad \begin{cases} 0 < r < R_f \\ R_g < r < R \end{cases}, \quad 0 < z < L, \quad 0 < t < t_f. \quad (\text{A.10})$$

There is no heat generation in the coolant; hence, $Q = 0$. Since C_p is essentially constant, then

$$H = \int_0^{T_c} C_p dT_c = C_p T_c.$$

Using this information, Eq. (A.9) applied to the coolant becomes

$$\frac{\partial}{\partial t} (\rho C_p T_c) + \frac{\partial}{\partial z} (\rho C_p v_3 T_c) = -\frac{1}{r} \frac{\partial}{\partial r} (r q_1).$$

Since there is no conduction in the coolant, the only nonzero heat flux occurs at the coolant-clad boundary. Because the coolant temperature is independent of r , this variable is integrated out as follows:

$$2\pi \int_R^{R_{\max}} \frac{\partial}{\partial t} (\rho C_p T_c) r dr + 2\pi \int_R^{R_{\max}} \frac{\partial}{\partial z} (\rho C_p v_3 T_c) r dr = -2\pi (r q_1) \Big|_R^{R_{\max}},$$

which simplifies to

$$A \frac{\partial}{\partial t} (\rho C_p T_c) + A \frac{\partial}{\partial z} (\rho C_p v_3 T_c) = 2\pi R q_1 \Big|_{r=R},$$

where $A = \pi(R_{\max}^2 - R^2)$ is the coolant channel cross-sectional area.

Assuming A is constant and defining the coolant mass flow rate $w = \rho A v_3$, this final form is obtained for the energy balance in the coolant

$$\frac{\partial}{\partial t} (A \rho C_p T_c) + \frac{\partial}{\partial z} (w C_p T_c) = 2\pi R q_1(R, z, t), \quad 0 < z < L, \quad 0 < t < t_f. \quad (A.11)$$

Auxiliary conditions are also obtained from assumptions (2.1). Combining (2.1 a) and (2.1 e) gives

$$\left. \frac{\partial T}{\partial r} \right|_{r=0} = 0.$$

The coolant-clad boundary and the fuel-clad interface have the conventional heat transfer conditions,

$$-k \left. \frac{\partial T}{\partial r} \right|_{r=R} = h_c (T|_{r=R} - T_c) \quad (A.12)$$

$$-k \left. \frac{\partial T}{\partial r} \right|_{r=R_f^-} = h_g (T|_{r=R_f^-} - T|_{r=R_g^+}).$$

Conservation of energy in the fuel-clad gap provides the interface condition

$$\left(rk \frac{\partial T}{\partial r} \right) \Big|_{r=R_f^-} = \left(rk \frac{\partial T}{\partial r} \right) \Big|_{r=R_g^+},$$

while the coolant boundary condition is derived from the known coolant inlet temperature,

$$T_c|_{z=0} = T_{cl}(l).$$

Initial conditions for both fuel pin and coolant are determined from the solution of a steady state problem with these same boundary conditions.

As a final note, consider again the coolant equation (A.11). Substitution of the boundary condition (A.12) into Eq. (A.11) gives this alternate representation, which is of greater practical value,

$$\frac{\partial}{\partial t} (A \rho C_p T_c) + \frac{\partial}{\partial z} (w C_p T_c) = 2\pi R h_c (T|_{r=R} - T_c),$$

$$0 < z < L, \quad 0 < t < t_f.$$

APPENDIX B

TYPICAL PROBLEM PARAMETERS

Parameters can appear in the problem in several forms. The simplest is to consider each of the physical quantities, ρ , C_p , k , Q , h_g , h_c , A , and w as a constant scale factor multiplying a function that may vary with temperature, such as

$$\begin{aligned} k(T) &= \bar{k} \cdot u(T) \\ h_c(T_c) &= \bar{h}_c \cdot v(T_c) \\ \rho &= \bar{\rho} . \end{aligned}$$

In the above cases, $\bar{k}$, $\bar{h}_c$, and $\bar{\rho}$ are possible α 's. Often problem data are given by explicit functions such as

$$\begin{aligned} k(T) &= a + b \exp(cT) , \\ C_p(T_c) &= d + eT_c + fT_c^2 . \end{aligned}$$

Here the coefficients a , b , c , d , e , and f are possible candidates for α . Many problem parameters occur implicitly. For instance, the heat source Q depends on literally thousands of nuclear cross-section data. Although consideration of this type of parameter is beyond the scope of the present work, it does illustrate the potential applicability of differential sensitivity theory.

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX C

DERIVATION OF THE SYSTEM OF EQUATIONS SATISFIED
BY SENSITIVITY VARIABLES ϕ AND χ

To begin, differentiate Eq. (2.2), remembering that (ρC_p) and k may depend on α explicitly as well as implicitly through the temperature T ,

$$\begin{aligned} \frac{\partial T}{\partial t} \left[\frac{\partial}{\partial T} (\rho C_p) \frac{\partial T}{\partial \alpha} + \frac{\partial}{\partial \alpha} (\rho C_p) \right] + \rho C_p \frac{\partial}{\partial t} \frac{\partial T}{\partial \alpha} \\ - \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial k}{\partial \alpha} \right) \frac{\partial T}{\partial r} + rk \frac{\partial}{\partial r} \frac{\partial T}{\partial \alpha} \right] = \frac{\partial Q}{\partial \alpha}. \end{aligned} \quad (C.1)$$

Using previous differentiability assumptions, Eq. (C.1) exhibits the equality of mixed partial derivatives by interchanging $\frac{\partial}{\partial \alpha} \frac{\partial}{\partial t}$ with $\frac{\partial}{\partial t} \frac{\partial}{\partial \alpha}$ and $\frac{\partial}{\partial \alpha} \frac{\partial}{\partial r}$ with $\frac{\partial}{\partial r} \frac{\partial}{\partial \alpha}$, the latter occurring twice. Evaluating Eq. (C.1) at $\alpha = \alpha_0$ and rearranging yields

$$\begin{aligned} \left[\frac{\partial T}{\partial t} \frac{\partial}{\partial T} (\rho C_p) \right]_{\alpha=\alpha_0} \phi + (\rho C_p) \Big|_{\alpha=\alpha_0} \frac{\partial \phi}{\partial t} \\ - \frac{1}{r} \frac{\partial}{\partial r} \left[r \left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial r} \right) \Big|_{\alpha=\alpha_0} \phi + rk \Big|_{\alpha=\alpha_0} \frac{\partial \phi}{\partial r} \right] \\ = \left[\frac{\partial Q}{\partial \alpha} - \frac{\partial T}{\partial t} \frac{\partial}{\partial \alpha} (\rho C_p) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \right]_{\alpha=\alpha_0}. \end{aligned} \quad (C.2)$$

For simplicity, the notational reference to α_0 is suppressed and the following terms are condensed:

$$\frac{\partial T}{\partial t} \frac{\partial}{\partial T} (\rho C_p) \phi + \rho C_p \frac{\partial \phi}{\partial t} = \phi \frac{\partial}{\partial t} (\rho C_p) + \rho C_p \frac{\partial \phi}{\partial t} = \frac{\partial}{\partial t} (\rho C_p \phi)$$

$$\frac{\partial k}{\partial T} \frac{\partial T}{\partial r} \phi + k \frac{\partial \phi}{\partial r} = \frac{\partial k}{\partial r} \phi + k \frac{\partial \phi}{\partial r} = \frac{\partial}{\partial r} (k\phi).$$

Defining

$$S_\phi = S_\phi(r, z, t) \equiv \left[\frac{\partial Q}{\partial \alpha} - \frac{\partial T}{\partial t} \frac{\partial}{\partial \alpha} (\rho C_P) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \right]_{\alpha=\alpha_0}, \quad (C.3)$$

Eq. (C.2) can be rewritten as

$$\frac{\partial}{\partial t} (\rho C_P \phi) - \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} (k \phi) \right] = S_\phi, \quad \left\{ \begin{array}{l} 0 < r < R_f \\ R_g < r < R \end{array} \right\}, \quad 0 < z < L, \quad 0 < t < t_f. \quad (C.4)$$

Differentiating the initial condition (2.3) gives

$$\phi(r, z, 0) = \frac{\partial T}{\partial \alpha}(r, z, 0; \alpha_0) = \frac{\partial T_0}{\partial \alpha}(r, z; \alpha_0) \equiv \phi_0(r, z). \quad (C.5)$$

By an earlier assumption, the boundary condition (2.4) holds for all α in some neighborhood of α_0 ; hence,

$$\left. \frac{\partial}{\partial \alpha} \left(k \frac{\partial T}{\partial r} \right) \right|_{r=0} = 0 \quad \alpha=\alpha_0$$

or

$$\left[\left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial k}{\partial \alpha} \right) \frac{\partial T}{\partial r} + k \frac{\partial}{\partial r} \frac{\partial T}{\partial \alpha} \right]_{r=0} = 0. \quad \alpha=\alpha_0$$

Simplifying and rearranging yields

$$\frac{\partial}{\partial r} (k \phi) \Big|_{r=0} = 0. \quad (C.6)$$

Next, differentiate the interface condition (2.5) and evaluate at $\alpha = \alpha_0$,

$$R_f \left[\left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial k}{\partial \alpha} \right) \frac{\partial T}{\partial r} + k \frac{\partial}{\partial r} \frac{\partial T}{\partial \alpha} \right]_{r=R_f^-} = R_g \left[\left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial k}{\partial \alpha} \right) \frac{\partial T}{\partial r} + k \frac{\partial}{\partial r} \frac{\partial T}{\partial \alpha} \right]_{r=R_g^+} \quad \alpha=\alpha_0$$

Rearranging and simplifying gives

$$\left[r \frac{\partial}{\partial r} (k\phi) \right]_{r=R_f^-} = \left[r \frac{\partial}{\partial r} (k\phi) \right]_{r=R_g^+} + a, \quad (C.7)$$

where

$$a = a(z, t) \equiv \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_g^+} - \left(r \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_f^-}. \quad (C.8)$$

Differentiation of the second interface condition (2.6) yields

$$\begin{aligned} & \left[\left(\frac{\partial k}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial k}{\partial \alpha} \right) \frac{\partial T}{\partial r} + k \frac{\partial}{\partial r} \frac{\partial T}{\partial \alpha} + \left(\frac{\partial h_g}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial h_g}{\partial \alpha} \right)_T + h_g \frac{\partial T}{\partial \alpha} \right]_{r=R_f^-} \\ & = \left[\left(\frac{\partial h_g}{\partial T} \frac{\partial T}{\partial \alpha} + \frac{\partial h_g}{\partial \alpha} \right)_T + h_g \frac{\partial T}{\partial \alpha} \right]_{r=R_g^+}, \end{aligned}$$

which is evaluated at $\alpha = \alpha_0$ and simplified, producing

$$\left[\frac{\partial(k\phi)}{\partial r} + h_g' \phi \right]_{r=R_f^-} = \left[h_g' \phi \right]_{r=R_g^+} + b, \quad (C.9)$$

where

$$h'_g = h'_g(z, t) \equiv h_g + T \frac{\partial h_g}{\partial T} \quad (C.10)$$

and

$$b = b(z, t) \equiv \left(\frac{\partial h_g}{\partial \alpha} T \right) \Big|_{r=R_g^+} - \left(\frac{\partial h_g}{\partial \alpha} T + \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right) \Big|_{r=R_f^-} \quad (C.11)$$

Analogous treatment of the boundary condition (2.7) results in

$$\left[\frac{\partial (k\phi)}{\partial r} + h_c \phi \right]_{r=R} = h'_c \chi + c, \quad (C.12)$$

where

$$h'_c = h'_c(z, t) = h_c - \frac{\partial h_c}{\partial T_c} (T - T_c) \Big|_{r=R} \quad (C.13)$$

and

$$c = c(z, t) = \left[- \frac{\partial h_c}{\partial \alpha} (T - T_c) - \frac{\partial k}{\partial \alpha} \frac{\partial T}{\partial r} \right]_{r=R} \quad (C.14)$$

Turning now to the second partial differential Eq. (2.8), again differentiate with respect to α ,

$$\begin{aligned} \frac{\partial}{\partial t} \left\{ \left[\frac{\partial}{\partial T_c} (A\rho C_p) \frac{\partial T_c}{\partial \alpha} + \frac{\partial}{\partial \alpha} (A\rho C_p) \right] T_c + (A\rho C_p) \frac{\partial T_c}{\partial \alpha} \right\} \\ + \frac{\partial}{\partial z} \left\{ \left[\frac{\partial}{\partial T_c} (wC_p) \frac{\partial T_c}{\partial \alpha} + \frac{\partial}{\partial \alpha} (wC_p) \right] T_c + (wC_p) \frac{\partial T_c}{\partial \alpha} \right\} + \end{aligned}$$

$$+ 2\pi R \left\{ \left[\frac{\partial h_c}{\partial T_c} \frac{\partial T_c}{\partial \alpha} + \frac{\partial h_c}{\partial \alpha} \right] T_c + h_c \frac{\partial T_c}{\partial \alpha} \right\} = 2\pi R \left\{ \left[\frac{\partial h_c}{\partial T_c} \frac{\partial T_c}{\partial \alpha} + \frac{\partial h_c}{\partial \alpha} \right] T + h \frac{\partial T}{\partial \alpha} \right\} \Big|_{r=R}.$$

Evaluating at $\alpha = \alpha_0$ and rearranging gives

$$\frac{\partial}{\partial t} [(A\rho C_p)'\chi] + \frac{\partial}{\partial z} [(wC_p)'\chi] + 2\pi R h_c' \chi = 2\pi R h_c \phi(R, z, t) + S_\chi, \quad (C.15)$$

$$0 < z < L, \quad 0 < t < t_f,$$

where

$$(A\rho C_p)' = (A\rho C_p)'(z, t) \equiv T_c \frac{\partial}{\partial T_c} (A\rho C_p) + (A\rho C_p) \quad (C.16)$$

$$(wC_p)' = (wC_p)'(z, t) \equiv T_c \frac{\partial}{\partial T_c} (wC_p) + (wC_p) \quad (C.17)$$

$$S_\chi = S_\chi(z, t) \equiv 2\pi R \frac{\partial h_c}{\partial \alpha} (T - T_c) \Big|_{r=R} - \frac{\partial}{\partial t} \left[T_c \frac{\partial}{\partial \alpha} (A\rho C_p) \right] - \frac{\partial}{\partial z} \left[T_c \frac{\partial}{\partial \alpha} (wC_p) \right] \quad (C.18)$$

and h_c' is given by Eq. (C.13).

Differentiation of Eqs. (2.9) and (2.10) yields the following initial and boundary conditions for χ :

$$\chi(z, 0) = \frac{\partial T_c}{\partial \alpha}(z, 0; \alpha_0) = \frac{\partial T_{c0}}{\partial \alpha}(z; \alpha_0) \equiv \chi_0(z) \quad (C.19)$$

$$\chi(0, t) = \frac{\partial T_c}{\partial \alpha}(0, t; \alpha_0) = \frac{\partial T_{c1}}{\partial \alpha}(t; \alpha_0) \equiv \chi_1(t). \quad (C.20)$$

Combining Eqs. (C.4), (C.5), (C.6), (C.7), (C.9), (C.12), (C.15), (C.19), and (C.20), the functions ϕ and χ appearing in Eq. (2.14) must satisfy the following system:

$$\frac{\partial}{\partial t} (\rho C_p \phi) - \frac{1}{r} \frac{\partial}{\partial r} \left[r \frac{\partial}{\partial r} (k \phi) \right] = S_\phi, \quad \begin{cases} 0 < r < R_f \\ R_g < r < R \end{cases}, \quad 0 < z < L, \quad 0 < t < t_f$$

$$\phi(r, z, 0) = \phi_0(r, z), \quad 0 < r < R, \quad 0 < z < L$$

$$\left. \begin{aligned} \frac{\partial}{\partial r} (k \phi) \Big|_{r=0} &= 0 \\ \left[r \frac{\partial}{\partial r} (k \phi) \right]_{r=R_f^-} &= \left[r \frac{\partial}{\partial r} (k \phi) \right]_{r=R_g^+} + a \\ \left[\frac{\partial}{\partial r} (k \phi) + h_g \phi \right]_{r=R_f^-} &= \left[h_g \phi \right]_{r=R_g^+} + b \\ \left[\frac{\partial}{\partial r} (k \phi) + h_c \phi \right]_{r=R} &= h_c \chi + c \end{aligned} \right\} \quad 0 < z < L, \quad 0 < t < t_f \quad (C.21)$$

$$\frac{\partial}{\partial t} [(A \rho C_p) \chi] + \frac{\partial}{\partial z} [(w C_p) \chi] + 2\pi R h_c \chi = 2\pi R h_c \phi(R, z, t) + S_\chi, \quad 0 < z < L, \quad 0 < t < t_f$$

$$\chi(z, 0) = \chi_0(z), \quad 0 < z < L$$

$$\chi(0, t) = \chi_1(t), \quad 0 < t < t_f$$

APPENDIX D

DERIVATION OF THE ADJOINT RESPONSE REPRESENTATION

Multiplying Eqs. (2.16) and (2.17) by 2π , then adding both to Eq. (2.18) and rearranging gives

$$\begin{aligned}
& 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi L^* \phi^* r \, dr \, dz \, dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi L^* \phi^* r \, dr \, dz \, dt \\
& + \int_0^{t_f} \int_0^L \chi M^* \chi^* \, dz \, dt \\
& = 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* L \phi \, r \, dr \, dz \, dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* L \phi \, r \, dr \, dz \, dt \\
& + \int_0^{t_f} \int_0^L \chi^* M \chi \, dz \, dt - 2\pi \int_0^L \int_0^{R_f} (\rho C_p \phi \phi^*) \Big|_0^{t_f} r \, dr \, dz \\
& - 2\pi \int_0^L \int_{R_g}^R (\rho C_p \phi \phi^*) \Big|_0^{t_f} r \, dr \, dz - \int_0^L [\chi^* \chi (A \rho C_p)^{-1}]_0^{t_f} \, dz \\
& - 2\pi \int_0^{t_f} \int_0^L \left\{ \left[rk\phi \frac{\partial \phi^*}{\partial r} - r\phi^* \frac{\partial}{\partial r} (k\phi) \right] \right\}_0^{R_f^-} \\
& + \left\{ \left[rk\phi \frac{\partial \phi^*}{\partial r} - r\phi^* \frac{\partial}{\partial r} (k\phi) \right] \right\}_{R_g^+}^R \, dz \, dt - \int_0^{t_f} [\chi^* \chi (w C_p)^{-1}]_0^L \, dt ,
\end{aligned}$$

which can be simplified using the differential equations and auxiliary conditions of systems (2.15) and (2.19),

$$\begin{aligned}
& 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} f \phi r \, dr \, dz \, dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R f \phi r \, dr \, dz \, dt + \int_0^{t_f} \int_0^L g X \, dz \, dt \\
& = 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* S_\phi r \, dr \, dz \, dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* S_\phi r \, dr \, dz \, dt \\
& + \int_0^{t_f} \int_0^L X^* S_X \, dz \, dt + 2\pi \int_0^L \int_0^{R_f} (\rho C_p \phi \phi^*) \Big|_{t=0} r \, dr \, dz \\
& + 2\pi \int_0^L \int_{R_g}^R (\rho C_p \phi \phi^*) \Big|_{t=0} r \, dr \, dz + \int_0^L [X^* X (A \rho C_p)^{-}]_{t=0} \, dz \\
& + \int_0^{t_f} [X^* X (w C_p)^{-}]_{z=0} \, dt - \int_0^{t_f} \int_0^L 2\pi h_c X^* (r \phi^*) \Big|_{r=R} \, dz \, dt \\
& + \int_0^{t_f} \int_0^L 2\pi h_c X^* (r \phi) \Big|_{r=R} \, dz \, dt - 2\pi \int_0^{t_f} \int_0^z \left\{ \left[r k \phi \frac{\partial \phi^*}{\partial r} - r \phi^* \frac{\partial}{\partial r} (k \phi) \right] \right\}_{R_g^+}^{R_f^-} \\
& + \left[r k \phi \frac{\partial \phi^*}{\partial r} - r \phi^* \frac{\partial}{\partial r} (k \phi) \right]_{r=R} \Bigg\} dz \, dt . \tag{D.1}
\end{aligned}$$

Consider now the further simplification of the last three integrals in Eq. (D.1). Use of the interface conditions of systems (2.15) and (2.19) yields

$$\begin{aligned}
& \left[rk\phi \frac{\partial \phi^*}{\partial r} - r\phi^* \frac{\partial}{\partial r} (k\phi) \right]_{R_g^+}^{R_f^-} \\
&= \left[rk\phi \frac{\partial \phi^*}{\partial r} \right]_{R_f^-} - \phi \Big|_{R_g^+} \left[rk \frac{\partial \phi^*}{\partial r} \right]_{R_f^-} - \left[r\phi^* \frac{\partial}{\partial r} (k\phi) \right]_{R_f^-} \\
&\quad + \phi^* \Big|_{R_g^+} \left[r \frac{\partial}{\partial r} (k\phi) \right]_{R_f^-} - a \\
&= \left[rk \frac{\partial \phi^*}{\partial r} \right]_{R_f^-} \left[\phi \Big|_{R_f^-} - \phi \Big|_{R_g^+} \right] + \left[r \frac{\partial}{\partial r} (k\phi) \right]_{R_f^-} \left[\phi^* \Big|_{R_g^+} \right. \\
&\quad \left. - \phi^* \Big|_{R_f^-} \right] - a\phi^* \Big|_{R_g^+} \\
&= R_f h_g' \left[\phi^* \Big|_{R_g^+} - \phi^* \Big|_{R_f^-} \right] \left[\phi \Big|_{R_f^-} - \phi \Big|_{R_g^+} \right] \\
&\quad + R_f \left\{ h_g' \left[\phi \Big|_{R_g^+} - \phi \Big|_{R_f^-} \right] + b \right\} \left[\phi^* \Big|_{R_g^+} - \phi^* \Big|_{R_f^-} \right] - a\phi^* \Big|_{R_g^+} \\
&= (R_f b - a)\phi^* \Big|_{R_g^+} - R_f b\phi^* \Big|_{R_f^-},
\end{aligned}$$

and the coolant-clad boundary conditions give

$$\begin{aligned}
& -2\pi h_c' X(r\phi^*) \Big|_{r=R} + 2\pi h_c X^*(r\phi) \Big|_{r=R} - 2\pi \left[rk\phi \frac{\partial \phi^*}{\partial r} - r\phi^* \frac{\partial}{\partial r} (k\phi) \right]_{r=R} \\
&= 2\pi R \left\{ \phi^* \left[\frac{\partial}{\partial r} (k\phi) - h_c' X \right] - \phi \left[k \frac{\partial \phi^*}{\partial r} - h_c X^* \right] \right\} \Big|_{r=R} \\
&= 2\pi R [\phi^*(c - h_c \phi) - \phi(-h_c \phi^*)]_{r=R} = 2\pi c(r\phi^*) \Big|_{r=R}.
\end{aligned}$$

Substituting these results into Eq. (D.1) produces

$$\begin{aligned}
& 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} f \phi r dr dz dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R f \phi r dr dz dt + \int_0^{t_f} \int_0^L g \chi dz dt \\
& = 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* S_\phi r dr dz dt + 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* S_\phi r dr dz dt \\
& + \int_0^{t_f} \int_0^L \chi^* S_\chi dz dt + 2\pi \int_0^L \int_0^{R_f} (\rho C_p \phi \phi^*) \Big|_{t=0} r dr dz \\
& + 2\pi \int_0^L \int_{R_g}^R (\rho C_p \phi \phi^*) \Big|_{t=0} r dr dz + \int_0^L [\chi^* \chi (A \rho C_p)']_{t=0} dz \\
& + 2\pi \int_0^{t_f} \int_0^L \left[(a - R_f b) \phi^* \Big|_{R_g^+} + R_f b \phi^* \Big|_{R_f^-} + c(r \phi^*) \Big|_R \right] dz dt \\
& + \int_0^{t_f} [\chi^* \chi (w C_p)']_{z=0} dt .
\end{aligned} \tag{D.2}$$

APPENDIX E

DERIVATION OF THE FORWARD CONDUCTION
DIFFERENCE EQUATIONS

It is necessary to approximate the integrated conduction equation

$$\int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_0^{2\pi} \int_{v_i} \left[(\rho C_p) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) - Q \right] r dr d\theta dz dt = 0, \quad (E.1)$$

$$i = 1, 2, \dots, I; j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1.$$

This procedure makes extensive use of the following identities:

$$y'(x) = \frac{1}{\Delta x} [y(x + \Delta x) - y(x)] + O(\Delta x) = \frac{1}{\Delta x} [y(x) - y(x - \Delta x)] + O(\Delta x) \quad (E.2)$$

$$y'(x) = \frac{1}{2\Delta x} [y(x + \Delta x) - y(x - \Delta x)] + O[(\Delta x)^2] \quad (E.3)$$

$$y(x) = \frac{1}{2} [y(x + \Delta x) + y(x - \Delta x)] + O[(\Delta x)^2] \quad (E.4)$$

$$y(x) = y(x + \Delta x) + O(\Delta x) \quad (E.5)$$

$$\frac{1}{\Delta x} \int_x^{x+\Delta x} y(\xi) d\xi = y(x) + O(\Delta x) \quad (E.6)$$

$$\frac{1}{\Delta x} \int_{x-\Delta x}^{x+\Delta x} y(\xi) d\xi = y(x) + O[(\Delta x)^2] \quad (E.7)$$

$$\int_x^{x+\Delta x} y(\xi) \xi d\xi = \frac{1}{2} y(\bar{x}) [(x + \Delta x)^2 - x^2] + O[(\Delta x)^2], \quad \bar{x} \in [x, x + \Delta x], \quad (E.8)$$

which result from application of Taylor's Theorem to any function y which is twice differentiable in the interval $[x - \Delta x, x + \Delta x]$.

Because the problem is independent of θ , integration of this variable in Eq. (E.1) produces 2π , which is immediately divided out. Dividing by $\Delta z = z_{j+1} - z_j$ and applying Eq. (E.7) to integrals in both z and t produces

$$\Delta t \int_{V_i} \left[(\rho C_p) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) - Q \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr = O[(\Delta t)^3 + \Delta t (\Delta z)^2] , \quad (E.9)$$

$$i = 1, 2, \dots, I; \quad j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1.$$

The remaining integral is evaluated term by term. Assumption (2.1 e) implies that each term of Eq. (E.9) is continuous in r , since the integral is over a homogeneous region.

For interior radial points in each region (fuel and clad), Eq. (E.9) becomes

$$\Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[(\rho C_p) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) - Q \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr = O[(\Delta t)^3 + \Delta t (\Delta z)^2] . \quad (E.10)$$

Applying Eq. (E.8) to the first term of Eq. (E.10) gives

$$\begin{aligned} \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[(\rho C_p) \frac{\partial T}{\partial t} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr &= \frac{\Delta t}{2} V_i \left[(\rho C_p) \frac{\partial T}{\partial t} \right] (r_i, z_{j+\frac{1}{2}}, t_{k+\frac{1}{2}}) \\ &+ O[(\hat{r}_i - \hat{r}_{i-1})^2] . \end{aligned}$$

Use of identities (E.3) and (E.5) in the time variable yields

$$\left(\frac{\partial T}{\partial t}\right)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} = \frac{1}{\Delta t} \left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^k\right) + O[(\Delta t)^2] ,$$

$$\begin{aligned} (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} &= (\rho C_p) \left(T_{i,j+\frac{1}{2}}^{k+\frac{1}{2}}\right) = (\rho C_p) \left[\frac{T_{i,j+\frac{1}{2}}^{k+1} + T_{i,j+\frac{1}{2}}^k}{2} + O[(\Delta t)^2]\right] \\ &= (\rho C_p) \left[\frac{T_{i,j+\frac{1}{2}}^{k+1} + T_{i,j+\frac{1}{2}}^k}{2}\right] + O[(\Delta t)^2] . \end{aligned}$$

Thus, the first term of Eq. (E.10) can be approximated

$$\begin{aligned} \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[(\rho C_p) \frac{\partial T}{\partial t}\right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\ = \frac{V_i}{2} (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^k\right) + O[(\Delta t)^3 + \Delta t(\hat{r}_i - \hat{r}_{i-1})^2] . \end{aligned} \quad (E.11)$$

Consider now the second term in Eq. (E.10),

$$\begin{aligned} \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[-\frac{1}{r} \frac{\partial}{\partial r} \left(rk \frac{\partial T}{\partial r}\right)\right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\ = \Delta t \hat{r}_{i-1} \left(rk \frac{\partial T}{\partial r}\right)_{i-1,j+\frac{1}{2}}^{k+\frac{1}{2}} - \Delta t \hat{r}_i \left(rk \frac{\partial T}{\partial r}\right)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} . \end{aligned}$$

Use of the identity (E.4) produces the Crank-Nicolson approximation

$$\left(k \frac{\partial T}{\partial r}\right)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} = \frac{1}{2} \left[\left(k \frac{\partial T}{\partial r}\right)_{i,j+\frac{1}{2}}^{k+1} + \left(k \frac{\partial T}{\partial r}\right)_{i,j+\frac{1}{2}}^k\right] + O[(\Delta t)^2] ,$$

while identities (E.2) and (E.5) are applied to $\frac{\partial T}{\partial r}$ and k , respectively, to give

$$\begin{aligned} \left[\frac{\partial T}{\partial r} \right]_{\hat{r}_i, j+\frac{1}{2}}^k &= \frac{1}{\Delta r_i} \left(T_{i+1, j+\frac{1}{2}}^k - T_{i, j+\frac{1}{2}}^k \right) + O(\Delta r_i) , \\ k_{\hat{r}_i, j+\frac{1}{2}}^k &= k[T(\hat{r}_i, z_{j+\frac{1}{2}}, t_k)] = k \left[\frac{T_{i+1, j+\frac{1}{2}}^k + T_{i, j+\frac{1}{2}}^k}{2} + O(\Delta r_i) \right] \\ &= k \left[\frac{T_{i+1, j+\frac{1}{2}}^k + T_{i, j+\frac{1}{2}}^k}{2} \right] + O(\Delta r_i) . \end{aligned}$$

Thus, the second term of Eq. (E.10) can be approximated as

$$\begin{aligned} \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[-\frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr \\ = \frac{1}{2} P_{i-1} \left[k_{\hat{r}_{i-1}, j+\frac{1}{2}}^{k+1} \left(T_{i, j+\frac{1}{2}}^{k+1} - T_{i-1, j+\frac{1}{2}}^{k+1} \right) + k_{\hat{r}_{i-1}, j+\frac{1}{2}}^k \left(T_{i, j+\frac{1}{2}}^k - T_{i-1, j+\frac{1}{2}}^k \right) \right] \\ = \frac{1}{2} P_i \left[k_{\hat{r}_i, j+\frac{1}{2}}^{k+1} \left(T_{i+1, j+\frac{1}{2}}^{k+1} - T_{i, j+\frac{1}{2}}^{k+1} \right) + k_{\hat{r}_i, j+\frac{1}{2}}^k \left(T_{i+1, j+\frac{1}{2}}^k - T_{i, j+\frac{1}{2}}^k \right) \right] \\ + O[(\Delta t)^3 + \Delta t(\Delta r_{i-1} + \Delta r_i)] , \end{aligned} \quad (E.12)$$

where

$$P_i \equiv \Delta t \hat{r}_i / \Delta r_i , \quad i = 1, 2, \dots, I_f-1, I_f+1, \dots, I-1.$$

Using identity (E.8) gives the following approximation for the last term in Eq. (E.10)

$$\begin{aligned} \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} Q_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr &= \Delta t \frac{V_i}{2} Q(r_i, z_{j+\frac{1}{2}}, t_{k+\frac{1}{2}}) + O[\Delta t(\hat{r}_i - \hat{r}_{i-1})^2] \\ &\equiv \frac{1}{2} \tilde{Q}_{i, j+\frac{1}{2}}^{k+\frac{1}{2}} + O[\Delta t(\hat{r}_i - \hat{r}_{i-1})^2] . \end{aligned} \quad (E.13)$$

Combining the results (E.11)-(E.13) yields the difference equation

$$\begin{aligned}
 & V_i (\rho C_P)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^k \right) \\
 & + P_{i-1} \left[k_{i-1,j+\frac{1}{2}}^{k+1} \left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i-1,j+\frac{1}{2}}^{k+1} \right) + k_{i-1,j+\frac{1}{2}}^k \left(T_{i,j+\frac{1}{2}}^k - T_{i-1,j+\frac{1}{2}}^k \right) \right] \\
 & - P_i \left[k_{i,j+\frac{1}{2}}^{k+1} \left(T_{i+1,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^{k+1} \right) + k_{i,j+\frac{1}{2}}^k \left(T_{i+1,j+\frac{1}{2}}^k - T_{i,j+\frac{1}{2}}^k \right) \right] \\
 & = \hat{Q}_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t(\Delta r_{i-1} + \Delta r_i) + \Delta t(\hat{r}_i - \hat{r}_{i-1})^2 + \Delta t(\Delta z)^2] .
 \end{aligned} \tag{E.14}$$

For the nodal volume immediately surrounding $r = 0$, Eq. (E.9) becomes

$$\Delta t \int_{r_1}^{\hat{r}_1} \left[(\rho C_P) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(rk \frac{\partial T}{\partial r} \right) - Q \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr = O[(\Delta t)^3 + \Delta t(\Delta z)^2] , \tag{E.15}$$

$j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1,$

which will also be evaluated term by term.

Applying the same reasoning used to obtain Eq. (E.11), the first term in Eq. (E.15) is approximated

$$\begin{aligned}
 & \Delta t \int_{r_1}^{\hat{r}_1} \left[(\rho C_P) \frac{\partial T}{\partial t} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\
 & = \frac{1}{2} V_i (\rho C_P)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{1,j+\frac{1}{2}}^{k+1} - T_{1,j+\frac{1}{2}}^k \right) + O[(\Delta t)^3 + \Delta t \hat{r}_1^2] .
 \end{aligned} \tag{E.16}$$

To approximate the second term in Eq. (E.15), exact differentiation and Eqs. (E.2), (E.4), and (E.5) are used as in the case for interior nodes. By invoking the boundary condition (2.4), the following approximation is obtained:

$$\begin{aligned}
\Delta t \int_{r_1}^{\hat{r}_1} \left[-\frac{1}{2} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr &= -\Delta t \left[\left(r k \frac{\partial T}{\partial r} \right) \Big|_{r_1}^{\hat{r}_1} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\
&= -\frac{1}{2} P_1 \left[k_{1,j+\frac{1}{2}}^{k+1} (T_{2,j+\frac{1}{2}}^{k+1} - T_{1,j+\frac{1}{2}}^{k+1}) + k_{1,j+\frac{1}{2}}^k (T_{2,j+\frac{1}{2}}^k - T_{1,j+\frac{1}{2}}^k) \right] \\
&\quad + O[(\Delta t)^3 + \Delta t \Delta r_1].
\end{aligned} \tag{E.17}$$

As in Eq. (E.13), the heat source term is approximated

$$\begin{aligned}
\Delta t \int_{r_1}^{\hat{r}_1} Q_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr &= \frac{1}{2} V_1 \Delta t Q_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t \hat{r}_1^2] \\
&= \frac{1}{2} \tilde{Q}_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t \hat{r}_1^2].
\end{aligned} \tag{E.18}$$

Combining Eqs. (E.16)-(E.18) results in this difference approximation to Eq. (E.15)

$$\begin{aligned}
&V_1 (\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} (T_{1,j+\frac{1}{2}}^{k+1} - T_{1,j+\frac{1}{2}}^k) \\
&- P_1 \left[k_{1,j+\frac{1}{2}}^{k+1} (T_{2,j+\frac{1}{2}}^{k+1} - T_{1,j+\frac{1}{2}}^{k+1}) + k_{1,j+\frac{1}{2}}^k (T_{2,j+\frac{1}{2}}^k - T_{1,j+\frac{1}{2}}^k) \right] \\
&= \tilde{Q}_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t (\Delta r_1 + \hat{r}_1^2) + \Delta t (\Delta z)^2], \\
&j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1.
\end{aligned} \tag{E.19}$$

Turning now to the outermost radial interval of the fuel region, Eq. (E.9) becomes

$$\Delta t \int_{\hat{r}_{f-1}}^{\hat{r}_f} \left[(\rho C_p) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) - Q \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr = O[(\Delta t)^3 + \Delta t (\Delta z)^2], \tag{E.20}$$

$$j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1.$$

Approximation of the first and third terms in the integrand of Eq. (E.20) is analogous to the derivations of Eqs. (E.16) and (E.18), respectively,

$$\begin{aligned} \Delta t \int_{\hat{r}_{I_f-1}}^{\hat{r}_{I_f}} \left[(\rho C_p) \frac{\partial T}{\partial t} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\ = \frac{1}{2} V_{I_f} (\rho C_p)_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{I_f, j+\frac{1}{2}}^{k+1} - T_{I_f, j+\frac{1}{2}}^k \right) + O \left[(\Delta t)^3 + \Delta t \left(r_{I_f} - \hat{r}_{I_f-1} \right)^2 \right], \end{aligned} \quad (E.21)$$

$$\begin{aligned} \Delta t \int_{\hat{r}_{I_f-1}}^{\hat{r}_{I_f}} Q_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr = \frac{1}{2} V_{I_f} \Delta t Q_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} + O \left[(\Delta t)^3 + \Delta t \left(r_{I_f} - \hat{r}_{I_f-1} \right)^2 \right] \\ = \frac{1}{2} \tilde{Q}_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} + O \left[(\Delta t) + \Delta t \left(r_{I_f} - \hat{r}_{I_f-1} \right)^2 \right]. \end{aligned} \quad (E.22)$$

Using the interface condition (2.6), the second term of Eq. (E.20) is approximated as follows:

$$\begin{aligned} \Delta t \int_{\hat{r}_{I_f-1}}^{\hat{r}_{I_f}} \left[-\frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr = -\Delta t \left[\left(r k \frac{\partial T}{\partial r} \right) \Big|_{\hat{r}_{I_f-1}}^{\hat{r}_{I_f}} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} \\ = \frac{1}{2} P_{I_f-1} \left[k_{I_f-1, j+\frac{1}{2}}^{k+1} \left(T_{I_f, j+\frac{1}{2}}^{k+1} - T_{I_f-1, j+\frac{1}{2}}^{k+1} \right) + k_{I_f-1, j+\frac{1}{2}}^k \left(T_{I_f, j+\frac{1}{2}}^k - T_{I_f-1, j+\frac{1}{2}}^k \right) \right] \\ - \frac{1}{2} r_{I_f} \Delta t \left[h_{g, j+\frac{1}{2}}^{k+1} \left(T_{I_f+1, j+\frac{1}{2}}^{k+1} - T_{I_f, j+\frac{1}{2}}^{k+1} \right) + h_{g, j+\frac{1}{2}}^k \left(T_{I_f+1, j+\frac{1}{2}}^k - T_{I_f, j+\frac{1}{2}}^k \right) \right] \\ + O \left[(\Delta t)^3 + \Delta t \Delta r_{I_f-1} \right]. \end{aligned} \quad (E.23)$$

Combining Eqs. (E.21)-(E.23) gives the difference approximation for Eq. (E.20),

$$\begin{aligned}
& V_{I_f} (\rho C_P)_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{I_f, j+\frac{1}{2}}^{k+1} - T_{I_f, j+\frac{1}{2}}^k \right) \\
& + P_{I_f-1} \left[k_{I_f-1, j+\frac{1}{2}}^{k+1} \left(T_{I_f, j+\frac{1}{2}}^{k+1} - T_{I_f-1, j+\frac{1}{2}}^{k+1} \right) + k_{I_f-1, j+\frac{1}{2}}^k \left(T_{I_f, j+\frac{1}{2}}^k - T_{I_f-1, j+\frac{1}{2}}^k \right) \right] \\
& - r_{I_f} \Delta t \left[h_{g, j+\frac{1}{2}}^{k+1} \left(T_{I_f+1, j+\frac{1}{2}}^{k+1} - T_{I_f, j+\frac{1}{2}}^{k+1} \right) + h_{g, j+\frac{1}{2}}^k \left(T_{I_f+1, j+\frac{1}{2}}^k - T_{I_f, j+\frac{1}{2}}^k \right) \right] \\
& = Q_{I_f, j+\frac{1}{2}}^{k+\frac{1}{2}} + 0 \left[(\Delta t)^3 + \Delta t \Delta r_{I_f-1} + \Delta t \left(r_{I_f} - \hat{r}_{I_f-1} \right)^2 + \Delta t (\Delta z)^2 \right]. \quad (E.24)
\end{aligned}$$

For the first radial region in the cladding, Eq. (E.9) can be rewritten as

$$\Delta t \int_{r_{I_f+1}}^{\hat{r}_{I_f+1}} \left[(\rho C_P) \frac{\partial T}{\partial t} - \frac{1}{r} \frac{\partial}{\partial r} \left(r k \frac{\partial T}{\partial r} \right) - Q \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr = U [(\Delta t)^3 + \Delta t (\Delta z)^2], \quad (E.25)$$

$$j = 1, 2, \dots, J-1; \quad k = 0, 1, \dots, K-1.$$

Again, the approximation of the first and third terms of the integrand is straightforward; to approximate the second term, it is necessary to use both interface conditions, Eqs. (2.5) and (2.6). The difference approximation for Eq. (E.25) then takes the form

$$\begin{aligned}
& V_{I_f+1} (\rho C_P)_{I_f+1, j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{I_f+1, j+\frac{1}{2}}^{k+1} - T_{I_f+1, j+\frac{1}{2}}^k \right) \\
& + r_{I_f} \Delta t \left[h_{g, j+\frac{1}{2}}^{k+1} \left(T_{I_f+1, j+\frac{1}{2}}^{k+1} - T_{I_f, j+\frac{1}{2}}^{k+1} \right) + h_{g, j+\frac{1}{2}}^k \left(T_{I_f+1, j+\frac{1}{2}}^k - T_{I_f, j+\frac{1}{2}}^k \right) \right] \\
& - P_{I_f+1} \left[k_{I_f+1, j+\frac{1}{2}}^{k+1} \left(T_{I_f+2, j+\frac{1}{2}}^{k+1} - T_{I_f+1, j+\frac{1}{2}}^{k+1} \right) + k_{I_f+1, j+\frac{1}{2}}^k \left(T_{I_f+2, j+\frac{1}{2}}^k - T_{I_f+1, j+\frac{1}{2}}^k \right) \right] \\
& = Q_{I_f+1, j+\frac{1}{2}}^{k+\frac{1}{2}} + 0 \left[(\Delta t)^3 + \Delta t \Delta r_{I_f+1} + \Delta t \left(\hat{r}_{I_f+1} - r_{I_f+1} \right)^2 + \Delta t (\Delta z)^2 \right], \quad (E.26)
\end{aligned}$$

Because the coolant-clad boundary condition (2.7) is identical in form to the interface condition (2.6), the approximations made in Eqs. (E.21)-(E.23) can be applied to the outer-clad radial region to get the following analogue of Eq. (E.24):

$$\begin{aligned}
 & V_I (\rho C_P)_{I,j+\frac{1}{2}}^{k+\frac{1}{2}} (T_{I,j+\frac{1}{2}}^{k+1} - T_{I,j+\frac{1}{2}}^k) \\
 & + P_{I-1} \left[k_{I-1,j+\frac{1}{2}}^{k+1} (T_{I,j+\frac{1}{2}}^{k+1} - T_{I-1,j+\frac{1}{2}}^{k+1}) + k_{I-1,j+\frac{1}{2}}^k (T_{I,j+\frac{1}{2}}^k - T_{I-1,j+\frac{1}{2}}^k) \right] \\
 & + r_I \Delta t \left[h_{c,j+\frac{1}{2}}^{k+1} (T_{I,j+\frac{1}{2}}^{k+1} - T_{c,j+\frac{1}{2}}^{k+1}) + h_{c,j+\frac{1}{2}}^k (T_{I,j+\frac{1}{2}}^k - T_{c,j+\frac{1}{2}}^k) \right] \\
 & = \tilde{Q}_{I,j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t \Delta r_{I-1} + \Delta t (r_I - \hat{r}_{I-1})^2 + \Delta t (\Delta z)^2]. \quad (E.27)
 \end{aligned}$$

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

APPENDIX F

DIFFERENCE APPROXIMATION TO THE ADJOINT
FUEL CONDUCTION EQUATION

It is necessary to approximate the integrated adjoint conduction equation

$$\int_{\tau_k}^{\tau_{k+1}} \int_{\xi_j}^{\xi_{j+1}} \int_0^{2\pi} \int_{v_i} \left[(\rho C_p)^* \frac{\partial T^*}{\partial \tau} - \frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) - f^* \right] r \, dr \, d\theta \, d\xi \, d\tau = 0,$$

$$i = 1, 2, \dots, I; j = 1, 2, \dots, J-1; k = 0, 1, \dots, K-1.$$

As in the forward case, the integration in θ is merely a formality. It results in a factor of 2π , which is immediately divided out. Also analogous to the forward problem, the identity (E.7) is applied to the integrations in ξ and τ , but only for the first two terms. This produces

$$\begin{aligned} \Delta t \, \Delta z \int_{v_i} \left[(\rho C_p)^* \frac{\partial T^*}{\partial \tau} - \frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\ = \int_{\tau_k}^{\tau_{k+1}} \int_{\xi_j}^{\xi_{j+1}} \int_{v_i} f^* r \, dr \, d\xi \, d\tau + O[(\Delta t)^3 \Delta z + \Delta t (\Delta z)^3] . \quad (F.1) \end{aligned}$$

Because of the special nature of the weight function f^* , the axial and time integrations of this term will not be performed here. Dividing Eq. (F.1) by Δz gives

$$\begin{aligned} \Delta t \int_{v_i} \left[(\rho C_p)^* \frac{\partial T^*}{\partial \tau} - \frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\ = \frac{1}{\Delta z} F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} + O[(\Delta t)^3 + \Delta t (\Delta z)^2] , \quad (F.2) \end{aligned}$$

where the term $F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}}$ (to be evaluated later) is defined as

$$F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} \equiv \int_{\tau_k}^{\tau_{k+1}} \int_{\xi_j}^{\xi_{j+1}} \int_{v_i} f^* r dr d\xi d\tau . \quad (F.3)$$

The first term of Eq. (F.2) is approximated exactly as in the forward case, yielding for each radial region

$$\begin{aligned} \Delta t \int_{v_i} \left[(\rho C_p)^* \frac{\partial T^*}{\partial \tau} \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr \\ = V_i (\rho C_p)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} \left(T_{i,j+\frac{1}{2}}^{*k+1} - T_{i,j+\frac{1}{2}}^{*k} \right) + O[(\hat{r}_i - \hat{r}_{i-1})^2] . \end{aligned} \quad (F.4)$$

The radial integration of the second term cannot be performed exactly as was done in the forward problem; hence, the Integral Mean Value Theorem is used, producing

$$\begin{aligned} \Delta t \int_{v_i} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr \\ = -\Delta t \left[k^* \Big|_{r_i^*} \int_{v_i} \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) dr \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} , \quad r_i^* \in v_i . \end{aligned} \quad (F.5)$$

To approximate, set $r_i^* \sim r_i$ and use a Crank-Nicolson procedure in the time variable.

For interior radial intervals in each region ($i = 2, 3, \dots, I_f - 1, I_f + 2, \dots, I - 1$), Eq. (F.5) becomes

$$\begin{aligned}
& \Delta t \int_{\hat{r}_{i-1}}^{\hat{r}_i} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r \, dr \\
&= \Delta t \, k_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\left(r \frac{\partial T^*}{\partial r} \right) \right]_{\hat{r}_i}^{\hat{r}_{i-1}} \Big|_{j+\frac{1}{2}}^{k+\frac{1}{2}} + O[(\Delta r_{i-1} + \Delta r_i) \Delta t] \\
&= \frac{1}{2} P_{i-1} \left[k_{i,j+\frac{1}{2}}^{*k+1} (T_{i,j+\frac{1}{2}}^{*k+1} - T_{i-1,j+\frac{1}{2}}^{*k+1}) + k_{i,j+\frac{1}{2}}^{*k} (T_{i,j+\frac{1}{2}}^{*k} - T_{i-1,j+\frac{1}{2}}^{*k}) \right] \\
&\quad - \frac{1}{2} P_i \left[k_{i,j+\frac{1}{2}}^{*k+1} (T_{i+1,j+\frac{1}{2}}^{*k+1} - T_{i,j+\frac{1}{2}}^{*k+1}) + k_{i,j+\frac{1}{2}}^{*k} (T_{i+1,j+\frac{1}{2}}^{*k} - T_{i,j+\frac{1}{2}}^{*k}) \right] \\
&\quad + O[(\Delta r_{i-1} + \Delta r_i) \Delta t + (\Delta t)^3] . \tag{F.6}
\end{aligned}$$

Combining Eqs. (F.4) and (F.6) gives a difference approximation to Eq. (F.2),

$$\begin{aligned}
& \frac{1}{2} V_i (\rho C_p)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} (T_{i,j+\frac{1}{2}}^{*k+1} - T_{i,j+\frac{1}{2}}^{*k}) \\
&+ \frac{1}{2} P_{i-1} \left[k_{i,j+\frac{1}{2}}^{*k+1} (T_{i,j+\frac{1}{2}}^{*k+1} - T_{i-1,j+\frac{1}{2}}^{*k+1}) + k_{i,j+\frac{1}{2}}^{*k} (T_{i,j+\frac{1}{2}}^{*k} - T_{i-1,j+\frac{1}{2}}^{*k}) \right] \\
&- \frac{1}{2} P_i \left[k_{i,j+\frac{1}{2}}^{*k+1} (T_{i+1,j+\frac{1}{2}}^{*k+1} - T_{i,j+\frac{1}{2}}^{*k+1}) + k_{i,j+\frac{1}{2}}^{*k} (T_{i+1,j+\frac{1}{2}}^{*k} - T_{i,j+\frac{1}{2}}^{*k}) \right] \\
&= \frac{1}{\Delta z} F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} + O[(\Delta t)^3 + (\hat{r}_i - \hat{r}_{i-1})^2 + (\Delta r_{i-1} + \Delta r_i) \Delta t + (\Delta z)^2 \Delta t],
\end{aligned}$$

which can be arranged in the form (neglecting higher order terms)

$$A_{i,j}^{*k+1} T_{i-1,j+\frac{1}{2}}^{*k+1} + B_{i,j}^{*k+1} T_{i,j+\frac{1}{2}}^{*k+1} + C_{i,j}^{*k+1} T_{i+1,j+\frac{1}{2}}^{*k+1} = D_{i,j}^{*k} , \tag{F.7}$$

where

$$A_{i,j}^{*k+1} \equiv -P_{i-1} k_{i,j+\frac{1}{2}}^{*k+1}$$

$$B_{i,j}^{*k+1} \equiv V_i (\rho C_P)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} + P_{i-1} k_{i,j+\frac{1}{2}}^{*k+1} + P_i k_{i,j+\frac{1}{2}}^{*k+1}$$

$$C_{i,j}^{*k+1} \equiv -P_i k_{i,j+\frac{1}{2}}^{*k+1}$$

$$D_{i,j}^{*k} \equiv V_i (\rho C_P)_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{i,j+\frac{1}{2}}^{*k} - P_{i-1} k_{i,j+\frac{1}{2}}^{*k} (T_{i,j+\frac{1}{2}}^{*k} - T_{i-1,j+\frac{1}{2}}^{*k}) \\ + P_i k_{i,j+\frac{1}{2}}^{*k} (T_{i+1,j+\frac{1}{2}}^{*k} - T_{i,j+\frac{1}{2}}^{*k}) + \frac{2}{\Delta z} F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} .$$

Evaluating Eq. (F.5) for the innermost radial interval ($i = 1$) and applying the boundary condition at $r = 0$ yields

$$\Delta t \int_{r_1}^{\hat{r}_1} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr = -\Delta t k_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}} \left[\left(r \frac{\partial T^*}{\partial r} \right) \right]_{r_1}^{\hat{r}_1} \Big|_{j+\frac{1}{2}}^{k+\frac{1}{2}} + O(\Delta t \Delta r_1) \\ = -\frac{1}{2} P_1 \left[k_{1,j+\frac{1}{2}}^{*k+1} (T_{2,j+\frac{1}{2}}^{*k+1} - T_{1,j+\frac{1}{2}}^{*k+1}) + k_{1,j+\frac{1}{2}}^{*k} (T_{2,j+\frac{1}{2}}^{*k} - T_{1,j+\frac{1}{2}}^{*k}) \right] \\ + O[\Delta t \Delta r_1 + (\Delta t)^3] ,$$

which is also combined with Eq. (F.4), giving the difference equation

$$\frac{1}{2} V_1 (\rho C_P)_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}} (T_{1,j+\frac{1}{2}}^{*k+1} - T_{1,j+\frac{1}{2}}^{*k}) \\ - \frac{1}{2} P_1 \left[k_{1,j+\frac{1}{2}}^{*k+1} (T_{2,j+\frac{1}{2}}^{*k+1} - T_{1,j+\frac{1}{2}}^{*k+1}) + k_{1,j+\frac{1}{2}}^{*k} (T_{2,j+\frac{1}{2}}^{*k} - T_{1,j+\frac{1}{2}}^{*k}) \right] \\ = \frac{1}{\Delta z} F_{i,j+\frac{1}{2}}^{*k+\frac{1}{2}} + O[(\Delta t)^3 + \hat{r}_1^2 \Delta t + \Delta t \Delta r_1 + \Delta t (\Delta z)^2] .$$

Rearranging gives this final form of the difference equation at the innermost radial interval,

$$B_{1,j}^{*k+1} T_{1,j+\frac{1}{2}}^{*k+1} + C_{1,j}^{*k+1} T_{2,j+\frac{1}{2}}^{*k+1} = D_{1,j}^{*k} , \quad (F.8)$$

where

$$B_{1,j}^{*k+1} \equiv V_1(\rho C_p)_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}} + P_1 k_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}}$$

$$C_{1,j}^{*k+1} \equiv -P_1 k_{1,j+\frac{1}{2}}^{*k+1}$$

$$D_{1,j}^{*k} \equiv V_1(\rho C_p)_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{1,j+\frac{1}{2}}^{*k} + P_1 k_{1,j+\frac{1}{2}}^{*k} (T_{2,j+\frac{1}{2}}^{*k} - T_{1,j+\frac{1}{2}}^{*k}) + \frac{2}{\Delta z} F_{1,j+\frac{1}{2}}^{*k+\frac{1}{2}}.$$

Using the first interface condition at the outermost fuel node
($i = I_f$), Eq. (F.5) becomes

$$\begin{aligned} \Delta t \int_{r_{I_f-1}}^{r_{I_f}} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr \\ = \frac{1}{2} P_{I_f-1} \left[k_{I_f,j+\frac{1}{2}}^{*k+1} (T_{I_f,j+\frac{1}{2}}^{*k+1} - T_{I_f-1,j+\frac{1}{2}}^{*k+1}) + k_{I_f,j+\frac{1}{2}}^{*k} (T_{I_f,j+\frac{1}{2}}^{*k} - T_{I_f-1,j+\frac{1}{2}}^{*k}) \right] \\ - \frac{1}{2} \Delta t r_{I_f} \left[h_{g,j+\frac{1}{2}}^{*k+1} (T_{I_f+1,j+\frac{1}{2}}^{*k+1} - T_{I_f,j+\frac{1}{2}}^{*k+1}) + h_{g,j+\frac{1}{2}}^{*k} (T_{I_f+1,j+\frac{1}{2}}^{*k} - T_{I_f,j+\frac{1}{2}}^{*k}) \right] \\ + 0 \left[(\Delta r_{I_f} \Delta t) + (\Delta t)^3 \right], \end{aligned}$$

which results in the difference equation

$$A_{I_f,j}^{*k+1} T_{I_f-1,j+\frac{1}{2}}^{*k+1} + B_{I_f,j}^{*k+1} T_{I_f,j+\frac{1}{2}}^{*k+1} + C_{I_f,j}^{*k+1} T_{I_f+1,j+\frac{1}{2}}^{*k+1} = D_{I_f,j}^{*k}, \quad (F.9)$$

where

$$A_{I_f,j}^{*k+1} \equiv -P_{I_f-1} k_{I_f,j+\frac{1}{2}}^{*k+1}$$

$$B_{I_f,j}^{*k+1} \equiv V_{I_f}(\rho C_p)_{I_f,j+\frac{1}{2}}^{*k+\frac{1}{2}} + P_{I_f-1} k_{I_f,j+\frac{1}{2}}^{*k+1} + \Delta t r_{I_f} h_{g,j+\frac{1}{2}}^{*k+1}$$

$$C_{I_f, j}^{*k+1} \equiv -\Delta t r_{I_f} h_{g, j+\frac{1}{2}}^{*k+1}$$

$$D_{I_f, j}^{*k} \equiv V_{I_f} (\rho C_p)_{I_f, j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{I_f, j+\frac{1}{2}}^{*k} - P_{I_f-1} k_{I_f, j+\frac{1}{2}}^{*k} \left(T_{I_f, j+\frac{1}{2}}^{*k} - T_{I_f-1, j+\frac{1}{2}}^{*k} \right) \\ + \Delta t r_{I_f} h_{g, j+\frac{1}{2}}^{*k} \left(T_{I_f+1, j+\frac{1}{2}}^{*k} - T_{I_f, j+\frac{1}{2}}^{*k} \right) + \frac{2}{\Delta z} F_{I_f, j+\frac{1}{2}}^{*k+\frac{1}{2}} .$$

Use of both interface conditions of system (2.22) results in the following evaluation of Eq. (F.5) at the innermost cladding mesh region ($i = I_f+1$):

$$\Delta t \int_{r_{I_f+1}}^{\hat{r}_{I_f+1}} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right]_{j+\frac{1}{2}}^{k+\frac{1}{2}} r dr \\ = -\frac{1}{2} P_{I_f+1} \left[k_{I_f+1, j+\frac{1}{2}}^{*k+1} \left(T_{I_f+2, j+\frac{1}{2}}^{*k+1} - T_{I_f+1, j+\frac{1}{2}}^{*k+1} \right) + k_{I_f+1, j+\frac{1}{2}}^{*k} \left(T_{I_f+2, j+\frac{1}{2}}^{*k} \right. \right. \\ \left. \left. - T_{I_f+1, j+\frac{1}{2}}^{*k} \right) \right] + \frac{1}{2} \Delta t r_{I_f} \left[h_{g, j+\frac{1}{2}}^{*k+1} \left(T_{I_f+1, j+\frac{1}{2}}^{*k+1} - T_{I_f, j+\frac{1}{2}}^{*k+1} \right) \right. \\ \left. + h_{g, j+\frac{1}{2}}^{*k} \left(T_{I_f+1, j+\frac{1}{2}}^{*k} - T_{I_f, j+\frac{1}{2}}^{*k} \right) \right] + 0 \left[\left(\Delta t \Delta r_{I_f+1} \right) + (\Delta t)^3 \right] .$$

Combining the above with Eq. (F.4) gives the difference equation

$$A_{I_f+1, j}^{*k+1} T_{I_f, j+\frac{1}{2}}^{*k+1} + B_{I_f+1, j}^{*k+1} T_{I_f+1, j+\frac{1}{2}}^{*k+1} + C_{I_f+1, j}^{*k+1} T_{I_f+2, j+\frac{1}{2}}^{*k+1} = D_{I_f+1, j}^{*k} , \quad (F.10)$$

where

$$A_{I_f+1, j}^{*k+1} \equiv -\Delta t r_{I_f} h_{g, j+\frac{1}{2}}^{*k+1}$$

$$B_{I_f+1,j}^{*k+1} \equiv V_{I_f+1} (\rho C_p)_{I_f+1,j+\frac{1}{2}}^{*k+\frac{1}{2}} + P_{I_f+1} k_{I_f+1,j+\frac{1}{2}}^{*k+1} + \Delta t r_{I_f} h_{g,j+\frac{1}{2}}^{*k+1}$$

$$C_{I_f+1,j}^{*k+1} \equiv -P_{I_f+1} k_{I_f+1,j+\frac{1}{2}}^{*k+1}$$

$$\begin{aligned} D_{I_f+1,j}^{*k+1} \equiv & V_{I_f+1} (\rho C_p)_{I_f+1,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{I_f+1,j+\frac{1}{2}}^{*k} \\ & + P_{I_f+1} k_{I_f+1,j+\frac{1}{2}}^{*k} \left(T_{I_f+2,j+\frac{1}{2}}^{*k} - T_{I_f+1,j+\frac{1}{2}}^{*k} \right) \\ & - \Delta t r_{I_f} h_{g,j+\frac{1}{2}}^{*k} \left(T_{I_f+1,j+\frac{1}{2}}^{*k} - T_{I_f,j+\frac{1}{2}}^{*k} \right) + \frac{2}{\Delta z} F_{I_f+1,j+\frac{1}{2}}^{*k+\frac{1}{2}} . \end{aligned}$$

Evaluating Eq. (F.5) at the outermost cladding node ($i = I$) and applying the coolant-clad boundary condition yields

$$\begin{aligned} \Delta t \int_{r_{I-1}}^{r_I} \left[-\frac{1}{r} k^* \frac{\partial}{\partial r} \left(r \frac{\partial T^*}{\partial r} \right) \right] r dr \\ = \frac{1}{2} P_{I-1} \left[k_{I,j+\frac{1}{2}}^{*k+1} \left(T_{I,j+\frac{1}{2}}^{*k+1} - T_{I-1,j+\frac{1}{2}}^{*k+1} \right) + k_{I,j+\frac{1}{2}}^{*k} \left(T_{I,j+\frac{1}{2}}^{*k} - T_{I-1,j+\frac{1}{2}}^{*k} \right) \right] \\ + \frac{1}{2} \Delta t r_I \left[h_{c,j+\frac{1}{2}}^{*k+1} \left(T_{I,j+\frac{1}{2}}^{*k+1} - T_{c,j+\frac{1}{2}}^{*k+1} \right) + h_{c,j+\frac{1}{2}}^{*k} \left(T_{I,j+\frac{1}{2}}^{*k} - T_{c,j+\frac{1}{2}}^{*k} \right) \right] \\ + O[(\Delta t \cdot \Delta r_{I-1}) + (\Delta t)^2] . \end{aligned}$$

As in the forward case, make the half-step approximation

$$T_{c,j+\frac{1}{2}}^{*k} = \frac{1}{2} \left(T_{c,j}^{*k} + T_{c,j+1}^{*k} \right) + O[(\Delta z)^2] .$$

The following approximation to Eq. (5.2) is then obtained:

$$\begin{aligned} A_{I,j}^{*k+1} T_{I-1,j+\frac{1}{2}}^{*k+1} + B_{I,j}^{*k+1} T_{I,j+\frac{1}{2}}^{*k+1} + C_{I,j}^{*k+1} T_{c,j+1}^{*k+1} \\ = D_{I,j+\frac{1}{2}}^{*k} - C_{I,j}^{*k+1} T_{c,j}^{*k+1} , \end{aligned} \quad (F.11)$$

where

$$A_{I,j}^{*k+1} \equiv -P_{I-1} k_{I,j+\frac{1}{2}}^{*k+1}$$

$$B_{I,j}^{*k+1} \equiv V_I (\rho C_p)_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}} + P_{I-1} k_{I,j+\frac{1}{2}}^{*k+1} + \Delta t r_I h_{c,j+\frac{1}{2}}^{*k+1}$$

$$C_{I,j}^{*k+1} \equiv -\frac{1}{2} \Delta t r_I h_{c,j+\frac{1}{2}}^{*k+1}$$

$$D_{I,j}^{*k} \equiv V_I (\rho C_p)_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}} T_{I,j+\frac{1}{2}}^{*k} - P_{I-1} k_{I,j+\frac{1}{2}}^{*k} (T_{I,j+\frac{1}{2}}^{*k} - T_{I-1,j+\frac{1}{2}}^{*k}) \\ - \Delta t r_I h_{c,j+\frac{1}{2}}^{*k} (T_{I,j+\frac{1}{2}}^{*k} - T_{c,j+\frac{1}{2}}^{*k}) + \frac{2}{\Delta z} F_{I,j+\frac{1}{2}}^{*k+\frac{1}{2}}.$$

APPENDIX G

PROOF OF DIAGONAL DOMINANCE OF DISCRETE
SOLUTION MATRICES

It is necessary to show that the matrices H_j^{k+1} and H_j^{*k+1} appearing in Eqs. (4.14) and (5.5), respectively, are strictly diagonally dominant for $j = 1, 2, \dots, J-1$ and $k = 0, 1, \dots, K-1$. This requires the knowledge that the physical quantities k , ρC_p , h_g , h_c , $A\rho C_p$, and wC_p are positive functions.¹³

To show that H_j^{k+1} is diagonally dominant, note that each row except the first and last have the diagonal element $B_{i,j}^{k+1}$ and nonzero off-diagonal elements $A_{i,j}^{k+1}$ and $C_{i,j}^{k+1}$, $i = 2, 3, \dots, I$. From the definitions of these elements [which appear in Eqs. (4.4), (4.7), (4.8), and (4.10)],

$$\begin{aligned} |B_{i,j}^{k+1}| &= |V_i (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1} + P_i k_{i,j+\frac{1}{2}}^{k+1}| \\ &> P_{i-1} k_{i-1,j+\frac{1}{2}}^{k+1} + P_i k_{i,j+\frac{1}{2}}^{k+1} = |A_{i,j}^{k+1}| + |C_{i,j}^{k+1}|, \\ i &= 2, 3, \dots, I_f-1, I_f+2, \dots, I-1 \end{aligned}$$

$$\begin{aligned} |B_{I_f,j}^{k+1}| &= |V_{I_f} (\rho C_p)_{I_f,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I_f-1} k_{I_f-1,j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g,j+\frac{1}{2}}^{k+1}| \\ &> P_{I_f-1} k_{I_f-1,j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g,j+\frac{1}{2}}^{k+1} = |A_{I_f,j}^{k+1}| + |C_{I_f,j}^{k+1}| \end{aligned}$$

$$\begin{aligned} |B_{I_f+1,j}^{k+1}| &= |V_{I_f+1} (\rho C_p)_{I_f+1,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I_f+1} k_{I_f+1,j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g,j+\frac{1}{2}}^{k+1}| \\ &> P_{I_f+1} k_{I_f+1,j+\frac{1}{2}}^{k+1} + r_{I_f} \Delta t h_{g,j+\frac{1}{2}}^{k+1} = |A_{I_f+1,j}^{k+1}| + |C_{I_f+1,j}^{k+1}| \end{aligned}$$

$$\begin{aligned} |B_{I,j}^{k+1}| &= |V_I (\rho C_p)_{I,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_{I-1} k_{I-1,j+\frac{1}{2}}^{k+1} + r_I \Delta t h_{c,j+\frac{1}{2}}^{k+1}| \\ &> P_{I-1} k_{I-1,j+\frac{1}{2}}^{k+1} + r_I \Delta t h_{c,j+\frac{1}{2}}^{k+1} > |A_{I,j}^{k+1}| + |C_{I,j}^{k+1}| \end{aligned}$$

and thus all interior rows of H_j^{k+1} satisfy the necessary condition for strict diagonal dominance. The first row also satisfies the requirement, since [using the coefficients of Eq. (4.6)]

$$|B_{1,j}^{k+1}| = |V_1(\rho C_p)_{1,j+\frac{1}{2}}^{k+\frac{1}{2}} + P_1 k_{1,j+\frac{1}{2}}^{k+1}| > P_1 k_{1,j+\frac{1}{2}}^{k+1} = |C_{1,j}^{k+1}| ,$$

where $B_{1,j}^{k+1}$ is the diagonal element and $C_{1,j}^{k+1}$ is the only nonzero off-diagonal element. To show that the last row of H_j^{k+1} maintains the requirement for strict diagonal dominance, consider the quantities $A_{I+1,j}^{k+1}$ and $B_{I+1,j}^{k+1}$ appearing in Eq. (4.13). The necessary condition is

$$|A_{I+1,j}^{k+1}| < |B_{I+1,j}^{k+1}| ,$$

or

$$\alpha_1 u_{j+1}^{k+1} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+1}^{k+1} + \alpha_1 \alpha_2 \Delta t x_{j+1}^{k+1} > \alpha_2 \Delta t \left[\alpha_1 x_{j+1}^{k+1} + (1 - \alpha_1) x_j^{k+1} \right] .$$

This simplifies to

$$\alpha_1 u_{j+1}^{k+1} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+1}^{k+1} - (1 - \alpha_1) \alpha_2 \Delta t x_j^{k+1} > 0 ,$$

which holds easily for $\alpha_1 \geq \frac{1}{2}$, $\Delta z \leq 10$ cm, and $\Delta t \leq 0.2$ sec. — trivial restrictions for most applications. (This conclusion requires examination of the physical data functions u , v , and x , and will not be shown in detail here.) Thus, each row of H_j^{k+1} has a diagonal element greater in absolute value than the sum of the absolute values of the off-diagonal elements, proving H_j^{k+1} is strictly diagonally dominant.

It is important to note that although a unique solution exists, the forward matrix equation (4.14) cannot be determined exactly, but must be solved by iteration. Preliminary results indicate that the iteration converges easily to several digits of accuracy in less than 10 iterations.

In addition, it is certain that at each iteration the matrix H_j^{k+1} is diagonally dominant — the above proof is based on the common occurrence of data functions in the coefficients $A_{i,j}^{k+1}$, $B_{i,j}^{k+1}$, and $C_{i,j}^{k+1}$, and not on any particular time level or temperature; hence, the same proof can be applied to each iteration of H_j^{k+1} .

Examination of the coefficient functions h_g' , h_c' , $(ApC_p)'$, and $(wC_p)'$ reveals that each is positive;¹³ hence, strict diagonal dominance of H_j^{*k+1} follows in an analogous manner. As in the forward case, it is easily seen that

$$|B_{1,j}^{*k+1}| > |C_{1,j}^{*k+1}|$$

$$|B_{1,j}^{*k+1}| > |A_{1,j}^{*k+1}| + |C_{i,j}^{*k+1}|, \quad i = 2, 3, \dots, I,$$

where the elements $A_{i,j}^{*k+1}$, $B_{i,j}^{*k+1}$, and $C_{i,j}^{*k+1}$ are those found in Eq. (5.2).

Analysis of the last row of H_j^{*k+1} requires knowledge of the coefficients $A_{I+1,j}^{*k+1}$ and $B_{I+1,j}^{*k+1}$ appearing in Eq. (5.4). For strict diagonal dominance, the necessary condition is $|A_{I+1,j}^{*k+1}| < |B_{I+1,j}^{*k+1}|$, or

$$\alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} < \alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_1 \alpha_2 \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}},$$

which reduces to

$$\alpha_1 u_{j+\frac{1}{2}}^{*k+\frac{1}{2}} + \alpha_2 \frac{\Delta t}{\Delta z} v_{j+\frac{1}{2}}^{*k+\frac{1}{2}} - \alpha_2 (1 - \alpha_1) \Delta t x_{j+\frac{1}{2}}^{*k+\frac{1}{2}} > 0.$$

This inequality requires slightly more stringent conditions than in the forward case, $\Delta z \leq 10$ cm, $\alpha_1 \geq \frac{1}{2}$, and $\Delta t \leq 0.1$ sec.; however, even these requirements are easily satisfied in practice. Thus, conclude that H_j^{*k+1} is also strictly diagonally dominant.

**THIS PAGE
WAS INTENTIONALLY
LEFT BLANK**

APPENDIX H

COMPUTATION OF SENSITIVITY INTEGRALS

Appearing in Eq. (2.21) are fourteen integrals representing as many distinct sensitivity quantities. As in the discussion following Eq. (2.21), the sensitivity of P to α is calculated for each relevant scale factor α , resulting in the following independent integral computations (all barred variables signify the appropriate scale factor):

$$\frac{dP}{d\bar{Q}_f} \cdot \frac{\bar{Q}_f}{P} = \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* Q r dr dz dt \quad (H.1)$$

$$\frac{dP}{d\bar{Q}_c} \cdot \frac{\bar{Q}_c}{P} = \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* Q r dr dz dt \quad (H.2)$$

$$\frac{dP}{d(\rho\bar{C}_p)_f} \cdot \frac{(\rho\bar{C}_p)_f}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_0^{R_f} \phi^* (\rho C_p) \frac{\partial T}{\partial t} r dr dz dt \quad (H.3)$$

$$\frac{dP}{d(\rho\bar{C}_p)_c} \cdot \frac{(\rho\bar{C}_p)_c}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_{R_g}^R \phi^* (\rho C_p) \frac{\partial T}{\partial t} r dr dz dt \quad (H.4)$$

$$\frac{dP}{d\bar{k}_f} \cdot \frac{\bar{k}_f}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_0^{R_f} k \frac{\partial \phi^*}{\partial r} \frac{\partial T}{\partial r} r dr dz dt \quad (H.5)$$

$$\frac{dP}{d\bar{k}_c} \cdot \frac{\bar{k}_c}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L \int_{R_g}^R k \frac{\partial \phi^*}{\partial r} \frac{\partial T}{\partial r} r dr dz dt \quad (H.6)$$

$$\frac{dP}{d\bar{h}_g} \cdot \frac{\bar{h}_g}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L R_f h_g \left(T \Big|_{R_f^-} - T \Big|_{R_g^+} \right) \left(\phi^* \Big|_{R_f^-} - \phi^* \Big|_{R_g^+} \right) dz dt \quad (H.7)$$

$$\frac{dP}{d\bar{h}_c} \cdot \frac{\bar{h}_c}{P} = - \frac{2\pi}{P} \int_0^{t_f} \int_0^L h_c [r(T - T_c)(\phi^* - \chi^*)]_{r=R} dz dt \quad (H.8)$$

$$\frac{dP}{d\bar{T}_{0f}} \cdot \frac{\bar{T}_{0f}}{P} = \frac{2\pi}{P} \int_0^L \int_0^{R_f} T_0 (\rho C_p \phi^*) \Big|_{t=0} r dr dz \quad (H.9)$$

$$\frac{dP}{d\bar{T}_{0c}} \cdot \frac{\bar{T}_{0c}}{P} = \frac{2\pi}{P} \int_0^L \int_{R_g}^R T_0 (\rho C_p \phi^*) \Big|_{t=0} r dr dz \quad (H.10)$$

$$\frac{dP}{d(\bar{A}\rho C_p)} \cdot \frac{(\bar{A}\rho C_p)}{P} = - \frac{1}{P} \int_0^{t_f} \int_0^L \chi^* \frac{\partial}{\partial t} (A\rho C_p T_c) dz dt \quad (H.11)$$

$$\frac{dP}{d(\bar{w}C_p)} \cdot \frac{(\bar{w}C_p)}{P} = - \frac{1}{P} \int_0^{t_f} \int_0^L \chi^* \frac{\partial}{\partial z} (wC_p T_c) dz dt \quad (H.12)$$

$$\frac{dP}{d\bar{T}_{c0}} \cdot \frac{\bar{T}_{c0}}{P} = \frac{1}{P} \int_0^L T_{c0} [\chi^* (A\rho C_p)]_{t=0} dz \quad (H.13)$$

$$\frac{dP}{dT_{C_1}} \cdot \frac{T_{C_1}}{P} = \frac{1}{P} \int_0^{t_f} T_{C_1} [X^*(wC_P)]_{z=0} dt . \quad (H.14)$$

In addition, recall the three integrals constituting the response (2.11),

$$P_{fuel} = 2\pi \int_0^{t_f} \int_0^L \int_0^{R_f} f T r dr dz dt \quad (H.15)$$

$$P_{clad} = 2\pi \int_0^{t_f} \int_0^L \int_{R_g}^R f T r dr dz dt \quad (H.16)$$

$$P_{coolant} = \int_0^{t_f} \int_0^L g T_c dz dt . \quad (H.17)$$

The forward and adjoint functions are known only at the discrete solution points; hence, computation of the sensitivity integrals must be done by numerical approximation. Computer storage limitations also pose restrictions, as only a few time levels of solution values can be stored in core at one time. With these factors in mind, consider two simple numerical integration procedures, the *trapezoidal rule* and the *midpoint rule*. For a single independent variable, integration over one interval is approximated as follows:⁴

$$(\text{Trapezoidal Rule}) \quad \int_a^b y(x) dx \doteq \frac{1}{2} [y(a) + y(b)] (b - a) ,$$

(Midpoint Rule)
$$\int_a^b y(x) dx \doteq y \left(\frac{a+b}{2} \right) (b-a) .$$

Often it is necessary to use a "compound rule," formed by merging both the trapezoidal and midpoint rules,

(Compound Rule)
$$\int_a^b w(x)y(x) dx \doteq \frac{1}{2} [w(a) + w(b)] y \left(\frac{a+b}{2} \right) (b-a) .$$

Using various combinations of these basic approximations on integrals in each independent variable, the single, double, and triple integrals in Eqs. (H.1)-(H.14) can be determined. Table H-I lists the sensitivity quantities and the method used to calculate each integral. Consistent with this information, the sensitivity integrals can be approximated as follows:

$$\begin{aligned} \frac{dP}{d\bar{Q}_f} \cdot \frac{\bar{Q}_f}{P} &= \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} \phi^* Q \, r dr dz dt \\ &= \frac{\pi \Delta z}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \left(\phi_{i,j+\frac{1}{2}}^{*k+1} + \phi_{i,j+\frac{1}{2}}^{*k} \right) \tilde{Q}_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \end{aligned}$$

$$\begin{aligned} \frac{dP}{d\bar{Q}_c} \cdot \frac{\bar{Q}_c}{P} &= \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} \phi^* Q \, r dr dz dt \\ &= \frac{\pi \Delta z}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \left(\phi_{i,j+\frac{1}{2}}^{*k+1} + \phi_{i,j+\frac{1}{2}}^{*k} \right) \tilde{Q}_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \end{aligned}$$

Table H-I. Integration Methods for Sensitivity Integrals

	Integral Approximation Method ^a		
	r	z	t
Equation 6.1			
Scale-factor $\bar{Q}_f$	M^b	M	C
Equation 6.2			
Scale-factor $\bar{Q}_c$	M^b	M	C
Equation 6.3			
Scale-factor $(\rho\bar{C}_p)_f$	M^b	M	C
Equation 6.4			
Scale-factor $(\rho\bar{C}_p)_c$	M^b	M	C
Equation 6.5			
Scale-factor $\bar{k}_f$	M	M	T
Equation 6.6			
Scale-factor $\bar{k}_c$	M	M	T
Equation 6.7			
Scale-factor $\bar{h}_g$	-	M	T
Equation 6.8			
Scale-factor $\bar{h}_c$	-	M	T
Equation 6.9			
Scale-factor $\bar{T}_{of}$	M	M	-
Equation 6.10			
Scale-factor $\bar{T}_{oc}$	M	M	-
Equation 6.11			
Scale-factor $(\bar{A}\rho C_p)$	-	M	C
Equation 6.12			
Scale-factor $(\bar{w}C_p)$	-	M	T
Equation 6.13			
Scale-factor $\bar{T}_{c0}$	-	M	-
Equation 6.14			
Scale-factor $\bar{T}_{c1}$	-	-	T
Equation 6.15			
Weight function f_{fuel}	T	M	C
Equation 6.16			
Weight function f_{clad}	T	M	C
Equation 6.17			
Weight function g	-	M	C

^aT = trapezoidal, M = midpoint, C = compound.

^bModified slightly at endpoints.

$$\frac{dP}{d(\rho\bar{C}_p)_f} \cdot \frac{(\rho\bar{C}_p)_f}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} \phi^*(\rho C_p) \frac{\partial T}{\partial t} r dr dz dt$$

$$= - \frac{\pi \Delta Z}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \left(\phi_{i,j+\frac{1}{2}}^{*k+1} + \phi_{i,j+\frac{1}{2}}^{*k} \right)$$

$$\left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^k \right) (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} V_i$$

$$\frac{dP}{d(\rho\bar{C}_p)_c} \cdot \frac{(\rho\bar{C}_p)_c}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} \phi^*(\rho C_p) \frac{\partial T}{\partial t} r dr dz dt$$

$$= - \frac{\pi \Delta Z}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \left(\phi_{i,j+\frac{1}{2}}^{*k+1} + \phi_{i,j+\frac{1}{2}}^{*k} \right)$$

$$\left(T_{i,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^k \right) (\rho C_p)_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} V_i$$

$$\frac{dP}{d\bar{k}_f} \cdot \frac{\bar{k}_f}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{r_i}^{r_{i+1}} k \frac{\partial \phi^*}{\partial r} \frac{\partial T}{\partial r} r dr dz dt$$

$$= - \frac{\pi \Delta Z}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f-1} P_i \left[k_{i,j+\frac{1}{2}}^{k+1} \left(T_{i+1,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^{k+1} \right) \left(\phi_{i+1,j+\frac{1}{2}}^{*k+1} - \phi_{i,j+\frac{1}{2}}^{*k+1} \right) + k_{i,j+\frac{1}{2}}^k \left(T_{i+1,j+\frac{1}{2}}^k - T_{i,j+\frac{1}{2}}^k \right) \left(\phi_{i+1,j+\frac{1}{2}}^{*k} - \phi_{i,j+\frac{1}{2}}^{*k} \right) \right]$$

$$\frac{dP}{d\bar{k}_c} \cdot \frac{\bar{k}_c}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^{I-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{r_i}^{r_{i+1}} k \frac{\partial \phi^*}{\partial r} \frac{\partial T}{\partial r} r dr dz dt$$

$$= - \frac{\pi \Delta Z}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^{I-1} P_i \left[k_{i,j+\frac{1}{2}}^{k+1} \left(T_{i+1,j+\frac{1}{2}}^{k+1} - T_{i,j+\frac{1}{2}}^{k+1} \right) \left(\phi_{i+1,j+\frac{1}{2}}^{*k+1} - \phi_{i,j+\frac{1}{2}}^{*k+1} \right) \right]$$

$$- \phi_{i,j+\frac{1}{2}}^{*k+1}) + k_{i,j+\frac{1}{2}}^k (T_{i+1,j+\frac{1}{2}}^k - T_{i,j+\frac{1}{2}}^k) (\phi_{i+1,j+\frac{1}{2}}^{*k} - \phi_{i,j+\frac{1}{2}}^{*k}) \Big]$$

$$\frac{dP}{d\bar{h}_g} \cdot \frac{\bar{h}_g}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} R_f h_g (T|_{R_f^-} - T|_{R_g^+}) (\phi^*|_{R_f^-} - \phi^*|_{R_g^+}) dz dt$$

$$= - \frac{\pi r_{I_f} \Delta z \Delta t}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \left[h_{g,j+\frac{1}{2}}^{k+1} (T_{I_f,j+\frac{1}{2}}^{k+1} - T_{I_f+1,j+\frac{1}{2}}^{k+1}) \right. \\ \left. (\phi_{I_f,j+\frac{1}{2}}^{*k+1} - \phi_{I_f+1,j+\frac{1}{2}}^{*k+1}) + h_{g,j+\frac{1}{2}}^k (T_{I_f,j+\frac{1}{2}}^k - T_{I_f+1,j+\frac{1}{2}}^k) \right. \\ \left. (\phi_{I_f,j+\frac{1}{2}}^{*k} - \phi_{I_f+1,j+\frac{1}{2}}^{*k}) \right]$$

$$\frac{dP}{d\bar{h}_c} \cdot \frac{\bar{h}_c}{P} = - \frac{2\pi}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} h_c [r(T - T_c)(\phi^* - \chi^*)]_{r=R} dz dt$$

$$= - \frac{\pi r_I \Delta z \Delta t}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \left[h_{c,j+\frac{1}{2}}^{k+1} (T_{I,j+\frac{1}{2}}^{k+1} - T_{c,j+\frac{1}{2}}^{k+1}) (\phi_{I,j+\frac{1}{2}}^{*k+1} \right. \\ \left. - \chi_{j+\frac{1}{2}}^{*k+1}) + h_{c,j+\frac{1}{2}}^k (T_{I,j+\frac{1}{2}}^k - T_{c,j+\frac{1}{2}}^k) (\phi_{I,j+\frac{1}{2}}^{*k} - \chi_{j+\frac{1}{2}}^{*k}) \right]$$

$$\frac{dP}{d\bar{T}_{0f}} \cdot \frac{\bar{T}_{0f}}{P} = \frac{2\pi}{P} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \int_{z_j}^{z_{j+1}} \int_{v_i} (T \phi^* \rho C_p) \Big|_{t=0} r dr dz$$

$$= \frac{\pi \Delta z}{P} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} T_{i,j+\frac{1}{2}}^0 \phi_{i,j+\frac{1}{2}}^{*0} (\rho C_p)_{i,j+\frac{1}{2}}^0 v_i$$

$$\frac{dP}{d\bar{T}_{0c}} \cdot \bar{T}_{0c} = \frac{2\pi}{P} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \int_{z_j}^{z_{j+1}} \int_{v_i} (T\phi^* \rho C_p) \Big|_{t=0} r dr dz$$

$$= \frac{\pi \Delta Z}{P} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} T_{i,j+\frac{1}{2}}^0 \phi_{i,j+\frac{1}{2}}^{*0} (\rho C_p)_{i,j+\frac{1}{2}}^0 v_i$$

$$\frac{dP}{d(\bar{A}\rho C_p)} \cdot \frac{(\bar{A}\rho C_p)}{P} = -\frac{1}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \chi^* \frac{\partial}{\partial t} (A\rho C_p T_c) dz dt$$

$$= -\frac{\Delta Z}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} (\chi_{j+\frac{1}{2}}^{*k+1} + \chi_{j+\frac{1}{2}}^{*k})$$

$$\left[(A\rho C_p T_c)_{j+\frac{1}{2}}^{k+1} - (A\rho C_p T_c)_{j+\frac{1}{2}}^k \right]$$

$$\frac{dP}{d(\bar{w}C_p)} \cdot \frac{(\bar{w}C_p)}{P} = -\frac{1}{P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \chi^* \frac{\partial}{\partial z} (wC_p T_c) dz dt$$

$$= -\frac{\Delta t}{2P} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \left\{ \chi_{j+\frac{1}{2}}^{*k+1} \left[(wC_p T_c)_{j+1}^{k+1} - (wC_p T_c)_j^{k+1} \right] \right. \\ \left. + \chi_{j+\frac{1}{2}}^{*k} \left[(wC_p T_c)_{j+1}^k - (wC_p T_c)_j^k \right] \right\}$$

$$\frac{dP}{d\bar{T}_{co}} \cdot \frac{\bar{T}_{co}}{P} = \frac{1}{P} \sum_{j=1}^{J-1} \int_{z_j}^{z_{j+1}} T_{co} [\chi^* (A\rho C_p)^{-1}]_{t=0} dz$$

$$= \frac{\Delta Z}{P} \sum_{j=1}^{J-1} T_{co,j+\frac{1}{2}}^0 \chi_{j+\frac{1}{2}}^{*0} (A\rho C_p)^{-1}_{j+\frac{1}{2}}^0$$

$$\begin{aligned}
\frac{dP}{d\bar{T}_{c1}} \cdot \frac{\bar{T}_{c1}}{P} &= \frac{1}{P} \sum_{k=0}^{K-1} \int_{t_k}^{t_{k+1}} T_{c1} [X^*(wC_p)]_{z=0} dt \\
&= \frac{\Delta t}{2P} \sum_{k=0}^{K-1} \left[T_{c,1}^k X_1^{*k} (wC_p)_1^k + T_{c,1}^{k+1} X_1^{*k+1} (wC_p)_1^{k+1} \right].
\end{aligned}$$

The three response integrals are also approximated using the trapezoidal, midpoint, and composite rules. The method of integration in each independent variable is listed in Table H-I. Application of these procedures results in the following approximations for Eqs. (5.15), (5.16), and (5.17):

$$\begin{aligned}
P_{fuel} &= 2\pi \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} f T r dr dz dt \\
&= \pi \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=1}^{I_f} F_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{i,j+\frac{1}{2}}^{k+1} + T_{i,j+\frac{1}{2}}^k \right) \\
P_{clad} &= 2\pi \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} \int_{v_i} f T r dr dz dt \\
&= \pi \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \sum_{i=I_f+1}^I F_{i,j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{i,j+\frac{1}{2}}^{k+1} + T_{i,j+\frac{1}{2}}^k \right) \\
P_{coolant} &= \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} \int_{t_k}^{t_{k+1}} \int_{z_j}^{z_{j+1}} g T_c dz dt \\
&= \frac{\Delta z \Delta t}{2} \sum_{k=0}^{K-1} \sum_{j=1}^{J-1} g_{j+\frac{1}{2}}^{k+\frac{1}{2}} \left(T_{c,j+\frac{1}{2}}^{k+1} + T_{c,j+\frac{1}{2}}^k \right).
\end{aligned}$$

THIS PAGE
WAS INTENTIONALLY
LEFT BLANK

ORNL/TM-6900
Distribution Category UC-79p
Breeder Reactor Safety

INTERNAL DISTRIBUTION

1. L. S. Abbott	48. L. J. Ott
2. R. G. Alsmiller, Jr.	49. J. V. Pace
3. V. C. Baker	50. C. V. Parks
4. M. A. Bjerke	51. R. W. Peelle
5. T. F. Bott	52. F. G. Perey
6. T. J. Burns	53. R. B. Perez
7-8. D. G. Cacuci	54. T. W. Pickel
9. G. de Saussure	55. R. W. Roussin
10. H. L. Dodds	56. J. P. Sanders
11. G. F. Flanagan	57. D. L. Selby
12. M. H. Fontana	58. D. G. Thomas
13. W. E. Ford III	59. E. T. Tomlinson
14. T. A. Gabriel	60. D. R. Vondy
15. U. Gat	61. J. L. Wantland
16. H. Goldstein (Consultant)	62-84. C. F. Weber
17. N. M. Greene	85. C. R. Weisbin
18. P. M. Haas	86. R. M. Westfall
19. D. T. Ingersoll	87. M. L. Williams
20. T. S. Kress	88. P. Greebler (Consultant)
21. R. A. Lillie	89. W. B. Loewenstein (Consultant)
22. J. L. Lucius	90. R. Wilson (Consultant)
23. R. E. Maerker	91-92. Central Research Library
24. F. C. Maienschein	93. ORNL Y-12 Technical Library
25. J. H. Marable	94-95. Laboratory Records Department
26. F. R. Mynatt	96. Laboratory Records - ORNL RC
27. L. C. Oakes	97. ORNL Patent Office
28-47. E. M. Oblow	

EXTERNAL DISTRIBUTION

- 98-99. Director, Division of Reactor Research and Technology, DOE, Washington, D.C. 20545.
100. Office of the Assistant Manager for Research and Development, DOE-ORO, Oak Ridge, Tennessee 37830.
- 101-376. Given distribution as shown in TID-4500, Distribution Category UC-79p, Breeder Reactor Safety (Base).