MODELING OF BWR WATER CHEMISTRY

by

JOHN HWAN CHUN

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Electrical Engineering and Computer Sciences
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Signature of Author________________________________
Department of Nuclear Engineering
July 9, 1990

Certified by________________________________
Ronald G. Ballinger
Professor of Nuclear Engineering and Materials Science and Engineering
Thesis Supervisor

Certified by________________________________
Michael J. Driscoll
Professor Emeritus of Nuclear Engineering
Thesis Reader

Accepted by________________________________
Allan F. Henry
Chairman, Department Committee on Graduate Students

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Abstract

A computer simulation of Boiling Water Reactor (BWR) coolant chemistry with particular attention to dissolved O_2 and H_2 concentrations has been conducted and results showing concentration profiles at various regions in a simulation of the Dresden-2 power plant are presented. Simulations include both normal water chemistry (NWC) and hydrogen water chemistry (HWC) studies.

For this project a general purpose computer program RADIation Chemistry Analysis Loop code (RADICAL) was developed in FORTRAN 77. RADICAL calculates concentrations of chemical species in water, including radicals as well as stable species, as the coolant flows through various components of a BWR. The code is derived from the species balance in a two-phase flowing control volume and is applicable to any arbitrary combination of single and two-phase systems in series or parallel arrangement.

A sensitivity analysis routine has been developed in conjunction with the concentration calculation routine to provide a quantitative measure of how input parameters affect the calculated results. Unlike parametric studies, the sensitivity routine utilizes the adjoint and response of the concentration function to obtain a quite precise differential sensitivity of concentrations with respect to input parameters. This is particularly important since most of the input parameters used in this simulation are not known accurately. Thus sensitivity results provide quantitative guidance in determining which parameters should be more accurately re-evaluated or measured in experiments to come up with better simulation results.

The simulation results showed that hydrogen injection decreases O_2 concentration in all regions of a BWR, but to a lesser degree in the core boiling region where the dissolved H_2 is rapidly stripped to the gas phase. Simulation showed that the oxygen concentration in the recirculation line, which is of particular interest in intergranular stress corrosion cracking (IGSCC) studies, was reduced to below 20 ppb by injecting 0.3 ppm of H_2 in the feedwater. This agrees reasonably well with the measured concentration of 50 ppb at 0.4 ppm of H_2 injection at the Dresden-2 power plant.

Thesis Supervisor :	Ronald G. Ballinger Professor of Nuclear Engineering and Materials Science and Engineering
Thesis Reader :	Michael J. Driscoll Professor Emeritus of Nuclear Engineering

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CHAPTER • 1

Introduction

Environmentally assisted cracking of structural material in high temperature aqueous systems has been of significant concern in the power industry for some time. A particular type of environmentally-assisted cracking of austenitic stainless steel, which has occurred predominantly in BWRs, is known as intergranular stress corrosion cracking (IGSCC). IGSCC has been known to occur only under the following three necessary conditions: (1) sensitized microstructure, i.e., chromium depletion at the grain boundaries during welding; (2) over yield tensile stress; and (3) oxygenated (200 ppb) high temperature (288 °C) water [Gordon 1987]. Therefore, removing any of these three conditions will prevent IGSCC, extending the power plant life and increasing availability.

While the local crack environment is the controlling variable in crack propagation, the bulk environment has a significant influence in IGSCC as a boundary condition. This is especially true in the case where neutron and gamma radiation results in radiolysis of the water which, in turn, has a strong influence on the electrochemical potential. As a result of water radiolysis, liquid-vapor phase equilibrium and recirculation, the coolant in the BWR recirculation line contains 150 to 300 ppb of oxygen. It has been found that reducing the oxygen level to 1 to 10 ppb, which results in a decrease in the electrochemical potential to < -230 mV (SHE), can effectively eliminate IGSCC in austenitic stainless steels. Based on prior work in the laboratory and at reactors, it was determined that the oxygen concentration can effectively be reduced by the use of hydrogen and that IGSCC can be stopped. This prompted the development of a water chemistry model that is capable of predicting the necessary level of hydrogen to effectively suppress the oxygen level.

A radiolysis code MITIRAD was developed at MIT by Scott Simonson in 1988 to predict the environmental chemistry of underground nuclear waste packages. MITIRAD was a suitable starting point to carry out this project of developing a BWR water chemistry simulator . In the present work, a new radiolysis model was derived from species balances in a two-phase flowing control volume. New sets of differential equations have been derived which include such effects as chemical reactions, radiolytic generation, and thermalhydraulic effects. These contributions are described by chemical reactions between species, generation by radiolysis, decomposition of H_2O_2 by wall contact, mass transfer between liquid and gas phases, and convection. The model is capable of predicting the evolution of water radiolysis products as well as the effect of metal-ion species reactions.

In addition, the model is unique in its incorporation of a sensitivity analysis; the sensitivity of results with respect to small variations of input parameters is analytically calculated. This is a much more efficient and exact way of observing the response of the output to the change of the input compared to conventional parametric studies. This is a very valuable tool in evaluating the quantitative importance of data; this is especially true in BWR radiolysis calculations since most of the input parameters are not accurately known under the high-temperature, high-pressure conditions pertinent to BWR operations. Sensitivity analysis results may be used in guiding parameter selections; it becomes clear which parameters play a key role, thus these parameters should be more carefully evaluated experimentally.

Water chemistry simulation and sensitivity analysis have been implemented through a FORTRAN code RADICAL (RADIation Chemistry Analysis Loop code). The code takes input parameters, such as a chemical reaction matrix, radiolytic data, thermalhydraulic conditions, *etc*. and runs a differential equation solver which returns calculated concentrations as a function of position within various components of the BWR. The sensitivity analysis is also included in the code as a separate routine from the water chemistry calculations. RADICAL has been developed with versatility in mind, such that it not only works well for BWR water chemistry, but it is also applicable to other situations as well. For instance, RADICAL has been successfully used in PWR shutdown chemistry studies and in simulations of the BWR corrosion chemistry loop (BCCL), an experimental loop at MIT.

Modeling is an approximation of nature. This is normally carried out by defining a system of interest, analysis of the system, and development of a mathematical description of the system. Aside from philosophical questions, modeling nature completely is impractical and unnecessary for an engineer; hence many simplifying assumptions are made in a modeling process, so that the model is as simple as possible, while all important effects are accounted for. Modeling of radiation chemistry is no exception to this rule; no attempt of perfecting the science (or rather the art) of radiation chemistry has been made. In fact, the present model is a first-step approach and there is room for many improvements. The significance of this thesis is in development of a BWR water chemistry code which is available to everyone of interest and the incorporation of the sensitivity routines which have been unavailable until now. With proper improvements to the code, RADICAL should become a valuable tool in water chemistry studies.

CHAPTER • 2

BWR Water Chemistry

High purity water of neutral pH is used in BWRs as the coolant and neutron moderator. As the coolant flows through the regions with gamma and fast-neutron radiation fields, e.g. the core region, the water molecule decomposes into various species:

$$H_2O \ \text{--->}\ e^-_{aq}, H^+, H, OH, O, HO_2, H_2, H_2O_2$$

This phenomenon is called *radiolysis* and has an important effect on the coolant chemistry throughout the entire reactor. Most of these species are radicals and go through a number of rapid chemical reactions which eventually lead to the final production of stable species such as H_2 and O_2. As the coolant flows away from the high-radiation regions into the downcomer region, there is a significant concentration of dissolved O_2 in the coolant generated by both chemical reactions along the path and thermal and metal-catalyzed decomposition of H_2O_2. This high concentration of O_2 is known to set up an environment that causes intergranular stress corrosion cracking (IGSCC) of austenitic stainless steel components in the recirculation system. One method of mitigating IGSCC is to lower the oxygen concentration in the entire coolant system by adding hydrogen in the feedwater. This method, which is called hydrogen water chemistry (HWC) or hydrogen-alternate water chemistry (HAWC), has been proven not only to prevent IGSCC but also to arrest further cracking in already-initiated cracks [Gordon 1987] (Fig 2-1).

As an aid in the characterization of HWC, analytical models that attempt to calculate bulk concentrations of chemical species can play a valuable role. Due to high-temperature

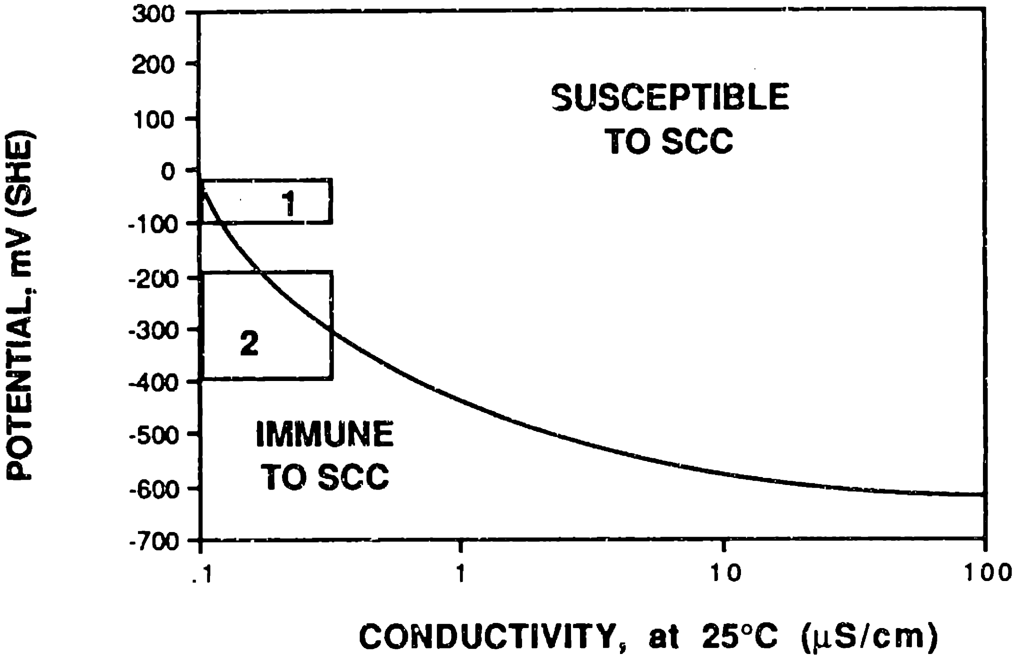

Figure 2-1 Typical stress corrosion cracking susceptibility curve with bulk and crevice regions of electrochemistry defined: (1) conditions in bulk solution with normal water chemistry; (2) conditions in bulk solution with hydrogen water chemistry.

and high-pressure, in combination with the high-radiation environment of BWRs, chemistry measurements are extremely difficult in most components under the operating conditions of BWRs , and thus analytical models are an essential tool for materials protection analysis and HWC evaluation.

Although accurate input data are necessary for simulations to be realistic, water chemistry simulations have suffered greatly from lack of reliable data. As mentioned before, actually measured parameters are scarce and their credentials are low. Often times some input parameters have to be estimated or adjusted to make the output fit to some known values.

There are two kinds of input parameters that are subject to uncertainties. The first kind is fundamental physical/chemical parameters that are relevant to radiolysis. These include g-values, chemical reactions, activation energies, and rate constants. These parameters can be determined with laboratory experiments and equally applied to all BWRs. The second kind of parameters are BWR plant specific. For instance, thermal power level, flow velocity, energy deposition rate, and residence time are unique for each BWR and its operating conditions. These parameters affect radiolysis through their thermalhydraulic characteristics. Unfortunately no complete set of input parameters are available for all of the above variables, and simulation models, hence results, are therefore subject to the discretion of the person running the simulator.

I. Previous Work in Water Chemistry Modeling

With the advent of the modern computer technology, a number of water chemistry simulators have been developed worldwide in the past two decades. Beginning with the WR20 which was developed by Schmidt of Argonne National Laboratory in 1970, various simulators using various mathematical algorithms have been introduced (see Table 2-1).

SIMFONY, AQUARY and FACSIMILE have been recently applied to BWR water chemistry studies, particularly to HWC simulations [Ibe, et al. 1986, 1987; Ruiz, et al.

Table 2-1 Development of Water Chemistry Simulators [Ibe and Uchida 1985]

Program Name	Publication Information	Principal Mathematical Method
WR20	Schmidt (1970)	5-th order Adams Bashforth Formulas
CHEK	Burns and Moore (1976)	Backward differentiation formulas (BDF)
FACSIMILE	Burns and Moore (1978)	• BDF combined with nonlinear algebraic equations • Sparse matrix routine
MAKSIMA	Boyd et al. (1979)	BDF with sparse matrix routine
AQUARY	Ibe and Uchida (1982)	Iterative procedures with BDF for a set of differential-integral equations
SIMFONY	Ibe and Uchida (1983)	• Extension of AQUARY • BDF
RADIOLYSIS MODEL	Takagi, et al. (1988)	• BDF

1989]. Although these simulations have yielded quantitative results, only qualitative interpretations have been given due to the uncertain nature of the parameters available and the lack of physical insights.

RADICAL, the code developed for the present study, utilizes an efficient mathematical solver package LSODE. LSODE was developed by Hindmarsh of Lawrence Livermore National Laboratory as a general tool in solving simultaneous nonlinear ordinary differential equations [Hindmarsh 1981, 1983; Painter 1981]. The thermalhydraulic derivations used in RADICAL are similar to those of SIMFONY.

II. G-Values

A quantitative measure of radiolysis is given by g-values which are the number of particular species produced by 100 eV of energy deposited by radiation. Each radiolysis product has its associated g-values for gamma and fast-neutron radiation. Though conceptually simple, actual measurement of such short-lived radical concentrations under BWR operating conditions is very difficult, and thus the g-values have been one of the major sources of uncertainties in radiolysis modeling. When experimental g-values are reported, only the g-values of the stable species O_2, H_2, and H_2O_2 are actually measured; then the g-values of radicals, e^-_{aq}, H^+, H, OH, O, O_2^-, HO_2 are calculated from a mass balance. Another difficulty is the temperature dependence of g-values. There are some confusing and conflicting reports on the temperature dependence of g-values [Ruiz 1989; McCracken 1990]. Gamma radiation and fast-neutron radiation seem to show a different temperature dependence. Among many sets of published g-values, those values by Burns [1976] and Christensen [1982] seem to be in wide use and both sets of values were used in the present study. McCracken has also provided recently reported g-values for gamma radiation which clearly show temperature dependence [Elliot, Chenier 1990]. McCracken suggested using the room temperature g-values for fast neutrons by Burns and his high-temperature g-values for gamma in BWR water chemistry modeling [1990] . Published g-values are sum-

Table 2-2 Summary of G-values [Ibe 1989].

Species	g-value (#/100eV)						
	Neutron			Gamma			
	A	B	C	A	B	C	D
e^-_{aq}	0.93	0.4	0.37	2.7	0.4	2.8	4.15
H^+	0.93	0.4	0.37	2.7	0.4	2.8	4.15
H	0.5	0.3	0.36	0.62	0.3	0.55	1.08
H_2	0.88	2.0	1.2	0.43	2.0	0.45	0.62
H_2O_2	0.99		0.97	0.62		0.72	1.25
HO_2	0.04		0.17	0.03			
OH	1.09	0.7	0.46	2.9	0.7	2.7	3.97
O		2.0			2.0		
-H2O	3.12	2.7	2.8	4.2	2.7	4.21	6.47

A : Burns' values for room temperature [1976].
B : Burns' values for elevated temperatures (300-410 °C) [1976].
C : Christensen's values based on Forsmark-2 [1982].
D : Elliot's values for elevated temperature (300 °C) [Elliot, Chenier 1990].

marized in Table 2-2. Mason performed numerous parametric studies on g-values which showed wide variations in calculated concentrations [1990].

III. Chemical Reactions

In RADICAL, a set of chemical reactions acts as a guide for chemical species; it tells the chemical species how to react with other species and result in some other species. A reaction consists of three parts: (1) reaction mechanism showing reactants and products; (2) rate constant which tells how fast a reaction proceeds; (3) activation energy which tells how difficult it is for a reaction to occur. All three parts should be known precisely to create a good reaction matrix for RADICAL.

Table 2-3 A Reaction Set Used in BWR Water Chemistry Simulations. See Appendix E for complete listing of various reaction sets [Simonson 1988].

CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES

	REACTIONS							RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
	Reactants			Products					
W 1	e-	H20		>H	OH-			0.16D+02	0.13D+02
W 2	e-	H+		>H				0.24D+11	0.13D+02
W 3	e-	OH		>OH-				0.24D+11	0.13D+02
W 4	e-	H2O2		>OH	OH-			0.13D+11	0.13D+02
W 5	H	H		>H2				0.10D+11	0.13D+02
W 6	e-	HO2		>HO2-				0.20D+11	0.13D+02
W 7	e-	O2		>O2-				0.19D+11	0.13D+02
I 1	H20	H20		>2H20				0.10D+01	0.00D+00
W 8	e-	e-	2H20	>OH-	OH-	H2		0.16D+07	0.13D+02
W 9	OH	OH		>H2O2				0.45D+10	0.13D+02
W10	OH-	H		>e-	H20			0.20D+08	0.19D+02

As radiolytic species are produced in regions with radiation, they quickly recombine to form stable species, and this is reflected in a reaction set. Reaction sets are usually given at room temperature and the rate constants are scaled using the Arrhenius law:

$$k = k_o \exp\left[\frac{E_a}{\mathrm{R}}\left(\frac{1}{T_o} - \frac{1}{T}\right)\right]$$

where k : rate constant
E_a : activation energy
R : the universal gas constant
T : temperature in kelvin

As in g-values, there are a number of reaction sets available, and the choice makes a difference. Again, the rule of thumb is to use the set of reactions that best describe actual plant chemistry measurements. Table 2-3 illustrates a reaction set used in BWR simulations. Mason also performed parametric studies on a number of reaction sets which, as for g-values, showed wide variations [1990].

Nitrogen chemistry has become an important consideration in HWC, partly due to

N-16 carry-over, i.e., hydrogen addition drives the formation of ammonia gas (NH_3), which evaporates radioactive N-16, and which transports through the steam line to the environment [Ibe 1989]. Although nitrogen chemistry is not considered in this thesis, it may be easily included in RADICAL by adding the nitrogen reaction set in Appendix E.

IV. Plant Operating Parameters

For each BWR, there is a unique set of parameters that describe the BWR unit's operating characteristics. These include thermalhydraulic parameters and the radiation profile. These parameters influence radiolysis directly and indirectly.

In RADICAL, temperature, flow velocity, pressure, void fraction profile, relative flowrate, and density are important thermalhydraulic parameters. Dose profile for both gamma and neutron radiation along the coolant flow path has to be input. This, along with the maximum dose rates, determines how much energy is deposited in the coolant through radiation, and this quantity is multiplied by g-values to give the number of radiolytic species produced.

It must be repeated that some of the plant-specific parameters are not precisely

Table 2-4 Reactions Involving Iron. See Appendix E for complete listing of reaction sets. [Simonson 1988].

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-------------------------------------------------------------------------------

      CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES

-------------------------------------------------------------------------------

                    IRON REACTIONS                            RATE  ACTIVATION
                                                           CONSTANT  ENERGIES
      Reactants                  Products                            (KJ/MOL-K)

F 1 FE2+     OH          >FE3+    OH-                     0.57D+09  0.13D+02
F 2 FE2+     e-          >FE+                             0.55D+11  0.13D+02
F 3 FE+      OH          >FEOH+                           0.70D+09  0.13D+02
F 4 FE+      H2O2        >FE2+    OH-      OH             0.13D+03  0.13D+02
F 5 FE+      O2-         >FE2+    OH-      OH      H2O2   0.88D+09  0.13D+02
-------------------------------------------------------------------------------
```

known. At the moment, dose shapes for both gamma and neutron radiation are the least known quantities. Since these affect radiolysis directly, this introduces significant uncertainties in simulation results. Often radiation levels are 'fit' to come up with a reasonable output.

V. Effects of Metal Impurities

Besides pure water species, the coolant contains impurities such as copper, iron, and zinc which dissolve from reactor materials. The overall chemistry of the coolant may be altered significantly by the presence of these impurities [Ruiz 1989]. The effect of these metallic species may be accounted for by including reactions involving these species. However, not enough data is available at the moment to interpret the effects quantitatively. Table 2-4 illustrates a possible reaction set involving iron impurities. More reaction sets involving other metallic species are listed in Appendix E.

CHAPTER • 3

Description of the BWR

Boiling water reactors (BWRs) comprise approximately 30% of the nuclear power reactors currently in use worldwide. BWRs operate with a reactor vessel pressure of approximately 6.9 MPa (1000 psia), at 300 °C (545 °F). Since the steam which drives the turbine is produced in the reactor vessel, BWRs do not require the secondary steam generator loop required by pressurized water reactors (PWRs). This simplifies the design and increases the heat transfer efficiency. The disadvantage, however, is that the steam,

Table 3-1 Design Parameters for BWR Reactor Vessel [Rust 1979].

Base Material	Low Alloy Steel
Cladding Material	Stainless Steel
Design Pressure	1250 psig (8.6 MPa)
Design Temperature	575 °F (302 °C)
Operating Pressure	1040 psia (7.2 MPa)
I. D.	238 in (6.0 m)
Wall Thickness, min./max.	5.7 in./6.46 in. (14 cm/16 cm)
Height	71 ft. (22 m)
Number Recirculation Loops	2
Number of Jet Pumps	20
Recirculation Line Pipe Sizes, I. D.	24 in. (61 cm)
Recirculation Pump Flow	35,400 GPM
Number of Steam Separators	263
Steam Separator Pressure Drop	7.3 psi (50 kPa)
Flow per Separator	3.99×10^5 lb/hr
Vessel Exit Steam Quality	99.6 %
Vessel Weight	975 tons

which has passed through the reactor core, is itself radioactive; thus additional shielding for the piping and turbines is required.

Typical design parameters for a BWR reactor vessel are given in Table 3-1, and thermalhydraulic characteristics for a General Electric BWR/6 are summarized in Table 3-2.

Table 3-2 BWR Core Geometry and Thermalhydraulic Characteristics-BWR/6 [Rust 1979].

Thermal Output	3579 MWt
Active Height	148 in. (3.76 m)
Equivalent Active Diameter	144 in. (3.66 m)
Height/Diameter	1.03
Active Core Volume	2260 ft^3 (64 m^3)
Average Core Power Density	1580 kW/ft^3 (55.8 W/cc)
Fuel Weight	138,000 kg
Specific Power	25.9 kW/kgU
Burnup	27,500 MWD/MTU
Number of Fuel Assemblies	732
Fuel Element Array	8 x 8
Assembly Dimensions	5.52 in. x 5.52 in. (14.0 cm x 14.0 cm)
Assembly Pitch	6.0 in. (15 cm)
Number of Fuel Rods/Assembly	62
Total Number of Fuel Rods	45,384
Fuel Rod O. D.	0.493 in. (1.25 cm)
Fuel Rod Pitch	0.64 in. (1.6 cm)
Pitch/Diameter	1.3
Clad Thickness	0.034 in. (0.86 mm)
Fuel Pellet Diameter	0.416 in. (1.06 cm)
Pellet-Clad Gap	0.0045 in. (0.11 mm)
Fuel Enrichment	2.2-2.7 %
Pellet Density % Theoretical	~ 94 %
Fission Gas Plenum Length	12 in. (30 cm)
System Pressure	1040 psia (7.2 MPa)
Coolant Flow	1.05×10^8 lb/hr
Core Inlet Enthalpy	527.9 Btu/lb
Average Exit Quality	14.6 %
Core Average Void Fraction	42.6 %
Maximum Exit Void Fraction	76 %
Average Inlet Velocity	7.1 ft/sec (216 cm/sec)
Core Pressure Drop	25.9 psi (179 kPa)
Average Linear Heat Rate	6.0 kW/ft (0.2 kW/cm)
Maximum Linear Heat Rate	13.4 kW/ft (0.4 kW/cm)
Average Heat Flux	159,000 Btu/hr-ft^2
Maximum Heat Flux	354,000 Btu/hr-ft^2
Minimum CHFR	> 1.9
Inlet Temperature (Feedwater)	420 °F (216 °C)
Core Inlet Temperature	532 °F (278 °C)
Outlet Temperature	547 °F (286 °C)
Maximum Fuel Temperature	~ 3500 °F (1900 °C)

I. Primary Region of the BWR

The primary focus of this thesis is the coolant flow within the BWR pressure vessel. This region is divided into the core, upper plenum, steam/liquid separator, mixing plenum, downcomer, jet pump, and lower plenum regions. The core region is subdivided into a boiling region along the fuel channel, and a bypass region between the fuel bundles where boiling does not occur. The operating characteristics of each of these regions are quite distinct, and in modeling, attention must be given to each region separately, after

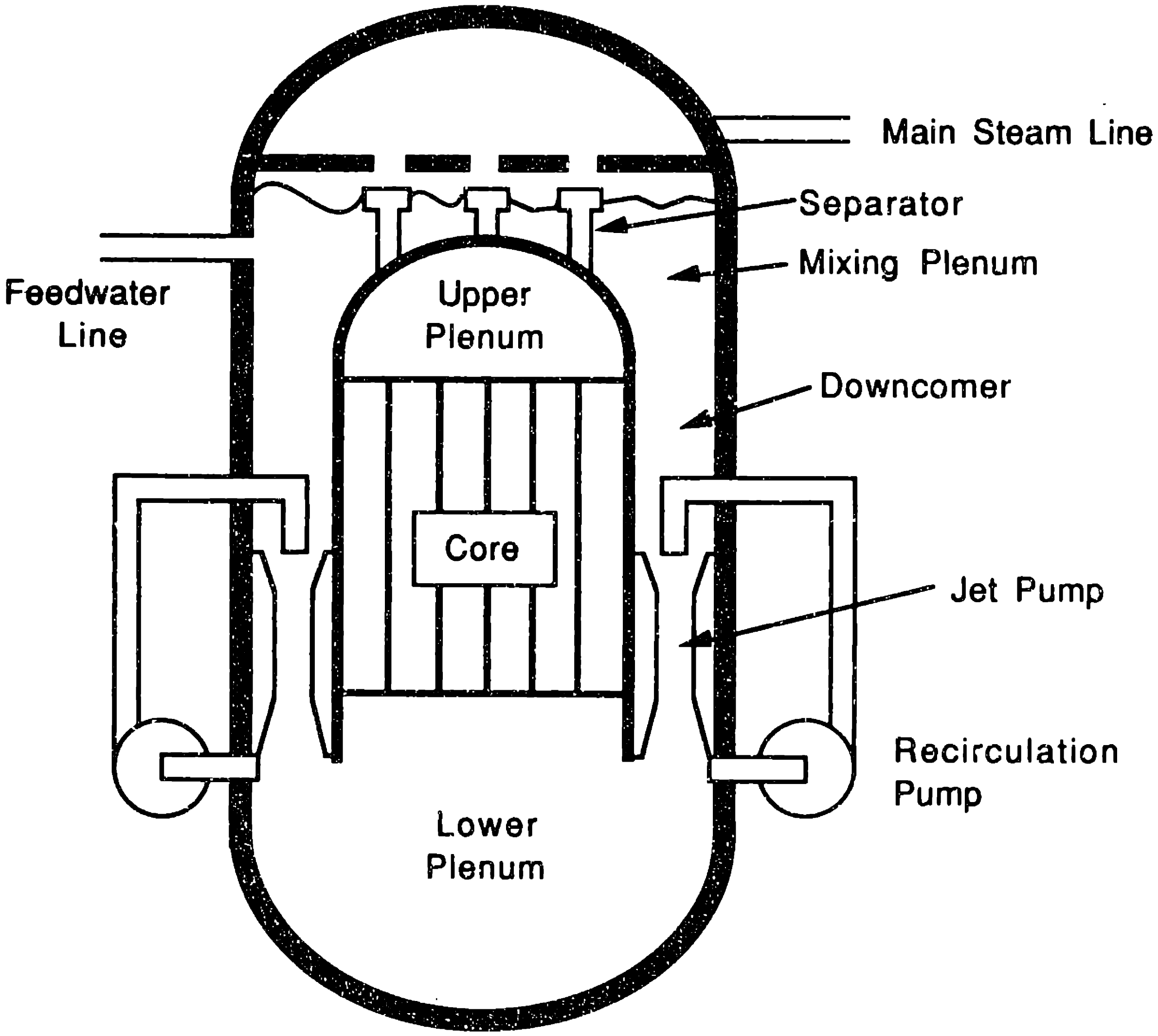

Figure 3-1 BWR Reactor Vessel

which they are combined into a loop.

II. BWR Coolant Flow Path

The flow pattern of the BWR primary region is, beginning with the feedwater inlet:

1. The feedwater is fed into the reactor vessel;
2. The feedwater is mixed with liquid in the mixing plenum;
3. The coolant flows into the downcomer region and through the jet pump;
4. A fraction of the coolant flow is fed into the recirculation line while the rest of the coolant emerges at the lower plenum and is fed into the core;

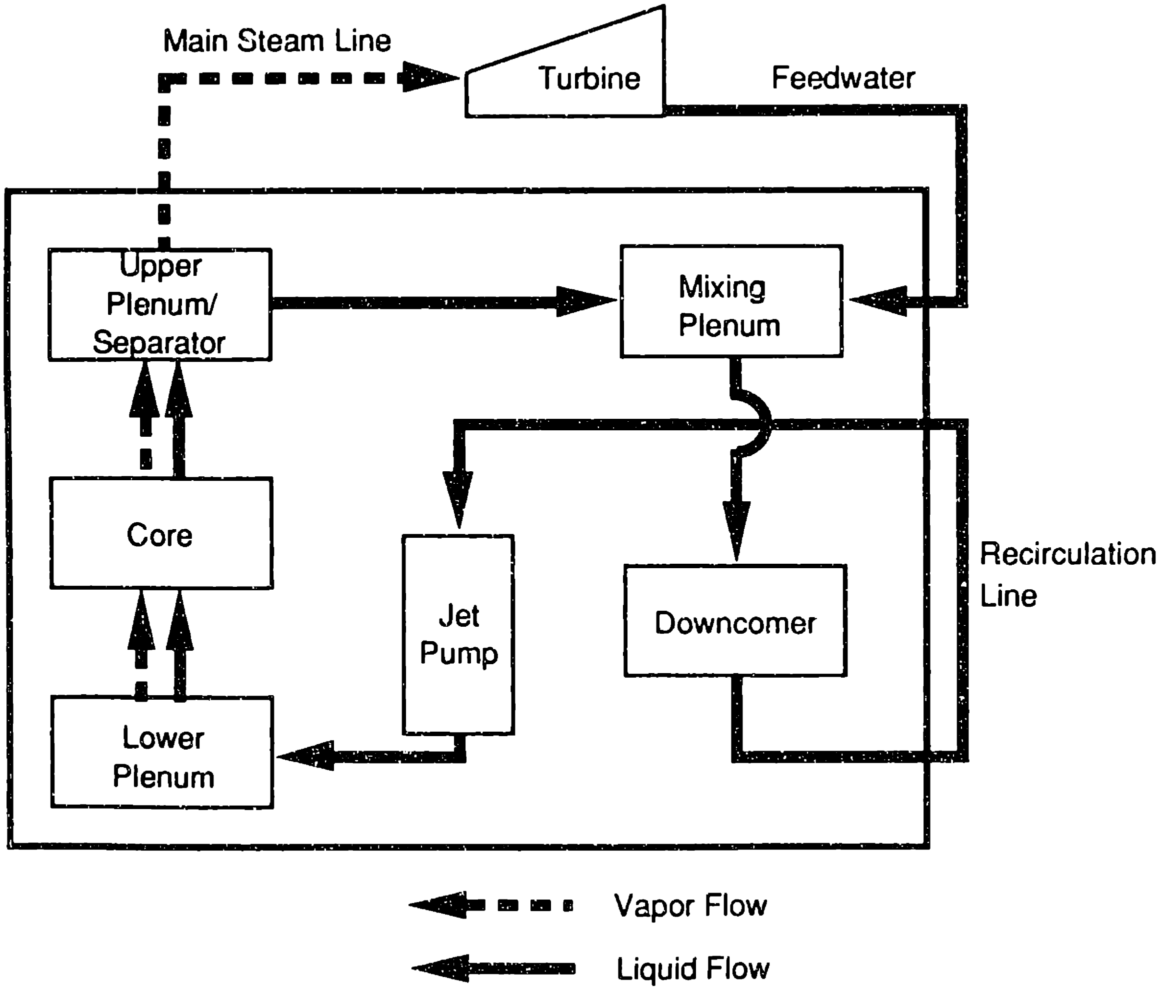

Figure 3-2 Schematic diagram of the coolant flow in the BWR pressure vessel. The boxed region is the pressure vessel.

5. A fraction of the coolant flow goes through the boiling fuel channel and turns into a two-phase mixture of steam and liquid. The rest of the coolant flow entering the core goes through the bypass region between the fuel bundles, where the temperature of the coolant rises but does not reach the boiling point.
6. Flow from the core boiling region and the core bypass region emerges at the upper plenum, where the steam and liquid are separated by the separator.
7. The steam emerges from the reactor vessel, and is fed into the turbines. The separated liquid returns to the mixing plenum, where it mixes with the feedwater... and the whole cycle repeats.

CHAPTER • 4

Theoretical Modeling of BWR Water Chemistry

Species balance equations of a differential volume element are derived for a two-phase flow system. These differential equations, which represent the change of concentrations as a function of position, dC/dx, serve as the basis of the radiolysis model.

I. Concentration Equation Derivation

To accurately account for the generation and annihilation of chemical species involved in radiolysis, molar balance equations were derived for a steady-state system using a control-volume approach (instead of the control-mass approach used by Ibe). In general, the mass balance for a radiolysis model of a two-phase flow system is given in terms of:

- Generation by chemical reactions
- Annihilation by chemical reactions
- Generation by radiolysis (i.e., gamma and neutron radiation)
- Convection
- Mass transfer between liquid and vapor phase.

One has the choice of writing the set of differential equations with respect to time (dC/dt where C = concentration of species in mole/liter) or space (dC/dx).* Space and time are related simply by the velocity of the coolant, for a single phase under uniform flow.

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* For instance, see p. 11 of *Fluid Mechanics* by White [1979] which describes Eulerian and Lagrangian descriptions of fluid motion.

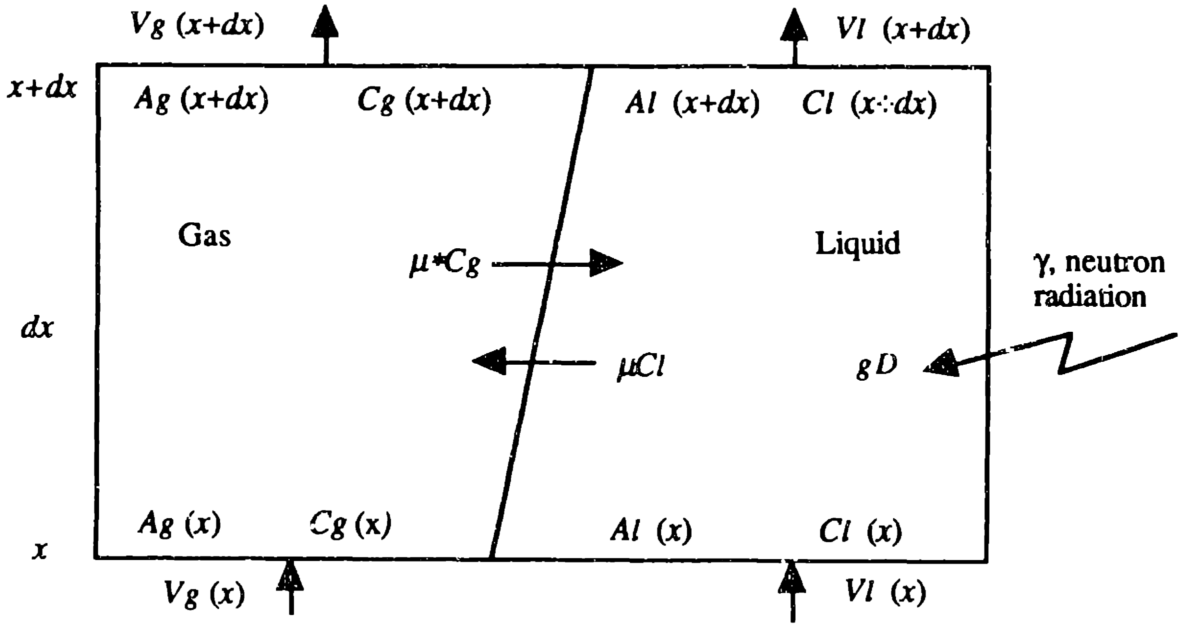

Figure 4-1 Two-phase species balance in a differential volume element.

However, for two-phase flow (e.g. in the core boiling region), the vapor phase and liquid phase flow at different velocities and the two phases develop a slip. If a time axis is used for derivation, liquid and vapor would be in different positions at a given time; this causes a considerable complication. In this respect, spatial derivation seemed to be a more appropriate choice since one is interested in spatial concentration profiles for water chemistry studies, and this eliminates the confusion caused by the slip. A differential volume element of two-phase flow used in balance equation derivations is depicted in Fig. 4-1.

The overall species balance for the liquid phase in a control volume at steady state is written as

$$\begin{aligned}\frac{d\left[C_i^l(x)\,A_l(x)\,dx\right]}{dt} &= A_l(x)dx\left[\overset{\text{chemical rx}}{\sum_{j=1}^{NRX} KOEF_{ji}\,k_j\prod_{m=1}^{3} C_{mi}^l(x)} + \overset{\text{generation by radiation}}{g_i\,Gc\,D}\right]\\ &+ C_i^l(x)V_l(x)A_l(x) - C_i^l(x+dx)V_l(x+dx)A_l(x+dx) \qquad \text{convection}\\ &+ A_g(x)dx\left[\,\mu_i^* C_i^g(x) - \mu_i C_i^l(x)\,\right] \qquad \text{gas-liquid transport}\\ &= 0 \end{aligned} \qquad (4.1)$$

where $C_i^l(x)$: concentration of i-th species in liquid phase at x (mol/l)
$A_l(x)$: cross-sectional area of liquid at x (cm^2)
NRX : number of chemical reactions
$KOEF_{ji}$: reaction coefficient of j-th reaction for i-th species
= 1 if i-th species is the first-order product in j-th reaction
= 2 if i-th species is the second-order product
=-1 if i-th species is the first-order reactant
=-2 if i-th species is the second-order reactant
k_j : rate constant for j-th reaction (liter/mol-s for a first-order reaction)
g_i : g-value of i-th species (#/100 eV), *ie.*, the number of molecules created by 100 eV of radiation (only one type of radiation is shown for simplicity).
Gc : g-value conversion factor from #/100 eV to mol/l-Rad
D : dose rate (Rad/s)

Expanding the convection term at $x + dx$ using a Taylor series and neglecting second and higher order terms,

$$C_i^l(x+dx)V_l(x+dx)A_l(x+dx)$$

$$\cong\left[C_i^l(x) + \frac{\partial C_l^i}{\partial x}dx\right]\left[V_l(x) + \frac{\partial V_l}{\partial x}dx\right]\left[A_l(x) + \frac{\partial A_l}{\partial x}dx\right]$$

$$= C_i^l(x)V_l(x)A_l(x) + C_i^l(x)V_l(x)\frac{\partial A_l}{\partial x}dx + C_i^l(x)A_l(x)\frac{\partial V_l}{\partial x}dx$$

$$+ V_l(x)A_l(x)\frac{\partial C_l^i}{\partial x}dx \tag{4.2}$$

Substituting Eq. (4.2) into Eq. (4.1) and rearranging gives

$$\boxed{\begin{aligned}\frac{d\,C_i^l(x)}{dx} = \frac{1}{V_l(x)}\Bigg\{ & \sum_{j=1}^{NRX} KOEF_{ji}\,k_j \prod_{m=1}^{3} C_{mi}^l(x) + g_i\,Gc\,D \\ & + \left[\mu_i^* C_i^g(x) - \mu_i C_i^l(x)\right]\frac{V_f(x)}{1 - V_f(x)} - C_i^l(x)\frac{\partial V_l}{\partial x} + \frac{C_i^l(x)V_l(x)}{1 - V_f(x)}\frac{\partial V_f(x)}{\partial x}\Bigg\}\end{aligned}} \tag{4.3}$$

The following relationship between the cross-sectional area and the void fraction were used in the above derivation:

$$\begin{aligned}
V_f(x) &= \frac{A_g(x)}{A_o} = \frac{A_o - A_l(x)}{A_o} = 1 - \frac{A_l(x)}{A_o} \\
A_l(x) &= [1 - V_f(x)]\, A_o \\
A_g(x) &= \frac{V_f(x)}{1 - V_f(x)} A_l(x) \\
\frac{\partial A_l(x)}{\partial x} &= -A_o \frac{\partial V_f(x)}{\partial x} \\
\frac{\partial A_g(x)}{\partial x} &= +A_o \frac{\partial V_f(x)}{\partial x}
\end{aligned} \tag{4.4}$$

For the gas species, the same species balance is used, except chemical reaction and radiolysis terms are neglected. Since the density of the vapor and therefore the radiation energy absorbed per unit volume is about one-twentieth that for the liquid, the radiolysis contribution in the gas phase is negligible [Ruiz 1989]. Proceeding as in the liquid-phase case the final form of the species balance for the vapor phase gives

$$\boxed{\begin{aligned}
\frac{dC_i^g(x)}{dx} = \frac{-1}{V_g(x)} \Bigg\{ & \left[\mu_i^* C_i^g(x) - \mu_i C_i^l(x) \right] + \frac{C_i^g(x) V_g(x)}{V_f(x)} \frac{\partial V_f(x)}{\partial x} \\
& + C_i^g(x) \frac{\partial V_g(x)}{\partial x} \Bigg\}
\end{aligned}} \tag{4.5}$$

Eqs. (4.3) and (4.5) completely describe the radiolysis of a two-phase flow system and are used as the basis of RADICAL. Detailed analysis of each mechanism is described below.

II. Chemical Reactions

In Eq. (4.1) the term

$$\sum_{j=1}^{NRX} KOEF_{ji}\, k_j \prod_{m=1}^{3} C_{mi}^l(x) \tag{4.6}$$

describes chemical reactions. This is a compact way of writing conventional chemical kinetics; e.g., consider the reaction

$$A + B \rightarrow C + D \tag{4.7}$$

The kinetics for the species C (i.e., generation of C) may be written as

$$\frac{d\,[C]}{dt} = k\,[A]\,[B] \tag{4.8}$$

where k is the rate constant for the reaction. For the species A, the kinetics for annihilation of A is written as

$$\frac{d\,[A]}{dt} = -\,k\,[A]\,[B] \tag{4.9}$$

Notice that the equations are the same, except for the sign, which depends on whether the species under consideration is a reactant or a product . Because of the ingenious way of keeping track of reactants and products by the coefficient *KOEF*, this single term Eq. (4.6) keeps track of both generation and annihilation of chemical species [Simonson 1988]. The product is carried out over all reactants and the summation is carried out over all reactions.

Chemical reactions are the dominant cause of concentration changes where the radiation level is low so that generation by radiation is negligible. Chemical reactions are described by writing out a standard chemical reaction equation with reactants and products. Each reaction is coupled with the reaction rate constant and the activation energy. There is a serious lack of precise high-temperature rate constants. This is especially true for BWR operating conditions, which involve high temperature (about 300 °C) and high pressure (about 6.9 MPa). Some researchers have reported a set of proposed reactions and rate constants specifically for BWR operating conditions, but there are some variations in these reported values [Burns 1976; Simonson 1988; Ibe 1986]. As mentioned earlier, there is no particular advantage of using one set over the other; the rule of thumb is to select a reaction set that best describes known results and apply it with discretion on a case-by-case basis.

Rate constants are adjusted for temperature using the Arrhenius law. Temperature gradients are assumed to be linear and at each position all rate constants are re-evaluated to reflect the proper temperature change.

Reaction sets are reported with H_2O either explicitly or implicitly declared. The implicit case assumes that H_2O concentration does not change over all positions and the density-corrected concentration of H_2O is multiplied into the rate constant. Therefore some reactions do not formally balance, but this does not introduce errors in actual computations. The explicit case declares H_2O explicitly in reactions. Both cases are equivalent, but this point should be kept in mind if one is to properly adjust rate constants. In RADICAL, *dC/dx* for H_2O is forced to zero, so that the water concentration is always kept constant.*

In RADICAL, up to three reactants and four products are accepted for each reaction and only up to second-order kinetics is considered. For instance,

```
A      A      C      >D      E      E      F
```

is acceptable but

```
X      X      X      >Y      Z
```

is not acceptable (X is third order).

---

* This is true as far as the way RADICAL is programmed. In some simulations, however, water concentration has been observed to change slightly and the cause has been traced to the internal calculations of LSODE. The error has not been fixed, but it should not introduce a significant problem.

III. Radiolysis

In Eq. (4.1) the term

$$g_i\,Gc\,D$$

accounts for radiolysis. Radiolysis is the production of chemical species by energetic radiations. For instance H_2O irradiated with gamma and fast neutrons dissociate into a number of radicals and stable species such as e^-_{aq}, H^+, H, OH, O, HO_2, H_2, and H_2O_2. Only water radiolysis is considered in BWR water chemistry modeling. How many of these species are created per unit of radiation energy is described by g-values, defined as the number of molecules produced by 100 eV of gamma or neutron irradiation. Though g-values are input in terms of #/100 eV, they are converted to mol/l-Rad for calculations inside RADICAL.

Both gamma and neutron radiations contribute to radiolysis. The dose rate of each of these radiations is input as polynomial functions of position within each component of the BWR. The polynomials may be of any order.

IV. Convection

The concentration gradient of the coolant in a two-phase flow is accounted for by the convection terms

$$C_i^l(x)V_l(x)A_l(x) - C_i^l(x+dx)V_l(x+dx)A_l(x+dx)$$

in Eq. (4.1). These terms state the time rate of change of concentration in the control volume due to the concentration gradient, velocity gradient, and the change of the cross-sectional area (Fig. 4-1). These terms are also valid for single-phase flow where the velocity and area remain uniform and only the concentration gradient is present. In RADICAL, the changes of coolant velocity and cross-sectional area are considered only for two-phase flow as a consequence of the void-fraction; these changes due to physical variation of the pipe diameter, e.g. flow through a horn-shaped flow channel, are not considered.

V. Mass Transfer Between Liquid and Vapor Phases

As the coolant goes through the boiling region, gas species are formed. Most of the volume in the gas phase is occupied by water vapor. In addition, hydrogen and oxygen gases are formed by mass transfer between the liquid and gas phases, which is expressed by the term

$$A_g(x)dx\left[\ \mu_i^* C_i^g(x) - \mu_i C_i^l(x)\ \right]$$

in Eq. (4.1). Gas release and absorption coefficients, μ_i^* and μ_i, are used to account for the mass transfer from the liquid phase to the gas phase and vice versa. Quantitative description of nucleation and boiling is quite complex and only a brief, simplified analysis, as used by Ibe [1985] is given below.[*]

As boiling starts to occur, bubbles are formed. Let's define the local gas release rate r_i from the liquid phase in the small differential volume of $S_O dx$ as

$$r_i = S_c(\ \phi_i - \phi_i^*\ ) \tag{4.10}$$

where r_i : local gas release rate from liquid to vapor phase through surface area S_c in small volume $S_O dx$ of liquid vapor mixture (mol/s)
S_c : sum of bubble surfaces in volume $S_O dx$ (cm^2)
ϕ_i : flux of i-th species from liquid to vapor (mol/s-cm^2)
ϕ_i^* : reverse flux of i-th species (mol/s-cm^2)
S_O : cross-sectional area of flow channel (cm^2)
x : distance from bottom of channel (cm)

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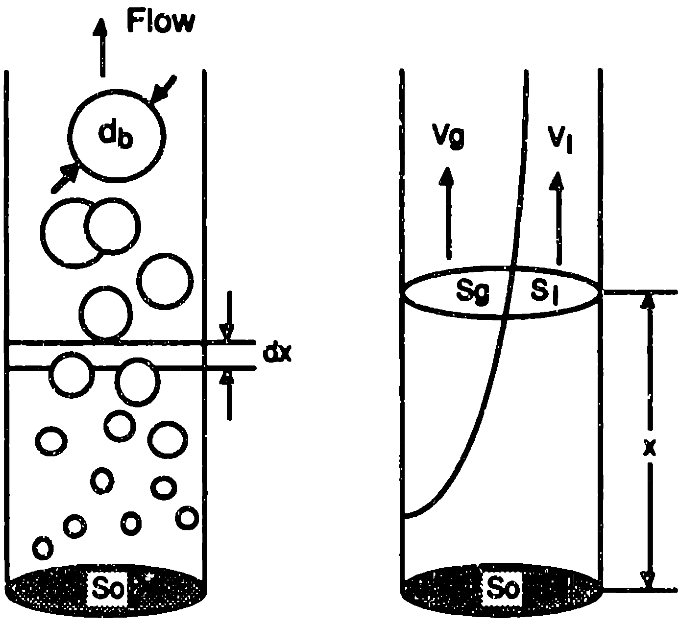
[*] See also *Nuclear Systems I* by Todreas and Kazimi [1990] for in-depth analyses of two-phase flow.



(a) Bubble Model (b) Separate Flow Model

Figure 4-2 Gaseous mass transfer models in boiling flow channel.

Assuming a uniform bubble diameter d_b, S_c is expressed as

$$S_c = \frac{6\,V_f}{d_b} S_0 dx \tag{4.11}$$

where V_f : void fraction

d_b : bubble diameter (cm)

The fluxes ϕ_i and ϕ_i^* are expressed by

$$\phi_i = k_i\,(C_i^l - C_i^{l+}) \tag{4.12}$$

$$\phi_i^* = k_i^*\,(C_i^v - C_i^{v+}) \tag{4.13}$$

where k_i, k_i^* : mass transfer coefficients of i-th species (s^{-1})

C_i^{l+} : concentration of i-th species in liquid at surface of bubbles (mol/l)

C_i^v : concentration of i-th species in bulk vapor phase (mol/l)

C_i^{v+} : concentration of i-th species in vapor phase at bubble surfaces (mol/l)

Since an exact evaluation of C_i^{l+} and C_i^{v+} is impractical, Ibe introduces proportional constants α and β and writes them as

$$C_i^{l+} = \alpha\, C_i^l \tag{4.14}$$

$$C_i^{v+} = \beta\, C_i^v \tag{4.15}$$

Then

$$r_i = S_o\, dx\, V_f\,(\, \mu_i C_i^l - \mu_i^* C_i^v\,) \tag{4.16}$$

where

$$\mu_i = \frac{6}{d_b}(\, k_i - \alpha\,)$$

$$\mu_i^* = \frac{6}{d_b}(\, k_i^* - \beta\,)$$

Since the local gas release rate r_i must equal the reduction rate of concentration in the liquid phase,

$$(\, 1 - V_f\,)\, S_o\, dx \frac{dC_i^l}{dt} = r_i = S_o\, dx\, V_f\,(\, \mu_i C_i^l - \mu_i^* C_i^v\,) \tag{4.17}$$

Rearranging

$$\frac{dC_i^l}{dt} = \frac{V_f}{1 - V_f}(\, \mu_i C_i^l - \mu_i^* C_i^v\,) \tag{4.18}$$

where μ_i : gas release coefficient for i-th species (s^{-1})
μ_i^* : gas absorption coefficient for i-th species (s^{-1})
C_i^v : concentration of i-th species in vapor phase (mol/l)

which is the form used in Eqs. (4.3) and (4.5).

Finally the gas release and absorption coefficients should be evaluated. These coefficients along with other physical constants, as suggested by Ibe, are tabulated in Table 4-1.

Table 4-1 Physical Constants Applied to BWR Water Radiolysis Simulation [Ibe 1985].

Henry's law constants, H [mol (kg H_2O)$^{-1}$/atm)]	
H_2	31.14×10^{-4}
O_2	50.62×10^{-4}
Gas release factor, μ (s^{-1})	
H_2	30
O_2	23
Gas absorption factor, μ^* (s^{-1})	
H_2	9.9
O_2	12.4
Specific volume (m^3/kg)	
Water	0.00135
Vapor	0.0276

VI. Void Fraction and Velocity Slip

As the coolant starts boiling, the void fraction starts increasing, and as a result, the net cross sectional area of the liquid phase decreases. This in turn increases the liquid velocity in keeping with the mass flowrate. The gas phase also flows faster as more bubbles are formed. This introduces velocity slip and convection which affect the concentrations of chemical species. The flow velocities of both the liquid and gas phases increase after the onset of boiling and they travel at different speeds at a given position; the difference between the two velocities is expressed in terms of the slip ratio. Slip ratio is the ratio between the liquid and gas velocities and it is a function of void fraction.

Assuming the heat flux distributes along the boiling channel in a cosine function and neglecting subcooled boiling, steam quality q can be expressed as

$$q = \begin{cases} 0 & (x < x_b) \\ \dfrac{q_t}{2h_{fg}} - \dfrac{h_f - h_i}{h_{fg}} - \dfrac{q_t}{2h_{fg}} \cos\left(\dfrac{\pi x}{h_L}\right) & (x \geq x_b) \end{cases} \tag{4.19}$$

where q_t : total heat added in channel = $h_f + q_e h_{fg} - h_i$ (kcal/kg)

h_f : enthalpy at channel exit (kcal/kg)
h_i : enthalpy at inlet (kcal/kg)
h_{fg} : latent heat (kcal/kg)
q_e : exit quality
h_L : length of channel (cm)
x_b : distance of boiling inception point from channel inlet

$$= \frac{h_L}{\pi} \cos^{-1}\left(\frac{h_i + q_e h_{fg} - h_f}{h_f + q_e h_{fg} - h_i}\right)$$

Once the quality profile is found, the two-phase flow model is described in terms of void fraction V_f and slip ratio S_l using Bankoff's equation:

$$V_f = \frac{K}{1 - \frac{\rho_g}{\rho_l}\left(1 - \frac{1}{q}\right)}$$

$$S_l = \frac{V_g}{V_l} = \frac{1 - V_f}{K - V_f} \tag{4.20}$$

$$A_g = V_f A_o$$

$$A_l = A_o - A_g$$

where K : flow parameter = $0.71 + 0.00143P$
P : pressure (atm)
ρ_l : density of liquid (g/cc)
ρ_g : density of vapor (g/cc)
A : corss sectional area (cm^2)
A_o : cross sectional area of the channel (cm^2) = $A_g + A_l$
V_0 : inlet velocity of liquid phase (cm/s)

From a mass balance

$$\rho_g V_f V_g + \rho_l (1 - V_f) V_l = \rho_l V_o \tag{4.21}$$

where V_o : Initial liquid velocity at channel inlet (cm/s)

Then

$$V_l = \frac{\rho_l V_o}{\rho_g V_f S_l + \rho_l (1 - V_f)} \tag{4.22}$$

$$V_g = S_l V_l \tag{4.23}$$

These equations completely describe the thermal-hydraulic condition of the BWR core. From these equations the differential equations describing radiolysis concentrations are evaluated. This means, for each component in the BWR primary region, the following operating conditions adequately describe the necessary parameters of radiolysis.

- Coolant Velocity
- Effective Length (actual physical length or calculated from residence time and coolant velocity)
- Void fraction profile (determined from Inlet and Outlet Enthalpy, Latent Heat, and Exit Quality)
- Pressure
- Density of Liquid and Vapor
- Temperature
- Radiation Level

These operating parameters are unique for each BWR and should be collected for each BWR being simulated.

VII. Decomposition of H_2O_2

Though stable at room temperature, hydrogen peroxide decomposes quickly at the operating temperatures of BWRs. The decomposition may be simply thermal, or this process may be catalyzed heterogeneously by metal surfaces and homogeneously by metal particles or ions in the coolant. H_2O_2, along with its decomposed counterpart O_2, creates an oxidizing environment in the coolant and its behavior is of considerable importance in water chemistry studies [Outwater 1990].

In RADICAL, H_2O_2 decomposition is accounted for by including a decomposition reaction with the pipe-diameter dependent rate constant suggested by Lin [1989]. The reaction is

$$2H_2O_2 \text{ ---> } O_2 + 2H_2O$$

Table 4-2 Estimated H_2O_2 Decomposition Rate Constants at 280 °C and Activation Energies in High-Purity Water [Lin 1989].

Reaction Chamber	Rate Constant at 280 °C (sec^{-1})	Activation Energy (Kcal/mol)
304 SS, 1/2" O.D.	0.15	15
304 SS, 1/4" O.D.	0.3	15-18
Titanium, 1/4" O.D.	0.3	16
Teflon, 0.13" I.D.	0.002	16-26
Teflon, 0.32" I.D.	0.003	14-16

Decomposition rates for various wall materials are summarized in Table 4-2. Decomposition experiments for stainless steel tubing were carried out at MIT recently, and they confirmed Lin's results [Mason 1990].

CHAPTER • 5

Computer Simulation of BWR Water Chemistry

Once the formulation of radiolysis equations is completed, the equations must be converted to a suitable form for computer calculations. In general, there are N simultaneous differential equations to solve, where N is the number of species under consideration. With the advent of fast and efficient computing tools, solving such simultaneous differential equations has become a routine task in engineering.

A standard, nonlinear differential equation solver LSODE developed by Hindmarsh at Lawrence Livermore National Laboratory is used in RADICAL [Hindmarsh 1983]. It uses Gear's method of solving a system of differential equations. The solver package is versatile, fast and almost transparent to the main routine of RADICAL. LSODE is used as a blackbox; parameters are input and the results are received by the main routine of RADICAL. Internal workings of LSODE go unnoticed by the main routine of RADICAL except when LSODE flags for an error condition; then LSODE writes the error message to the output file.

I. RADICAL Implementation of Radiolysis

RADICAL prepares the parameters necessary for radiolysis calculations from an input file. When all parameters are ready, RADICAL calls LSODE and requests solution of the concentration equations. For LSODE to know which equations it is supposed to solve, an external subroutine is prepared by RADICAL and passed to LSODE. The generic name for this subroutine is FRO and it contains the radiolysis differential equations developed in Chapter 4.

RADICAL marches through the coolant flow path and calculates the concentration of species at an interval specified by the input file. At each interval RADICAL updates all information and prepares new parameters. Then it calls LSODE which returns new calculation results. This process repeats until the calculation is completed.

For more detail, see the Appendices to this thesis, which contain the source listing of RADICAL along with the documentation.

II. Jacobian Derivation

Along with the differential equations in FRO, the Jacobian of the equations is input to LSODE. This is not a required input since LSODE is capable of evaluating the Jacobian internally, but providing a user-specified Jacobian speeds up calculations.

The Jacobian of $\frac{\partial C_i}{\partial x}$ is defined as $\frac{\partial}{\partial C_k}\left(\frac{\partial C_i}{\partial x}\right)$ where the subscripts i and k span all species. For the liquid phase the Jacobian of the concentration equation (4.5) is

$$
\begin{aligned}
\frac{\partial}{\partial C_k}\left(\frac{\partial C_i^l(x)}{\partial x}\right) = \frac{1}{V_l(x)}\Bigg\{ & \sum_{j=1}^{NRX} KOEF_{ij}\, k_j \frac{\partial}{\partial C_k} \prod_{m=1}^{3} C_{im}^l(x) \\
& + \frac{\partial}{\partial C_k}\left[\mu_i^* C_i^g(x) - \mu_i C_i^l(x) \right] \frac{V_f(x)}{1 - V_f(x)} \\
& - \frac{\partial C_i^l(x)}{\partial C_k}\left[\frac{\partial V_l}{\partial x} + \frac{V_l(x)}{1 - V_f(x)} \frac{\partial V_f(x)}{\partial x} \right]\Bigg\} \\
& \equiv \mathrm{Jac}\left(C_i^l,\, C_k \right)
\end{aligned}
\tag{5.1}
$$

where

$$\frac{\partial C_i^l(x)}{\partial C_k} = \begin{cases} 0 & \text{if } i \neq k \\ KOEF_{ii} & \text{if } i = k \end{cases}$$

Similarly, for the gas phase the Jacobian is

$$\frac{\partial}{\partial C_k}\left(\frac{\partial C_i^g(x)}{\partial x}\right) = \frac{-1}{V_g(x)}\left\{\frac{\partial}{\partial C_k}\left[\mu_i^* C_i^g(x) - \mu_i C_i^l(x)\right]\right.$$

$$\left. + \frac{\partial C_i^l(x)}{\partial C_k}\left[\frac{\partial V_g}{\partial x} + \frac{V_g(x)}{V_f(x)}\frac{\partial V_f(x)}{\partial x}\right]\right\}. \tag{5.2}$$

CHAPTER • 6

Sensitivity Analysis

A unique feature of RADICAL is its incorporation of a sensitivity analysis along with radiolysis calculations. This feature enables the user to determine which of the input parameters has the most significant influence on a particular concentration under examination. This not only serves as a quantitative guide in understanding the physical mechanism of radiolysis subject to a number of controlling variables, but also helps in reduction of many input parameters to a handful of the most significant ones; this helps the experimentalist in determining which parameters should be more carefully measured. Since most of the available parameters for water chemistry studies are hardly precise, the sensitivity analysis will prove itself to be a handy tool in the development of more reliable water chemistry simulators.

Among many numerical methods for sensitivity analysis for a system of equations, a straight-forward method of *adjoint* implementation given by Piepho [1981] is used in RADICAL. This method requires evaluation of the adjoint of the radiolysis equations, which in turn is used in evaluation of *response* equations. These response equations give the sensitivity of the concentration of a species under examination with respect to a number of input parameters. Therefore the sensitivity routine requires two sections; the first routine evaluates the adjoint using a backward integration of the concentration profile and the second routine evaluates the response from the concentration and adjoint profiles. LSODE is used in evaluating the integrals of the adjoint and response functions. This means we should derive not only the appropriate adjoint and response functions but also the Jacobian of these functions to be used in the numerical integration by LSODE. In the following sections, detailed derivations of these equations are shown step-by-step.

I. Sensitivity Derivation

This section gives a detailed derivation of the sensitivity equations, *ie.*, adjoint and response functions, as given by Piepho [1981] and adapted by Simonson [1988]. Time-dependence in the original derivations is converted to spatial-dependence.

A. Derivation of Importance Functions

Adjoint or importance theory in this context assumes a set of model equations in the form of ordinary differential equations (ODEs):

$$\frac{dC_i}{dx} = f_i\,(C, x, \eta) \tag{6.1}$$

where C : variables of interest
η : parameters of interest
x : position

The response functions for this system are defined, in general form, as

$$R = \int_0^{x_f} L\,(C, x, \eta)\,dx \tag{6.2}$$

where L : response function of interest. In this case L is defined as $L \equiv \frac{dC_{sens}}{dx}$
η : parameters
x_f : final position

This implies that

$$\dot{R} = L\,(C, x, \eta) \quad \text{with } R(0) = 0 \tag{6.3}$$

It is of interest to know how a change in the model will affect the response variable. The differential change in response is defined using the following definition:

$$\delta R = \sum_{i=1}^{n} C_i^*(x')\, \delta C_i' \tag{6.4}$$

where C_i^* : importance function associated with the i-th variable C_i
$\delta C_i'$: momentary change in C_i at x'

The following analysis provides a means of evaluating the importance functions and also the overall response to change in the model. Let the momentary change in one or more of the variables be denoted by

$$C_i(x) = \begin{cases} C_{io}(x) & x < x' \\ C_{io}(x) + \delta C_i' & x = x' \\ C_{io}(x) + \delta C_i(x) & x > x' \end{cases} \tag{6.5}$$

where one or more of the $\delta C_i'$ are non-zero at $x = x'$. We assume that the changes in the variables are small relative to the variable itself; therefore, the original system, Eq. (6.1), can be expanded in a Taylor series about the unperturbed value C_0, neglecting higher order terms of the series, to obtain

$$\frac{dC_{io}(x)}{dx} + \frac{d[\,dC_i(x)]}{dx} = f_i(C_o) + \left.\frac{\partial f_i}{\partial C_k}\right|_{C_o(x)} \delta C_k(x) \tag{6.6}$$

A summation over the index k is also not shown but should be assumed. Subtracting (6.1) from (6.5) gives

$$\frac{d[\,dC_i(x)]}{dx} = \left.\frac{\partial f_i}{\partial C_k}\right|_{C_o(x)} \delta C_k(x) \tag{6.7}$$

where

$$\delta C_k(x) = C_i' \tag{6.8}$$

Applying the same small changes to the response function, (6.2), and neglecting summation over the index i for the moment yields

$$\delta R = \int_0^{x_f} \left.\frac{\partial L}{\partial C_i}\right|_{C_o(x')} \delta C_i(x')\, dx' \tag{6.9}$$

This can be rewritten as

$$\delta R = \int_0^x \frac{\partial L}{\partial C_i}\, \delta\, C_i(x')\, dx' + \int_x^{x_f} \frac{\partial L}{\partial C_i}\, \delta\, C_i(x')\, dx' \tag{6.10}$$

where x is arbitrary on the interval from 0 to x_f. Arbitrary changes to the system prior to x are duplicated by assuming that an appropriate momentary change $\delta\, C_i(x')$ is made to the system at x. Therefore, substituting the definition of (6.4), we get

$$\int_0^{x_f} \frac{\partial L}{\partial C_i}\, \delta\, C_i(x')\, dx' = C_i^*(x)\, \delta\, C_i(x) \tag{6.11}$$

Introducing this result into (6.10) and differentiating with respect to x yields

$$0 = \frac{\partial L}{\partial C_i}\, \delta\, C_i(x') + \frac{d}{dx}\left[\, C_i^*\, \delta\, C_i \,\right] \tag{6.12}$$

Substituting (6.7) and rearranging gives

$$0 = \delta\, C_i \left[\frac{\partial L}{\partial C_i} + \frac{dC_i^*}{dx} + \sum_{k=1}^{n} C_k^* \frac{\partial f_k}{\partial C_i} \right] \tag{6.13}$$

This equation must hold for the case of small, finite, changes in δC_i, therefore, the parenthetical portion of (6.13) must go to zero, *ie.*,

$$0 = \frac{\partial L}{\partial C_i} + \frac{dC_i^*}{dx} + \sum_{k=1}^{n} C_k^* \frac{\partial f_k}{\partial C_i} \tag{6.14}$$

This is then a set of ordinary differential equations in C_i^*, with the boundary condition such that

$$C_i^*(x_f) = 0 \tag{6.15}$$

This states simply that things that occur at x_f have no effect on the response of the system. This new system is solved backwards in position; hence the name of ‘adjoint’ theory is often given to this type of analysis.

B. Total Sensitivity

An important result that is derived from the calculation of the importance functions is the total sensitivity equation. This equation can be used to get the total relative change in a particular response due to a change in particular variables or parameters of the model. The derivation of total sensitivity starts by differentiating (6.2) with respect to some parameter of interest, say α, and applying the chain rule

$$\frac{dR}{d\alpha} = \int_0^{x_f} \left[\frac{\partial L}{\partial \alpha} + \frac{\partial L}{\partial C}\frac{dC}{d\alpha} \right] dx \tag{6.16}$$

In this case there is no loss of generality by using only one process variable, C, to perform the derivation; the final form will be generalized to an arbitrary number of variables. Using (6.14) to eliminate the $\partial L/\partial C$ term from (6.16) gives

$$\frac{dR}{d\alpha} = \int \frac{\partial L}{\partial \alpha} dx - \int \frac{\partial C^*}{\partial x}\frac{\partial C}{\partial \alpha} dx - \int C^* \frac{\partial f}{\partial C}\frac{dC}{d\alpha} dx \tag{6.17}$$

The first term gives the explicit sensitivity of the total sensitivity and should be straightforward to calculate. The second term is reduced to simpler terms by an integration by parts;

$$\begin{aligned}
- \int \frac{\partial C^*}{\partial x}\frac{\partial C}{\partial \alpha} dx &= - \int dC^* \frac{dC}{d\alpha} \\
&= - C^* \frac{dC}{d\alpha}\Big|_0^{x_f} - \left[- \int C^* d\left(\frac{dC}{d\alpha}\right) \right] \\
&= - C^* \frac{dC}{d\alpha}(x_f) + C^* \frac{dC}{d\alpha}(0) + \int C^* \frac{d}{dx}\left(\frac{dC}{d\alpha}\right) dx \\
&= C^* \frac{dC}{d\alpha}(0) + \int C^* \frac{df}{d\alpha} dx \\
&= C^* \frac{dC}{d\alpha}(0) + \int \left[C^* \frac{df}{d\alpha} + C^* \frac{df}{dC}\frac{dC}{d\alpha} \right] dx
\end{aligned}$$

The third term of (6.17) is equal and opposite to the last term in (6.18). Cancelling these terms and rearranging (6.17) yields the total sensitivity equation, now with summation over multiple variables

$$\frac{\delta R}{\delta \alpha} = \sum_{k=1}^{NSP} \left[C_k^*(0) \frac{dC_k(0)}{d\alpha} \right] + \int_0^{x_f} \left[\frac{\partial L}{\partial \alpha} + \sum_{k=1}^{NSP} \left(C_k^* \frac{df_k}{d\alpha} \right) \right] dx \tag{6.19}$$

The C_k^*'s are calculated from (6.13) and (6.14); L is known explicitly (or should be); f_k is determined in the forward calculation, (6.1); and α is arbitrarily chosen as one of the model parameters or one of the variables. The only difficulty may lie in the calculation of the initial effects of α on the variables, *ie.*, the $dC_k(0)/d\alpha$ term. In general, the expression for C_k is not known explicitly (we know only dC_k/dx explicitly), but for most cases of interest this quantity can be estimated. If α is chosen as the initial condition of a variable ($\alpha = C_i(0)$) then

$$\frac{dC_k(0)}{d\alpha} = \delta_{ik} = \begin{cases} 1 & \text{if } i = k \\ 0 & \text{if } i \neq k \end{cases} \tag{6.20}$$

where δ_{ik} is the Kronecker delta. In other cases, this quantity will have to be estimated if it is deemed to be important to the calculation.

II. Adjoint Derivation

The adjoint of the concentration equation is given as

$$\frac{dC_m^*}{dx} = -\frac{\partial}{\partial C_m}\left(\frac{dC_{sens}}{dx}\right) - \sum_{n=1}^{NSP} C_n^* \frac{\partial}{\partial C_m}\left(\frac{dC_n}{dx}\right)$$

$$= -\frac{\partial L}{\partial C_m} - \sum_{n=1}^{NSP} C_n^* \frac{\partial f_n}{\partial C_m}$$

where

$$L \equiv \frac{dC_{sens}}{dx} \quad \text{and} \quad f_n \equiv \frac{dC_n}{dx}$$

Using the Jacobian notation defined in the previous section where Jac $(a,b) \equiv \frac{d}{db}\left(\frac{da}{dx}\right)$, the adjoint is simply written as

$$\frac{dC_m^*}{dx} = -\,\text{Jac}\,(C_{sens}, C_m) - \sum_{n=1}^{NSP} C_n^*\,\text{Jac}\,(C_n, C_m) \tag{6.21}$$

The Jacobian of the adjoint is given simply by inspection of (6.21) as

$$\frac{\partial}{\partial C_p^*}\left(\frac{dC_m^*}{dx}\right) = \frac{\partial}{\partial C_m}\left(\frac{dC_p}{dx}\right) = -\,\text{Jac}\,(C_p, C_m)$$

Therefore the Jacobian of the adjoint is the transpose of the Jacobian of the concentration equation.

III. Response Derivation

In calculating the sensitivity of various parameters, we are measuring how the concentration function responds to a small change of a particular parameter. Mathematically the response of a function is defined as

$$R = \int_0^{x_f} L\,(C, x, \eta)\,dx \tag{6.22}$$

where L : response function of interest. In this case L is defined as $L \equiv \frac{dC_{sens}}{dx}$

η : parameters

x_f : final position

Differentiating (6.22) with respect to a particular parameter of interest α

$$\frac{\delta R}{\delta \alpha} = \sum_{a=1}^{NSP}\left[C_a^*(0)\,\frac{dC_a(0)}{d\alpha}\right] + \int_0^{x_f}\left[\frac{\partial L}{\partial \alpha} + \sum_{a=1}^{NSP}\left(C_a^*\,\frac{df_a}{d\alpha}\right)\right]dx$$

where delta is used in the place of an ordinary differential symbol to denote that we are taking an approximate differentiation of the response function. The first term on the right-hand side is the initial values of the response differential. In this study the initial values are assumed to be zero and only the integral portion of the response is evaluated. This yields the response differential of the form

$$\frac{\delta R}{\delta \alpha} = \int_0^{x_f} \left\{ \frac{\partial}{\partial \alpha}\left(\frac{dC_{sens}}{dx}\right) + \sum_{a=1}^{NSP} \left[C_a^* \frac{\partial}{\partial \alpha}\left(\frac{dC_a}{dx}\right)\right]\right\} dx \tag{6.23}$$

where we expanded L and f to show the concentration equations explicitly. The sensitivity is calculated by evaluating this integral.

Three sensitivity calculations are evaluated in RADICAL: sensitivities with respect to rate constants, g-values and hydrogen concentrations. The differentials of the concentration equation with respect to each of these parameters are

$$\frac{\partial}{\partial k_j}\left(\frac{d\,C_i^l\,(x)}{dx}\right) = \frac{1}{V_l(x)}\; KOEF_{ij} \prod_{m=1}^{3} C_{mi}^l(x) \qquad \text{Rate constant}$$

$$\frac{\partial}{\partial g_j}\left(\frac{d\,C_i^l\,(x)}{dx}\right) = \frac{1}{V_l(x)}\; Gc\, D\;\; \delta_{ij} \qquad \text{G-value}$$

where δ_{ij} is the Kronecker delta.

$$\frac{\partial}{\partial [H_2]}\left(\frac{d\,C_i^l\,(x)}{dx}\right) = \mathrm{Jac}\left(C_i^l, [H_2]\right) \qquad \text{Hydrogen}$$

Eq. (6.23) gives absolute sensitivity. Relative sensitivity is found by

$$\text{Relative Sensitivity} \equiv \frac{\alpha}{R} \times \frac{\delta R}{\delta \alpha}\,.$$

For example, the differential response of oxygen to hydrogen level in terms of absolute sensitivity is

$$\text{Absolute Response of } [O_2] \text{ to } [H_2] \equiv \frac{\delta\,[O_2]}{\delta\,[H_2]}$$

and the corresponding relative sensitivity is

$$\text{Relative Response of } [O_2] \text{ to } [H_2] \equiv \frac{[H_2]}{[O_2]} \times \frac{\delta\,[O_2]}{\delta\,[H_2]}$$

In the relative sensitivity calculation, the initial concentrations of H_2 and O_2 at the inlet of the component are used.

The Jacobian of the response function is zero, as can be seen immediately from Eq. (6.23).

CHAPTER • 7

Code Verification

RADICAL produces many numbers that would be meaningless unless the code performs desired calculations correctly. Because of the enormous amount of number-crunching and the presence of nonlinear, simultaneous differential equations, verifying the code manually, even for the simplest case of BWR water chemistry, would be nearly impossible. In fact, solving analytically just two of the simultaneous nonlinear differential equations used in RADICAL would be extremely difficult.

Three methods have been employed to check the results. The first verifies the chemical kinetics and sensitivity routines [Simonson 1988]. This method uses the Bateman equations, which describe the kinetics of a radioactive decay chain. These equations are analytically solvable, including the sensitivity equations. This method, however, does not check the thermalhydraulic routines.

The second method checks chemical kinetics routines more rigorously than the relatively simple tests used in the first method. An input file which describes the burning of a cesium flare was tested in the present work, and the results agreed exactly with Simonson's [1988].

The third method is more of a brute-force one. Mason developed a simulator MITIRAD using an earlier version of RADICAL for the BWR coolant corrosion loop (BCCL), which is an experimental project at the MIT Nuclear Laboratory [Mason 1990]. After the two simulators were completed independently, they were run simultaneously with various input files and the results were compared. Many bugs were found in both codes and were corrected until both codes yielded similar, physically reasonable results. This tested the radiolysis part of the code as well as the thermalhydraulics (MITIRAD does not have sensitivity analysis routines). Though many combinations of input parameters were tried in this test, the test is not fail-safe; the code is expected to be debugged further through continuous use.

The first verification method as described by Simonson is presented below.

I. Kinetics

A simple double-decay chain of parent, daughter, granddaughter nuclei is considered. The system is defined as

N_1 ---> N_2 rate = λ_1 = decay constant 1

N_2 ---> N_3 rate = λ_2 = decay constant 2

or in differential form, neglecting N_3,

$$\frac{dN_1}{dt} = -\lambda_1 N_1 \tag{7.1}$$

$$\frac{dN_2}{dt} = \lambda_1 N_1 - \lambda_2 N_2 \, . \tag{7.2}$$

Also assume that the initial value is N_{1o} for N_1 and zero for the rest. Solving these simultaneously gives

$$N_1(t) = N_{1o}\, e^{-\lambda_1 t} \tag{7.3}$$

Table 7-1 Kinetics Results for Analytic and RADICAL Calculations.

	Analytic Calculation	RADICAL Calculation
N_1	1.375	1.375
N_2	0.4298	0.4298

$$N_2(t) = \frac{\lambda_1 N_{1o}}{\lambda_2 - \lambda_1}\left[e^{-\lambda_1 t} - e^{-\lambda_2 t} \right] \tag{7.4}$$

The simulation results using RADICAL matches exactly with the hand-calculated results (Table 7-1). The time dependence of these equations is easily converted to position dependence for RADICAL by setting the velocity to 1 cm/s, thus 1 cm in simulation is 1 sec in the hand calculation. The following values were used for these calculations: $N_{1o} = 2.0$, $\lambda_1 = 0.01$, $\lambda_2 = 0.02$, $t = 37.5$ sec.

II. Adjoint

For the sensitivity analysis, we will find the response of N_2 with respect to the decay constants λ_1 and λ_2, which can be written as

$$\frac{dN_2}{d\lambda_1} \text{ and } \frac{dN_2}{d\lambda_2} \,. \tag{7.5}$$

The adjoint is given by Eq. (5.5) as

$$\frac{dC_m^*}{dx} = -\,\mathrm{Jac}\,(C_{sens}, C_m) - \sum_{n=1}^{NSP} C_n^*\,\mathrm{Jac}\,(C_n, C_m) \tag{7.6}$$

where x is now understood as t. Here, both m and n span from 1 to 2. The Jacobian is easily found by inspection of Eqs. (7.1) and (7.2).

Then the adjoint differential equations are

$$\frac{dN_1^*}{dt} = \lambda_1 + \lambda_1 N_1^* - \lambda_1 N_2^* \qquad N_1^*(t_f) = 0 \tag{7.7}$$

$$\frac{dN_2^*}{dt} = \lambda_2 + \lambda_2 N_2^* \qquad N_2^*(t_f) = 0 \tag{7.8}$$

where the initial values are assumed zero (since adjoints are evaluated backward in time, initial values for adjoints are in fact final values in concentration calculations). These equations are solved simultaneously, beginning with (7.8), by integrating from t_f to t:

$$N_2^*(t) = e^{-\lambda_2 (t_f - t)} - 1 \tag{7.9}$$

Table 7-2 Adjoint Results for Analytic and RADICAL Calculations.

	Analytic Calculation	RADICAL Calculation
N_1^*	0.2149	0.2149
N_2^*	-0.5276	-0.5276

$$N_1^*(t) = \frac{\lambda_1}{\lambda_2 - \lambda_1}\left[e^{-\lambda_1(t_f - t)} - e^{-\lambda_2(t_f - t)} \right] \tag{7.10}$$

These adjoints are hand-calculated and compared with RADICAL calculations in Table 7-2. The following values were used in the adjoint calculations: $t_f = 37.5$ sec, $t = 0$.

III. Total Sensitivity

The total sensitivity we want to find is the sensitivity of N_2 with respect to the decay constants, λ_1 and λ_2, which is expressed by Eq. (7.5):

$$\frac{dN_2}{d\lambda_1} \text{ and } \frac{dN_2}{d\lambda_2}\ . \tag{7.11}$$

This can be found directly from Eqs. (7.4) and (7.5) by differentiating with respect to the decay constants:

$$\frac{dN_2}{d\lambda_1} = \frac{N_{1o}\, e^{-\lambda_1 t_f}}{\lambda_2 - \lambda_1}\left[\left(1 + \frac{\lambda_1}{\lambda_2 - \lambda_1} \right)\left(1 - e^{-(\lambda_2 - \lambda_1) t_f} \right) - \lambda_1 t_f \right] \tag{7.12}$$

$$\frac{dN_2}{d\lambda_2} = \frac{\lambda_1 N_{1o}\, e^{-\lambda_2 t_f}}{\lambda_2 - \lambda_1}\left[\frac{e^{(\lambda_2 - \lambda_1) t_f} - 1}{\lambda_2 - \lambda_1} + \lambda_f \right] \tag{7.13}$$

Now, using the adjoint theory, the total sensitivity is given by Eq. (5.9) as

$$\frac{\delta R}{\delta \alpha} = \int_0^{t_f} \left\{ \frac{\partial}{\partial \alpha}\left(\frac{dC_{sens}}{dx} \right) + \sum_{a=1}^{NSP} \left[C_a^* \frac{\partial}{\partial \alpha}\left(\frac{dC_a}{dx} \right) \right] \right\} dx \tag{7.14}$$

Table 7-3 Sensitivity Results for Analytic and RADICAL Calculations.

	Analytic Calculation	RADICAL Calculation
$dN_2/d\lambda_2$	34.42	34.42
$dN_2/d\lambda_1$	-7.557	-7.557

Here $R = C_{sens} = N_2$ which is the response variable, $\alpha = \lambda_1$ and λ_2, and a spans from 1 to 2. Then the response equations are, expanding Eq. (7.14),

$$\frac{\delta N_2}{\delta \lambda_1} = \int_0^{t_f} \left\{ \frac{\partial}{\partial \lambda_1}\left(\frac{dN_2}{dt}\right) + N_1^* \frac{\partial}{\partial \lambda_1}\left(\frac{dN_1}{dt}\right) + N_2^* \frac{\partial}{\partial \lambda_1}\left(\frac{dN_2}{dt}\right) \right\} dt \tag{7.15}$$

$$\frac{\delta N_2}{\delta \lambda_2} = \int_0^{t_f} \left\{ \frac{\partial}{\partial \lambda_2}\left(\frac{dN_2}{dt}\right) + N_1^* \frac{\partial}{\partial \lambda_2}\left(\frac{dN_1}{dt}\right) + N_2^* \frac{\partial}{\partial \lambda_2}\left(\frac{dN_2}{dt}\right) \right\} dt \tag{7.16}$$

These can be integrated in closed form by substituting the kinetics equations, (7.1) and (7.2), and the adjoint equations, (7.9) and (7.10). The integration results in exactly the same expressions as found by direct differentiation (Eqs. (7.12) and (7.13)).

The calculated values are compared in Table 7-3.

CHAPTER • 8

Simulation Results

The primary function of RADICAL is to simulate the water chemistry of boiling water reactors (BWRs). To test the functionality of RADICAL and also to provide a tutorial on the steps involved in running the simulator, a series of simulations was performed for both normal water chemistry (NWC) and hydrogen water chemistry (HWC) on the Dresden-2 power plant. The Dresden-2 unit is one of the first BWRs where HWC experiments were performed and the coolant chemistry has been studied more extensively than other BWRs by Ibe [1986, 1987] and Ruiz [1989]. These study results also provided a benchmark against which the results of RADICAL could be checked.

It was unfortunate, however, that the plant specifications for Dresden-2 were not consistent among the published reports. Even some plant conditions reported by the same author were different in earlier and later publications (see, for example, the core residence time in Ibe's 1986 and 1985 papers). This can be best explained by the fact that water chemistry modeling and related parameter selections are constantly improving, and changes are brought about each time. The parameters for the simulations in this chapter have been extracted from both Ibe's and Ruiz's papers. Ibe's parameters were used for the most part, including the selection of chemical reactions and g-values. Dr. Robinson, one of the co-authors of Ruiz's report, of General Electric also provided a list of input parameters used in his simulations, which was cross-checked with Ibe's parameters. Great efforts have been made to reproduce the previous simulation results exactly, but this was complicated by the enormous number of input parameters and contradicting plant specifications. The qualitative behavior of the water chemistry, however, turned out strikingly similar.

Considering all these points , the significance of the simulation results in this chapter should be interpreted on a qualitative basis only. Better simulation results are expected when more precise operating conditions and water chemistry parameters are determined. Extensive parametric studies were not performed in the present study, but the sensitivity of certain parameters has been determined using the built-in sensitivity analysis routine in RADICAL. More extensive use of RADICAL may be made on a case-by-case basis as the need arises.

I. Operating Conditions of Dresden-2

The operating parameters for the Dresden-2 unit are given in the input and output files for RADICAL in Appendix E, and summarized in Table 8-1. The values in the files have been extracted from the reports by Ibe [1986] and Ruiz [1989]. When conflicting values were reported, an arbitrary judgment was made to determine which one to use, or an independent estimate was made to come up with reasonable values. Simulators in the past have used time increments, whereas RADICAL uses position increments. Thus in earlier simulators a residence time is used to characterize the coolant flow in each component of the primary region. On the other hand, in RADICAL, a component is characterized by its flow path length and velocity. If the flow geometry is not uniform, an effective length should be calculated which is consistent with the residence time.

Table 8-1 Dresden-2 Operating Conditions.

Thermal power (MWt)		2418
Liquid density (g/cc)		0.741
Vapor density (g/cc)		0.0362
Pressure (atm)		70.75
Core height (cm)		370
Onset of boiling from core inlet (cm)		66
Fraction of core coolant in channel		0.8934
Fraction of core coolant in bypass		0.1066
Upper plenum flowrate (arbitrary*)		1.105
Feedwater flowrate (arb.)		0.125
Fraction of upper & lower downcomer flow in region 1		0.31
Fraction of upper & lower downcomer flow in region 2		0.33
Fraction of upper & lower downcomer flow in region 3		0.30
Fraction of upper & lower downcomer flow in region 4		0.06
Component	Length (cm)	Inlet Velocity (cm/s)
Core boiling	370	150
Core bypass	370	19.22
Upper plenum	40	20
Mixing plenum	130	30.23
Upper downcomer	40	40
Lower downcomer	80	24.242
Recirc	130	30.23
Jet pump	200	100
Lower plenum	140	30.435
Temperature (k)	Inlet	Outlet
Core	552	558
Upper plenum	558	555
Feedwater	555	555
Mixing plenum	555	552
All others	552	552
Maximum energy deposition rate (Rad/s)	Gamma	Neutron
Core	$Q_g = 3.00 \times 10^5$	$Q_n = 4.17 \times 10^5$
Upper plenum & separator	$Q_g, Q_n/1000$	
Mixing plenum	$Q_g, Q_n/10000$	
Recirculation line	0	
Jet pump	$Q_g, Q_n/1000$	
Lower plenum	$Q_g, Q_n/1000$	
Upper & Lower downcomer 1	$Q_g \times 10^{-2}$	$Q_n \times 10^{-3}$
Upper & Lower downcomer 2	$Q_g \times 10^{-3}$	$Q_n \times 10^{-4}$
Upper & Lower downcomer 3	$Q_g \times 10^{-4}$	$Q_n \times 10^{-5}$
Upper & Lower downcomer 4	$Q_g \times 10^{-4}$	$Q_n \times 10^{-6}$

---

* Only the ratio of a flowrate to the total flowrate is used in RADICAL and the unit is unimportant.

The model circuit is illustrated in Figure 8-1. There are a total of 17 components in this model including the multi-layered downcomer regions. The Spacer (component no. 14) is a dummy component that is used to avoid an infinite loop around the recirculation line; this is necessary because of the way RADICAL handles inlet/outlet connections. Simulation begins at the inlet of the core region with initial concentrations for O_2, H_2 and

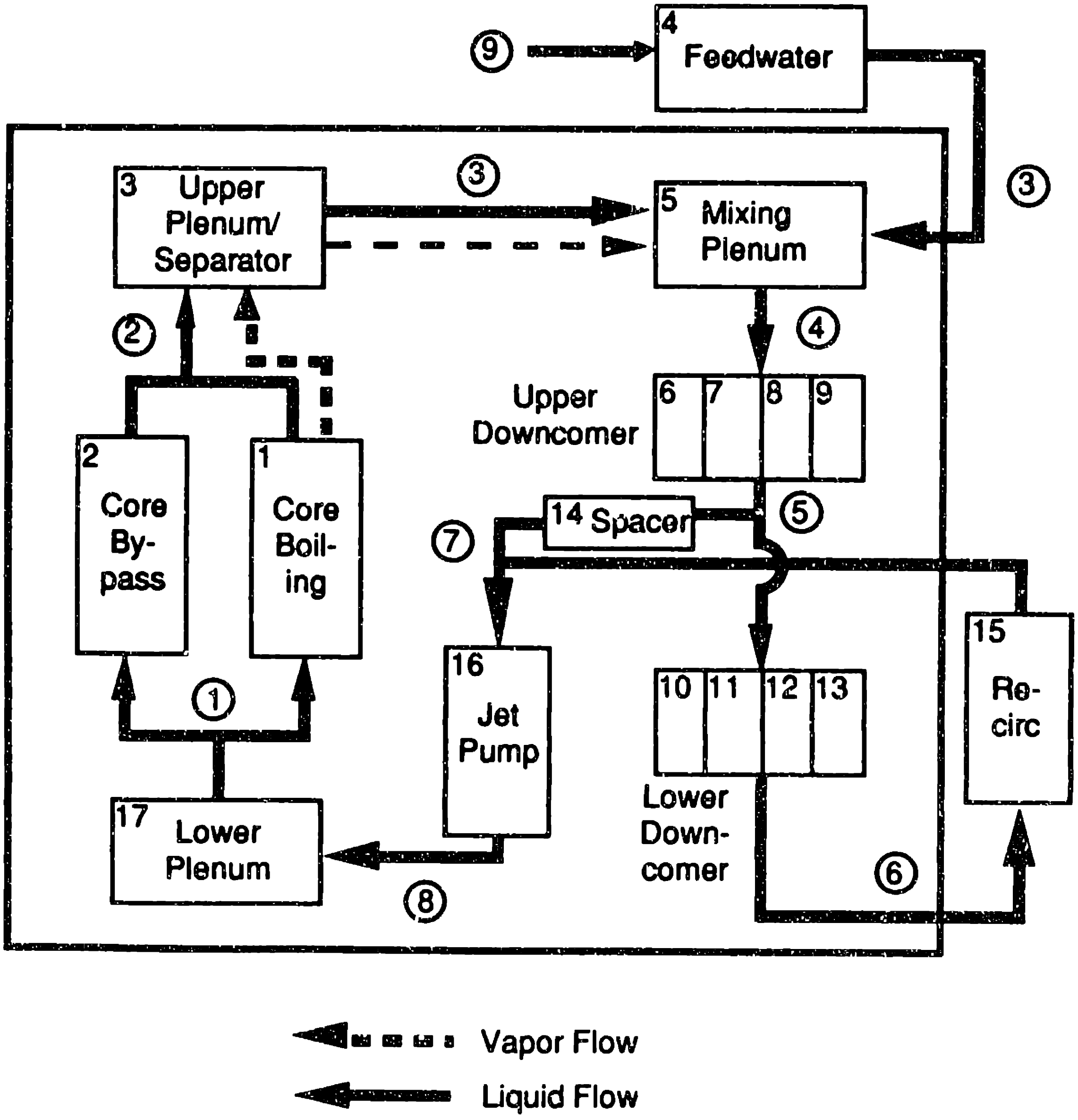


Figure 8-1 Schematic diagram of the primary region of the Dresden-2 power plant as simulated in this chapter. The circled numbers represent the node numbers as input into RADICAL. The numbers at the upper-left corner of each component are the component numbers.

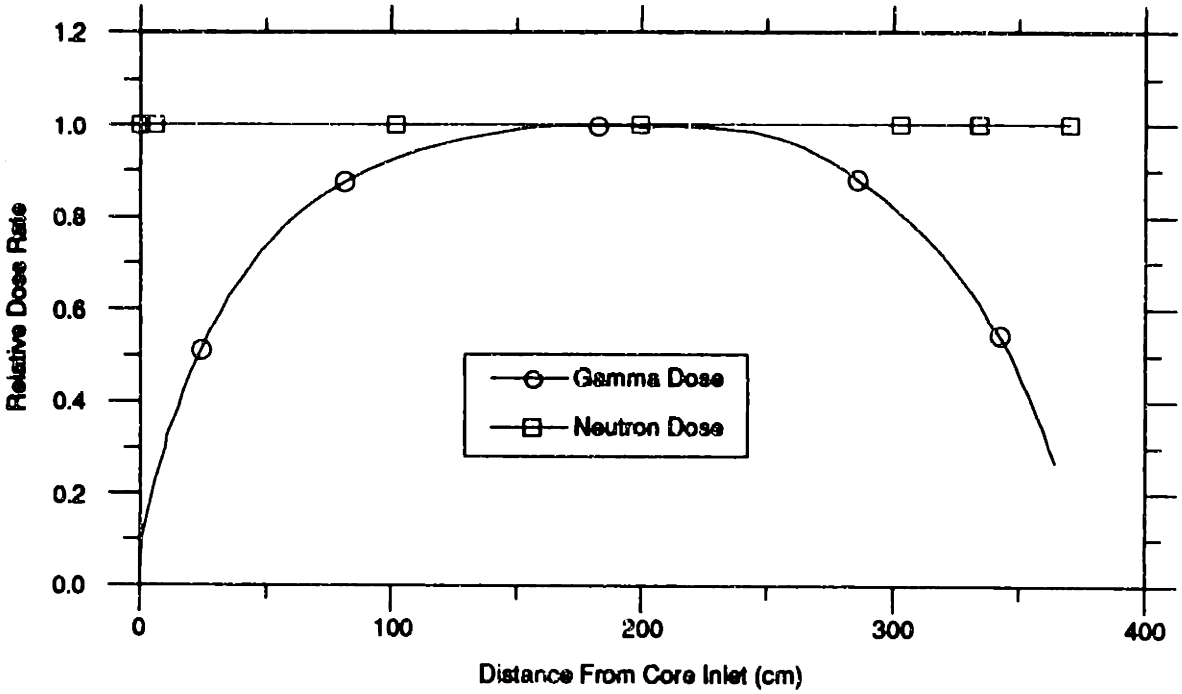


Figure 8-2 Dose rate profile of gamma and neutron radiation in the reactor core of Dresden-2. These profiles are multiplied by the doserate multipliers (GAMMARATE, NEUTRATE) to determine the actual dose rate at each point in the core.

H_2O_2 and proceeds along the circuit. When one complete cycle is made through the circuit, the process repeats one more cycle, this time with the calculated concentrations at the core inlet (these are the lower plenum exit concentrations). This repeated cycle helps better approximate the initial concentrations for radicals which are usually impractical to measure.

The core region is divided into two parallel components: the boiling channel and the bypass channel. The vapor phase is present only in the boiling channel, where the onset of boiling is specifically given in the input file (66 cm from the bottom of the core in this study). The bypass channel has a lower flowrate and the flow is single phase. The same doserate profile is used in both channels (see Fig. 8-2). These doserates are fit to 9-th order polynomials. At the exit of the core region, the concentrations are averaged by weighing them with respect to the flowrates and the average values are passed on to the upper plenum entrance.

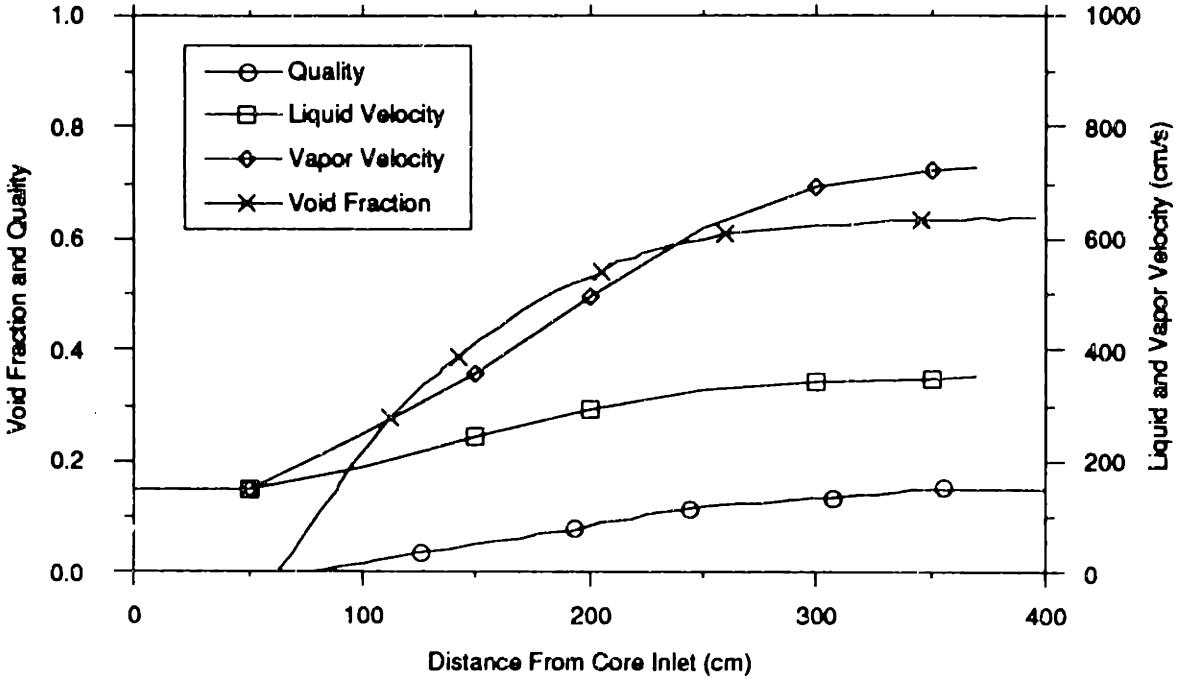


Figure 8-3 Void fraction and quality in the core boiling channel as obtained from the operating condition of Dresden-2. Liquid and vapor velocities are calculated from void fraction [Ibe 1985].

Void fraction in the core boiling region is also input through polynomial coefficients. Any arbitrarily ordered polynomial may be used to specify void fraction and doserates; in the present simulation, a 5-th order fit was used for void fraction. The liquid and gas velocities are calculated from void fraction through the slip ratio (see Fig. 8-3).

The carry-under in the separator is simulated by specifying negligible void fraction, which tapers off to almost zero in the mixing plenum. The feedwater inlet does two things: the concentrations in the separator are averaged with the concentrations from the feedwater; it also acts as a hydrogen injection point in HWC simulations. All HWC simulations use the same input file as NWC, except an appropriate H_2 concentration is specified in the feedwater inlet.

To illustrate the flexibility of RADICAL in laying out a circuit, a multi-layered downcomer is used in the simulation to better approximate the dose profile in the downcomer region. This approach was used by Ibe, and the same doserate values were used in the four-layered model in the present study. The downcomer region is also divided into upper and lower regions to simulate the partial flow into the jet pump.

Dose rates in the components besides the core boiling and bypass channels are scaled according to the dose levels in the core regions; the weighting fractions are shown in Table 8-1.

II. Water Chemistry Parameters

The reaction set reported by Ibe was used in the present study. Gas absorption and release factors are also included in the reaction matrix as rate constants for the two-phase pseudo-reactions. The negative activation energy in such reactions flags RADICAL to use appropriate routines for two-phase mass transfer.

The surface decomposition of H_2O_2 is also included in the reaction set as the last entry. This reaction is a modified first-order version of Lin's reaction model, which yields essentially the same results [Lin 1989, Mason 1990]. There may be more than one surface decomposition reaction (for instance, one for stainless steel and another for titanium) and these surface reactions should be the last entries in a reaction set. The reason is as follows: Lin reported that surface decomposition rate is a function of the pipe diameter; hence in the present work the rate constants for surface reactions are scaled according to the pipe diameter in centimeters in the input file, unlike other rate constants. The surface rate constant in the input file was adjusted from Lin's value for this scaling; Lin also reports his results in terms of outside diameters, but these were adjusted to correspond to inside diameters. Although the surface reaction was included in the reaction set, it was not considered in this simulation; the surface reaction can be turned on and off by setting the flag CalcSurf in the input file.

Burns' high-temperature g-values were used in this simulation, as was the case in Ibe's simulations. Ibe wrote "the g-values at elevated temperatures (573 - 683 K) are used for plant data simulations, since the g-values have given reasonable calculated concentrations for hydrogen, oxygen and hydrogen peroxide in the BWR primary systems" [Ibe 1989]. On the contrary, Ruiz et al. used the room temperature g-values. Mason performed a number of parametric studies on different g-values and reaction sets [1990]. It is recommended that a combination of g-values and a reaction set which best describes actual experiences be determined for each case study.

The reaction set and the g-values used are shown in the output file for this simulation along with other parameters in Appendix E.

III. Normal Water Chemistry

Normal water chemistry differs from hydrogen water chemistry in that no hydrogen is injected through the feedwater line. Under this normal operating condition for a BWR the feedwater contains about 35 ppb of dissolved oxygen in pure water and the concentrations of the rest of the species are assumed negligible.

A simulation was run for this case with the input file DRESDEN0.IN, which is given in Appendix E. Particular attention was given to the oxygen and hydrogen concentrations in the boiling and bypass channels in the core region and the recirculation line where IGSCC is important.

In the core region, radiolysis produces high concentrations of O_2 and H_2 (see Figs. 8-4 and 8-6). In the boiling region, however, the concentrations of both species decrease substantially as boiling starts; much of the dissolved gaseous species are now transferred to the vapor phase (see Fig. 8-5). In the bypass region, the concentrations monotonically increase until near the exit of the core, where the radiation level drops.

The pH of the coolant in the core is near 5.6 throughout the entire region in both the boiling region and the bypass region (see Fig. 8-8 and 8-9).

The effect of the multi-layered downcomer region is depicted in Figs. 8-10 and 8-11.

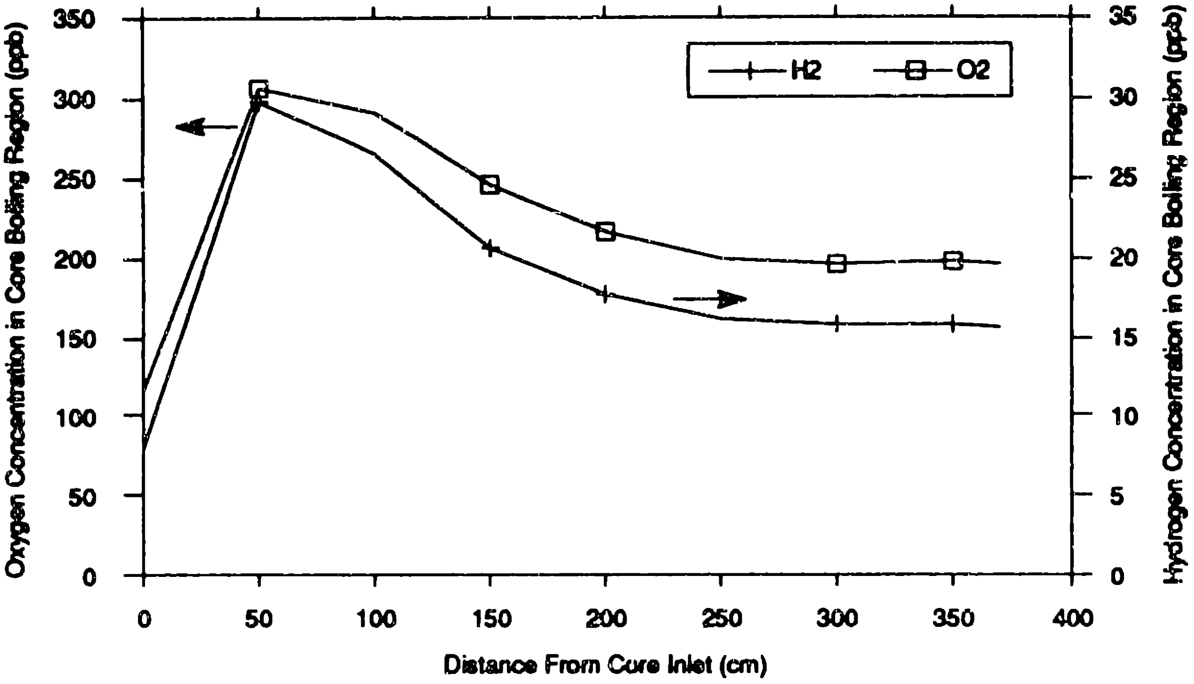


Figure 8-4 Vapor phase oxygen and hydrogen concentrations in the core boiling channel under NWC.

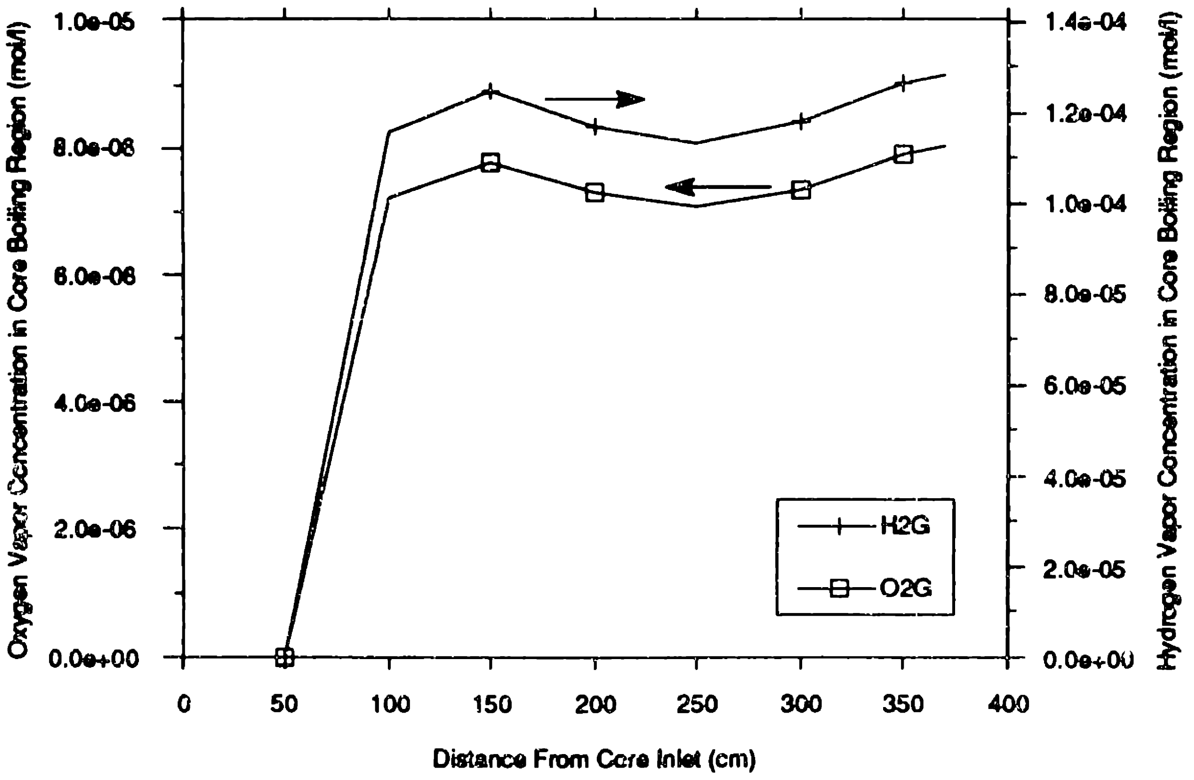


Figure 8-5 Vapor phase oxygen and hydrogen concentrations in the core boiling channel under NWC.

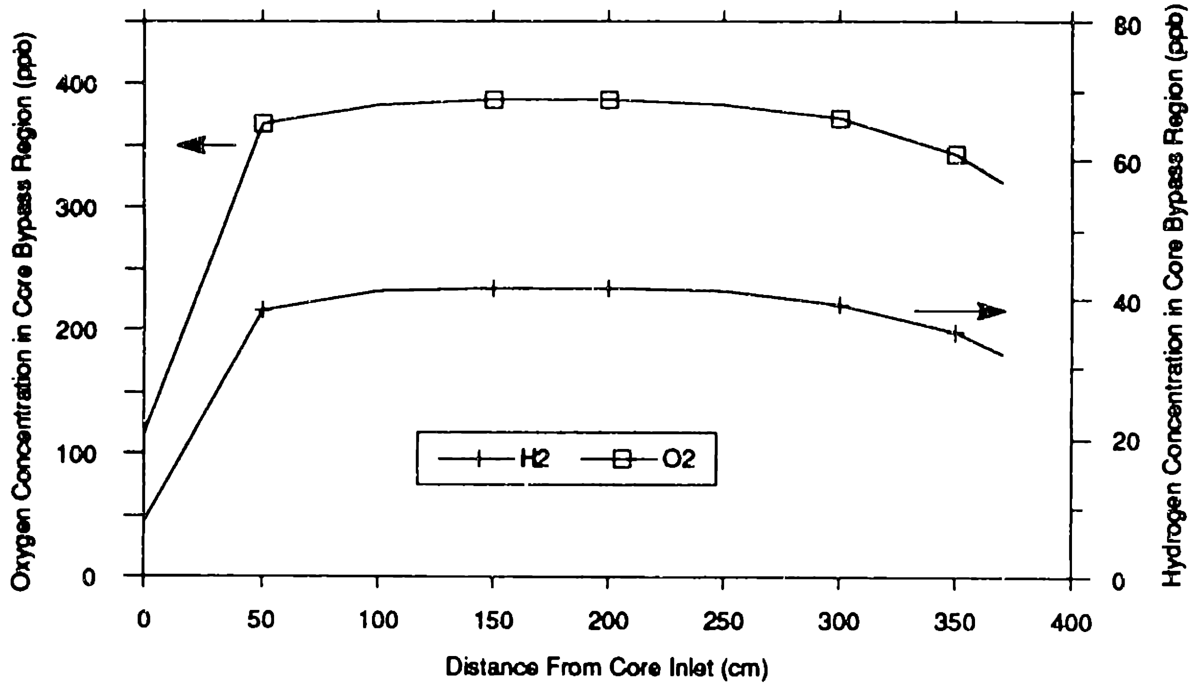


Figure 8-6 Oxygen and hydrogen concentrations in the core bypass region under NWC.

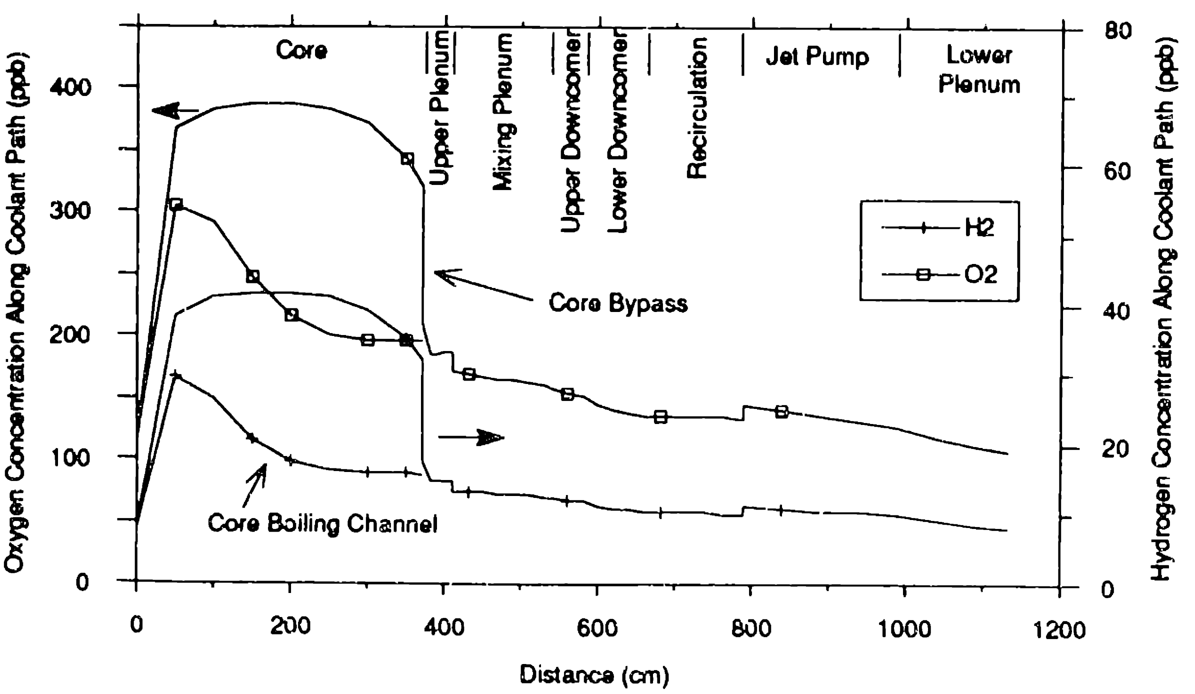


Figure 8-7 Oxygen and hydrogen concentrations throughout the entire flow path in the primary region of Dresden-2 under NWC.

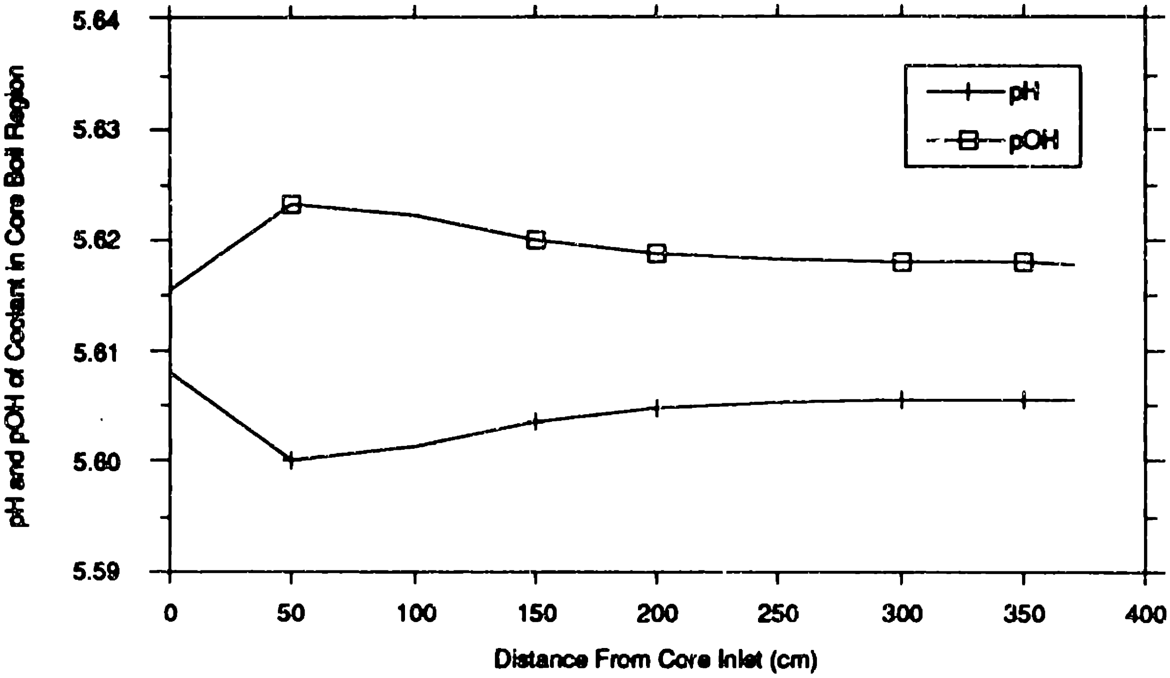


Figure 8-8 pH and pOH of the coolant in the core boiling channel under NWC.

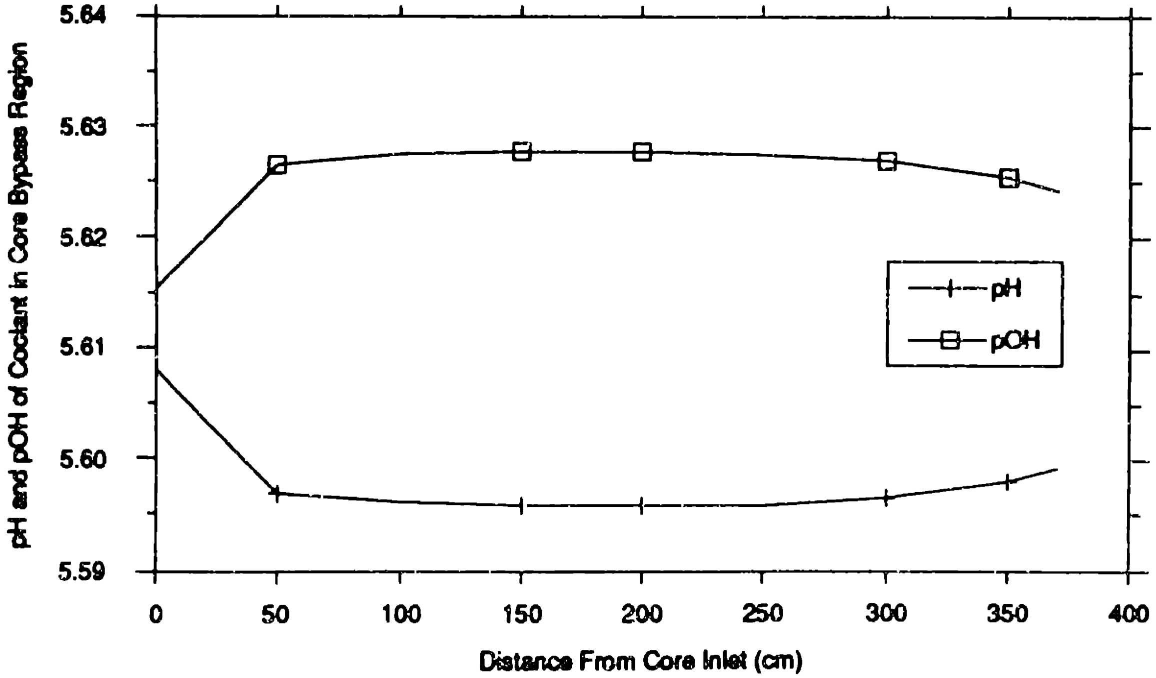


Figure 8-9 pH and pOH in the core bypass region under NWC.

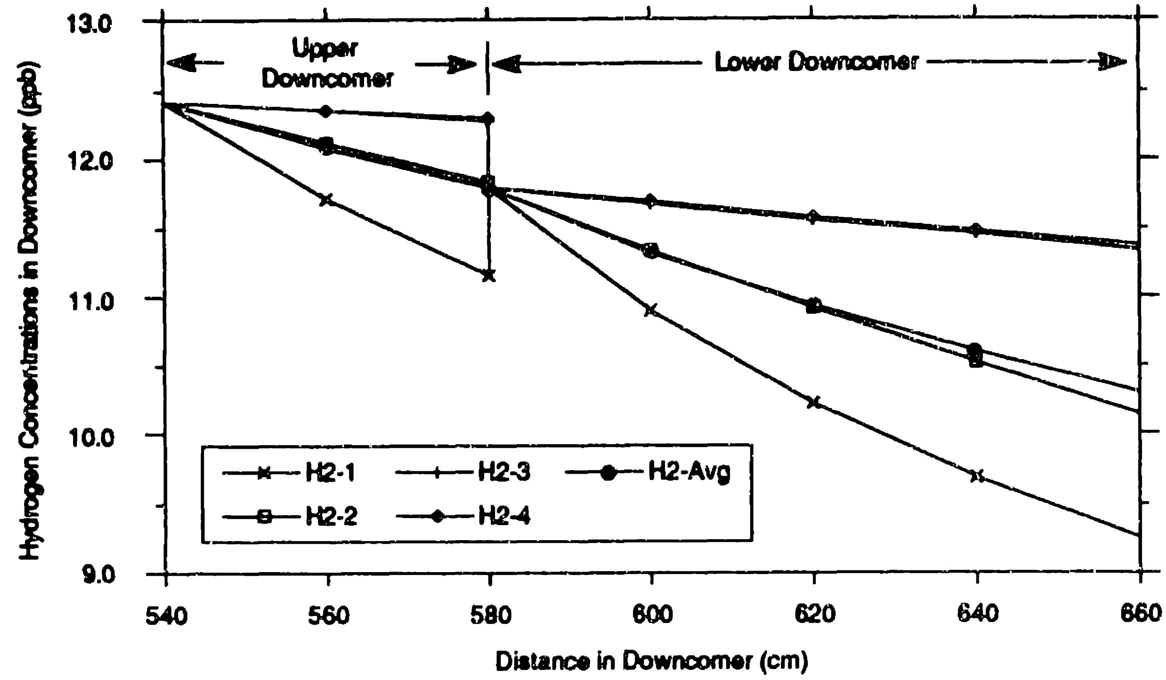


Figure 8-10 Hydrogen concentrations in the multi-layered downcomer region.

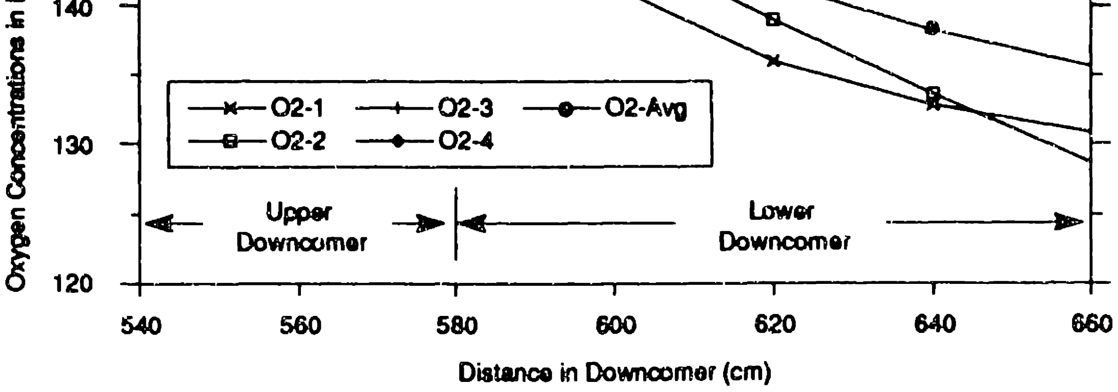


Figure 8-11 Oxygen concentrations in the multi-layered downcomer region.

IV. Hydrogen Water Chemistry

Hydrogen water chemistry was simulated by fixing the hydrogen concentration at the feedwater inlet; the rest of the input file remained the same as NWC. Four hydrogen injection levels were tested: 0.3, 0.5, 0.8, and 2.1 ppm. The response of the oxygen concentration in the core is illustrated in Fig. 8-12. In the boiling region suppression of oxygen level is less effective due to the mass transfer of hydrogen into the vapor phase. On the other hand, oxygen is suppressed to a negligible level in the bypass channel with only 0.3 ppm of hydrogen injection.

The oxygen level in the recirculation line is of significant importance because IGSCC has frequently occurred in this region. Fig. 8-13 indicates that 0.5 ppm of hydrogen injection is sufficient to decrease the oxygen level in the recirculation line below 10 ppb, which is supposedly the threshold oxygen level to mitigate IGSCC. Hydrogen injection of 0.8 ppm or more completely suppressed oxygen concentration in this region. This, however, is not consistent with measured results, which have shown that oxygen is still observed for higher hydrogen concentrations [Ibe 1987]. This may be caused by some effects which have not been accounted for in this model.

The oxygen responses in the core region to 0.3 ppm of hydrogen injection are depicted in Figs. 8-15 through 8-17. It is clearly shown in Fig. 8-15 that the oxygen concentration in the liquid phase of the boiling channel is completely suppressed up to the onset of boiling and starts increasing when the hydrogen concentration starts decreasing, due to mass transfer to the vapor phase. In the vapor phase not only the oxygen vapor concentration decreases but the hydrogen concentration decreases as well. Oxygen is completely depressed in the entire bypass region, where the dissolved hydrogen remains in the liquid phase.

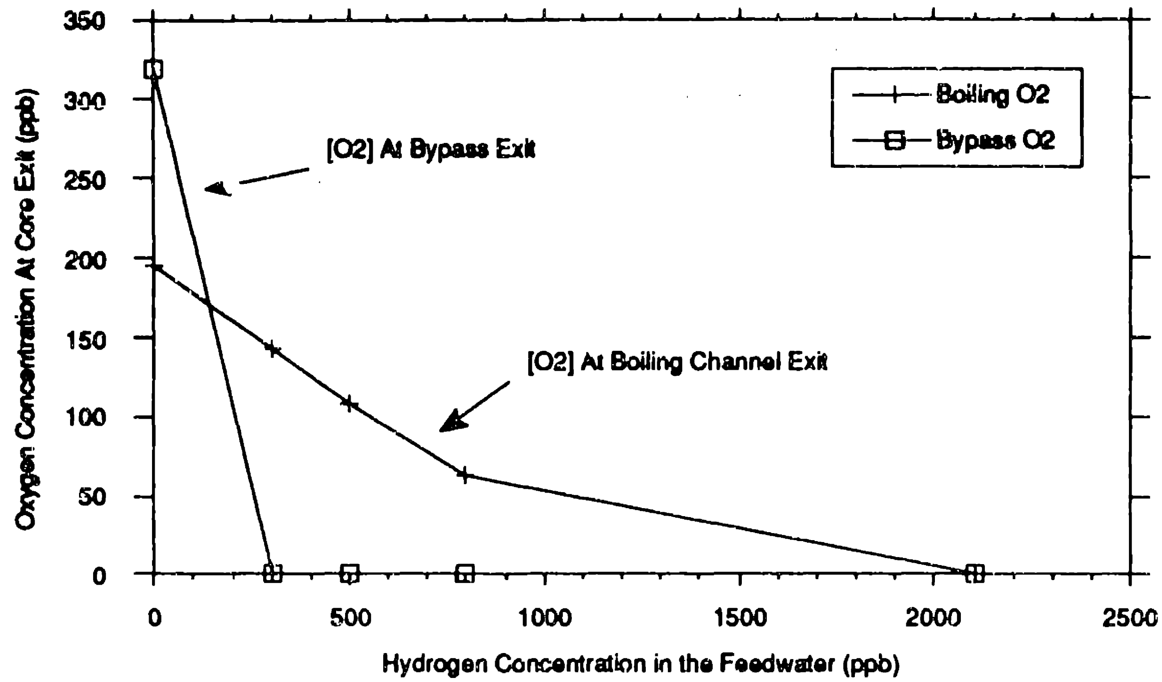


Figure 8-12 Oxygen concentrations in the core at various hydrogen injection levels in the feedwater.

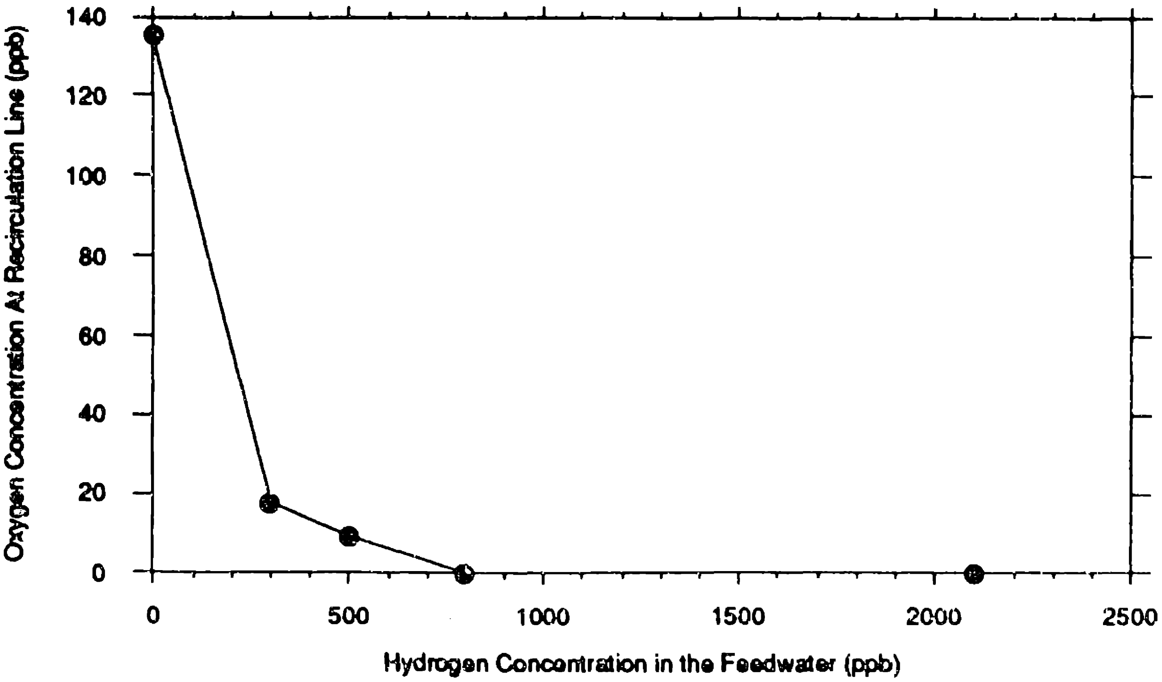


Figure 8-13 Oxygen concentrations in the recirculation line exit at various hydrogen injection levels in the feedwater.

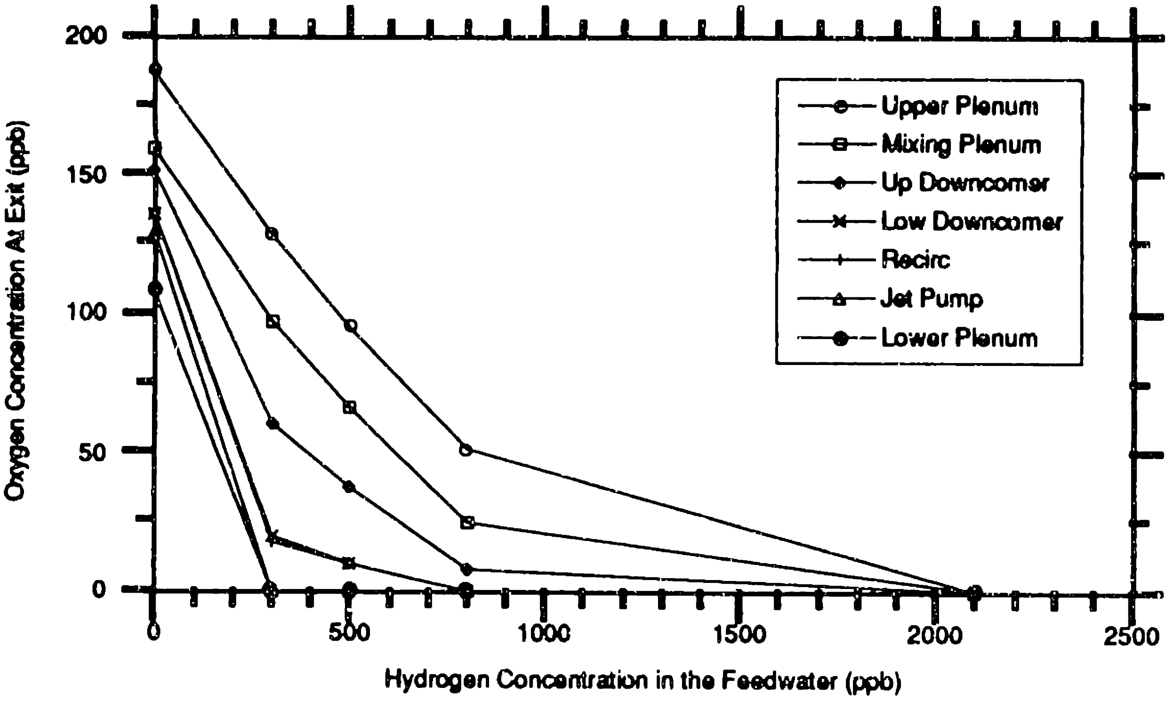


Figure 8-14 Oxygen concentration responses, at various components, to hydrogen injection in the feedwater.

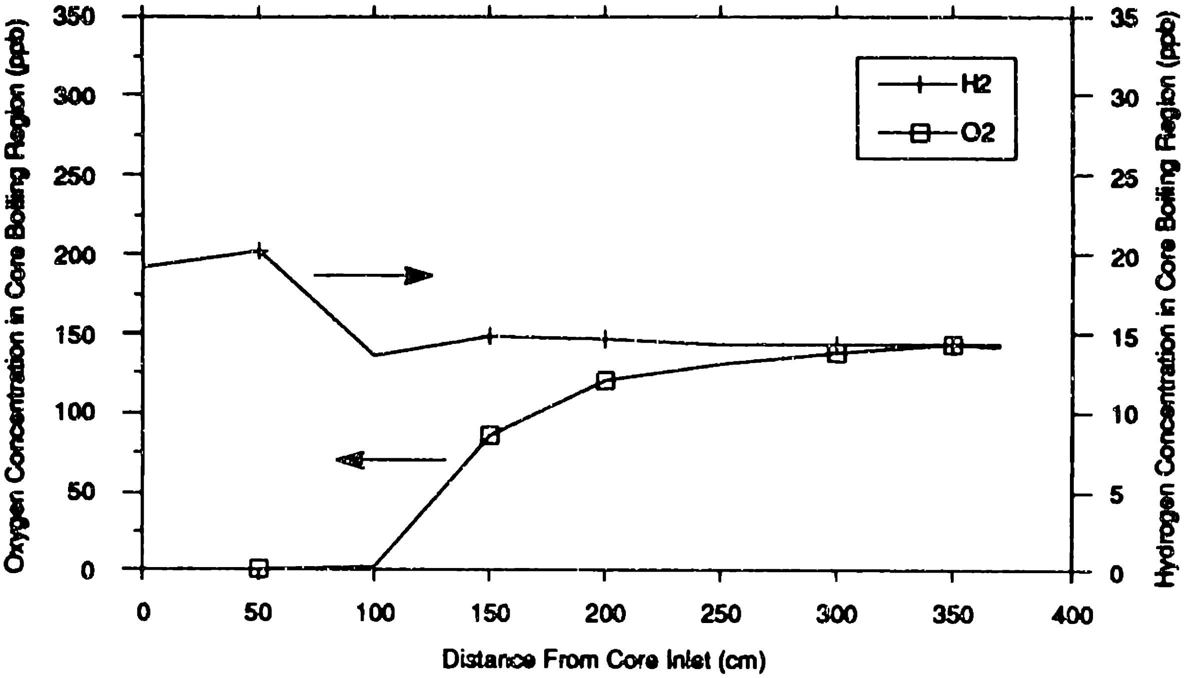


Figure 8-15 Liquid phase oxygen and hydrogen concentrations in the core boiling region with 0.3 ppm hydrogen injection in the feedwater.

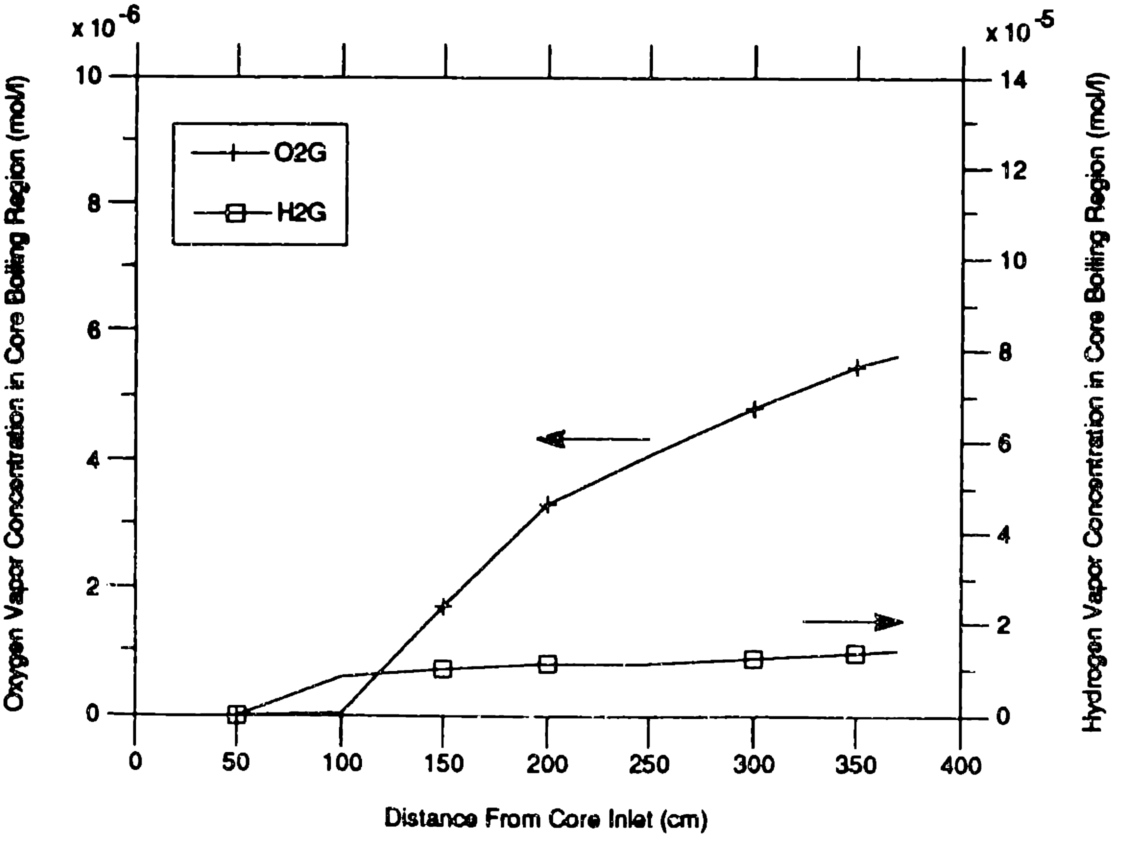


Figure 8-16 Vapor phase oxygen and hydrogen concentrations in the core boiling region with 0.3 ppm hydrogen injection in the feedwater.

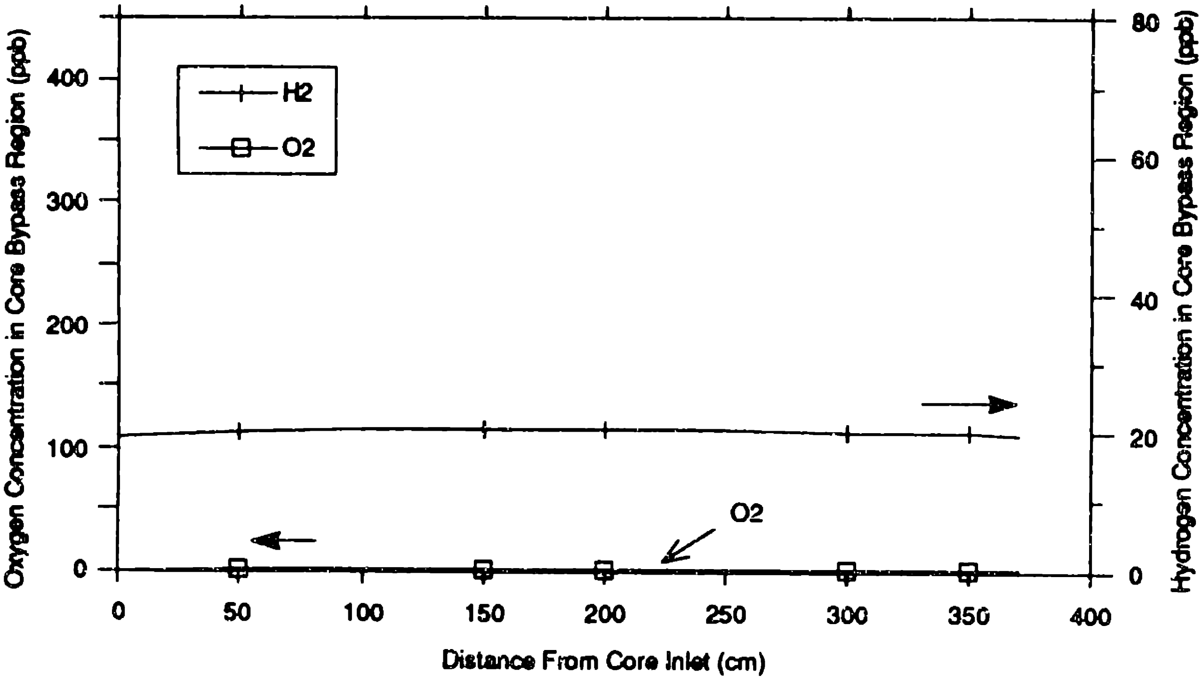


Figure 8-17 Oxygen and hydrogen concentrations in the core bypass region with 0.3 ppm hydrogen injection in the feedwater.

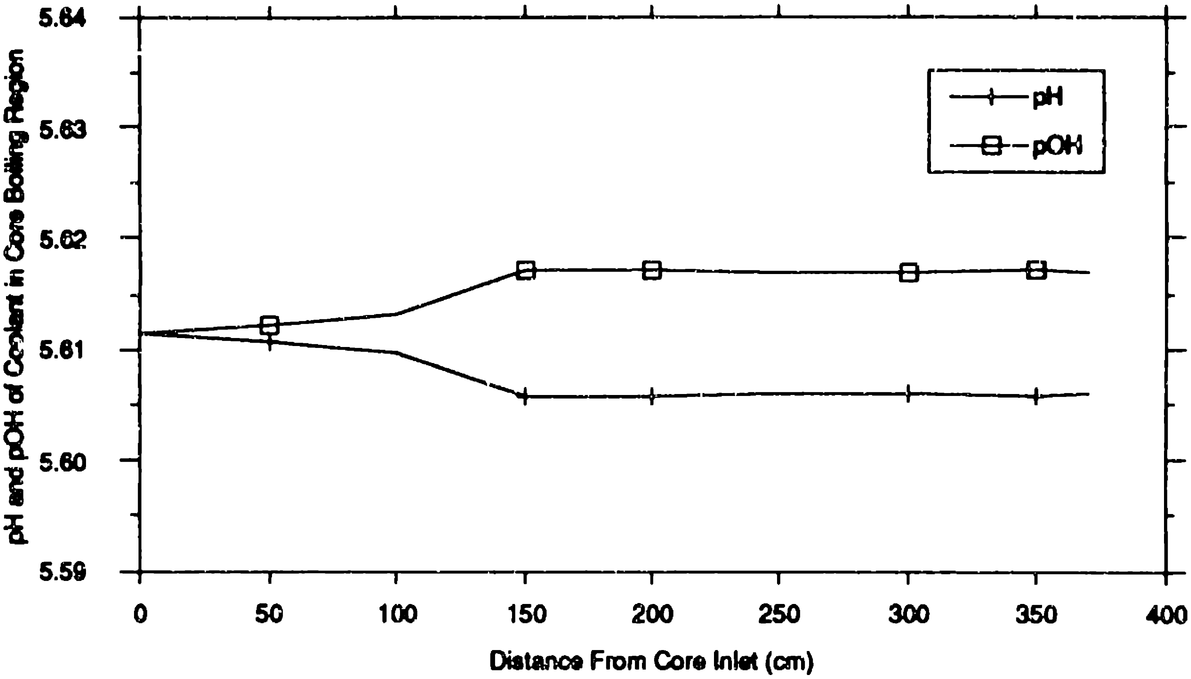


Figure 8-18 pH and pOH in the core boiling region with 0.3 ppm hydrogen injection in the feedwater.

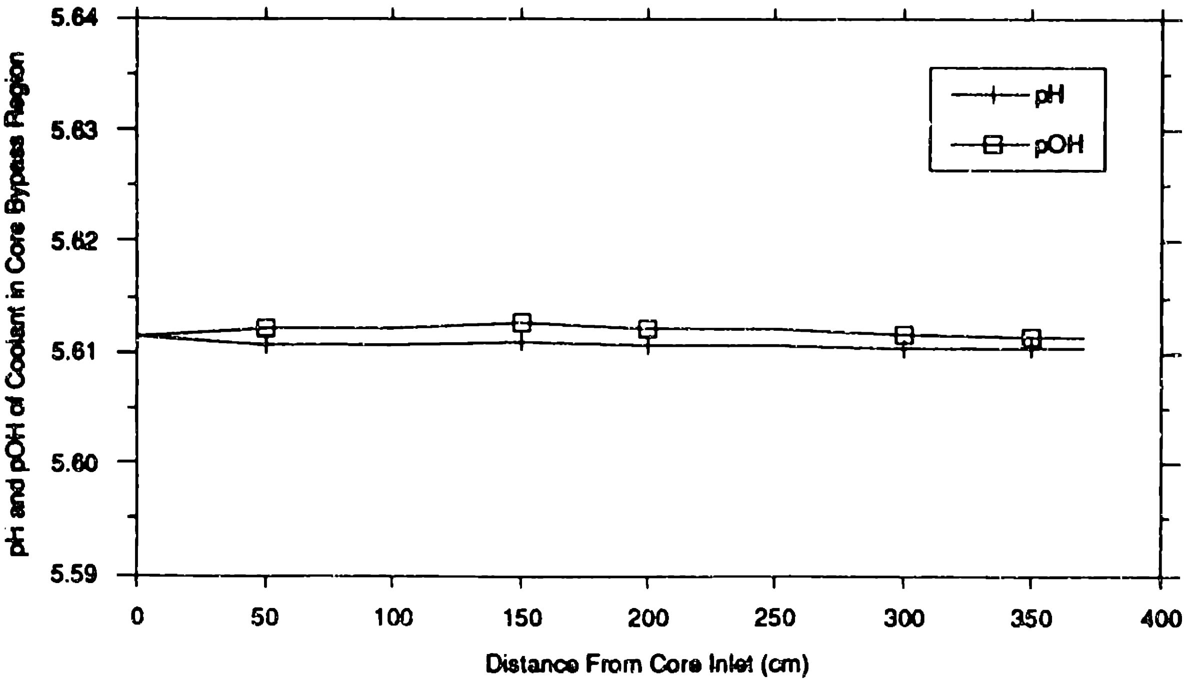


Figure 8-19 pH and pOH in the core bypass region with 0.3 ppm hydrogen injection in the feedwater.

V. Sensitivity Analysis

Sensitivity analysis was performed for oxygen in normal water chemistry and hydrogen water chemistry of 2.0 ppm to determine the differential response of oxygen concentration to various input parameters and hydrogen concentration. While sensitivity analysis can be evaluated for every component, it is best to limit the analysis to critical components to reduce the execution time; DRESDEN0.IN takes about 10 minutes to run on the MicroVAX-II computer, whereas the same input file with sensitivity analyses in the core region and the recirculation line may take two to three times longer. Also, a comparison of sensitivity plots in different regions reveals that the general characteristics of the graphs are quite similar; this can be interpreted to mean that some important parameters are important throughout all of the components.

In sensitivity analysis the response of a concentration with respect to rate constants, g-values, and concentrations are evaluated. In the present study the response of oxygen concentration in the core boiling and bypass region and the recirculation line was evaluated.

The sensitivity results may be interpreted as follows: if a curve is plotted in an x-y plane and the slope of the curve at x_0 and y_0 is measured, this slope is the absolute sensitivity. The slope gives a measure of how much y changes for a small change in x about x_0, i.e., Δy and Δx. If the slope is multiplied by x_0 and divided by y_0, this gives a dimensionless value, which is the relative sensitivity. Relative sensitivity gives the percent change in y_0 for a percent change in x_0, *i.e.*, $\Delta y/y_0$ and $\Delta x/x_0$. The larger the value of the sensitivity, the more sensitive is the response of y to a change in x.

Sensitivity results can be either positive or negative depending on whether the response is positive or negative to a given change of a parameter. In the sensitivity plots, however, the absolute values of sensitivity results are shown, so that the wide range of values can be plotted using a log scale. The sign may be found in the tables.

Remember that sensitivity analysis is a differential calculation and is valid over a very small range about x_0; if there has been a large change in the parameter, more than a few percent, the analysis should be rerun.

The general trend of the relative sensitivity results show that relative changes in g-values have the most significant effects on oxygen concentrations in all regions. Neutron g-values for H_2 and O have the most significant effect. The mass transfer coefficients also show significant effect in the core boiling channel. Among the reaction rate constants, rate constants for W17, W28, W31, W36, and W37 show the most significant effect in both the core boiling and bypass regions. The reactions are:

```
W17 H2      OH              >H       H2O
W28 H2O2    OH-             >HO2-    H2O
W31 HO2-    H2O             >H2O2    OH-
W36 H2O     O               >OH      OH
W37 OH      O               >HO2
```

The concentration sensitivity results show that in the core boiling region, the oxygen concentration is most sensitive to its own concentration and hydrogen concentrations, which seems obvious. In the single phase liquid regions, *ie.*, the core bypass region and the recirculation line, the oxygen concentration is most sensitive to OH-, HO_2-, and H_2O_2 concentrations.

Table 8-2 Sensitivity Results For O_2 In the Core Boiling Channel Under NWC.

```
________________________________________________________________________

            CORE BOILING     SENSITIVITY RESULTS FOR O2
________________________________________________________________________

            ============ ADJOINT RESULTS ============

e-      =   -0.169968E+01 **     OH-      =   -0.242486E+00 **
H2      =   -0.290595E+01 **     OH       =    0.145330E+01 **
HO2-    =    0.268444E+01 **     H2O2     =    0.292693E+01 **
O2-     =    0.414184E+01 **     O2       =    0.483807E+01 **
H       =   -0.145389E+01 **     H+       =    0.242486E+00 **
HO2     =    0.438432E+01 **     O2G      =    0.122240E+00 **
H2G     =   -0.539085E-01 **     O        =    0.290660E+01 **
H2O     =   -0.296610E-08 **     2H2O     =   -0.582393E-08 **


                                      ABSOLUTE       RELATIVE
          PARAMETER                  SENSITIVITY    SENSITIVITY
-------------------------           ------------   ------------

RATE CONST OF I 1                    0.85517E-05    0.18887E+01
RATE CONST OF I 2                   -0.85599E-05   -0.18905E+01
RATE CONST OF W 1                    0.68435E-10    0.25860E-02
RATE CONST OF W 2                    0.41482E-17    0.23512E+00
RATE CONST OF W 3                    0.28215E-18    0.15993E-01
RATE CONST OF W 4                   -0.22087E-16   -0.67811E+00
RATE CONST OF W 5                    0.43841E-19    0.10354E-02
RATE CONST OF W 6                   -0.31242E-18   -0.14757E-01
RATE CONST OF W 7                    0.12135E-16    0.54453E+00
RATE CONST OF W 8                    0.14261E-17    0.55235E-05
RATE CONST OF W 9                    0.46302E-14    0.54676E-04
RATE CONST OF W10                    0.85292E-17    0.24172E+00
RATE CONST OF W11                    0.54228E-16    0.15368E+01
RATE CONST OF W12                   -0.37790E-16   -0.17850E-02
RATE CONST OF W13                    0.25938E-18    0.27567E-03
RATE CONST OF W14                   -0.84689E-17   -0.12601E-02
RATE CONST OF W15                   -0.37485E-18   -0.12729E+00
RATE CONST OF W16                    0.10476E-17    0.49480E-01
RATE CONST OF W17                   -0.23723E-13   -0.67160E+01
RATE CONST OF W18                    0.12166E-13    0.10481E+01
RATE CONST OF W19                   -0.24005E-15   -0.81572E-01
RATE CONST OF W20                    0.22993E-16    0.10318E+01
RATE CONST OF W21                   -0.29066E-14   -0.54917E-02
RATE CONST OF W22                   -0.31309E-15   -0.36270E-01
RATE CONST OF W23                   -0.49267E-16   -0.10273E-02
RATE CONST OF W24                   -0.33643E-11   -0.14550E+00
RATE CONST OF W25                   -0.31500E-17   -0.14879E+00
RATE CONST OF W26                   -0.20048E-16   -0.94695E+00
RATE CONST OF W27                   -0.80831E-16   -0.11237E+00
RATE CONST OF W28                   -0.45789E-15   -0.17681E+01
RATE CONST OF W29                    0.25804E-05    0.12727E+00
```

PARAMETER	ABSOLUTE SENSITIVITY	RELATIVE SENSITIVITY
RATE CONST OF W30	0.46211E-19	0.54569E-02
RATE CONST OF W31	0.73326E-10	0.17698E+01
RATE CONST OF W32	-0.24589E-06	-0.41701E-03
RATE CONST OF W33	0.97093E-18	0.50447E-01
RATE CONST OF W34	-0.19059E-18	-0.90023E-02
RATE CONST OF W35	0.83464E-16	0.10764E-04
RATE CONST OF W36	-0.90400E-09	-0.40565E+01
RATE CONST OF W37	0.83953E-16	0.39655E+01
RATE CONST OF W38	-0.45949E-15	-0.34525E-03
RATE CONST OF W39	0.14587E-15	0.11469E-02
RATE CONST OF W40	-0.11358E-19	-0.53650E-03
RATE CONST OF H2G	0.53123E-04	0.20102E+03
RATE CONST OF H2L	-0.52583E-04	-0.66325E+02
RATE CONST OF O2G	-0.70184E-04	-0.20361E+03
RATE CONST OF O2L	0.55191E-04	0.83536E+02
GAMMA G-VALUE OF e-	-0.24582E-03	-0.21716E+02
NEUTRON G-VALUE OF e-	-0.46311E-03	-0.40912E+02
GAMMA G-VALUE OF H2	-0.39686E-03	-0.17530E+03
NEUTRON G-VALUE OF H2	-0.75340E-03	-0.33278E+03
GAMMA G-VALUE OF OH	0.20051E-03	0.30998E+02
NEUTRON G-VALUE OF OH	0.37990E-03	0.58731E+02
GAMMA G-VALUE OF H	-0.20260E-03	-0.13423E+02
NEUTRON G-VALUE OF H	-0.38302E-03	-0.25377E+02
GAMMA G-VALUE OF H+	0.39786E-04	0.35148E+01
NEUTRON G-VALUE OF H+	0.74586E-04	0.65890E+01
GAMMA G-VALUE OF O	0.40473E-03	0.17877E+03
NEUTRON G-VALUE OF O	0.76556E-03	0.33815E+03
CONCENTRATION OF e-	-0.50560E+03	-0.97017E-02
CONCENTRATION OF OH-	-0.35815E+01	-0.19068E+01
CONCENTRATION OF H2	-0.28317E+01	-0.36026E+01
CONCENTRATION OF OH	0.64331E+01	0.13341E+00
CONCENTRATION OF HO2-	0.23790E+04	0.17678E+01
CONCENTRATION OF H2O2	-0.20423E+02	-0.16176E+01
CONCENTRATION OF O2-	0.94950E+01	0.13720E+00
CONCENTRATION OF O2	0.46109E+01	0.46109E+01
CONCENTRATION OF H	-0.48615E+03	-0.96069E-01
CONCENTRATION OF H+	0.26628E+00	0.14582E+00
CONCENTRATION OF HO2	0.99284E+01	0.22417E-01
CONCENTRATION OF O2G	0.11790E+00	0.20890E+00
CONCENTRATION OF H2G	-0.51337E-01	-0.17844E+00
CONCENTRATION OF O	0.48204E+01	0.88921E-03
CONCENTRATION OF H2O	0.19136E-06	0.17390E+01
CONCENTRATION OF 2H2O	-0.61672E-08	-0.23083E+01

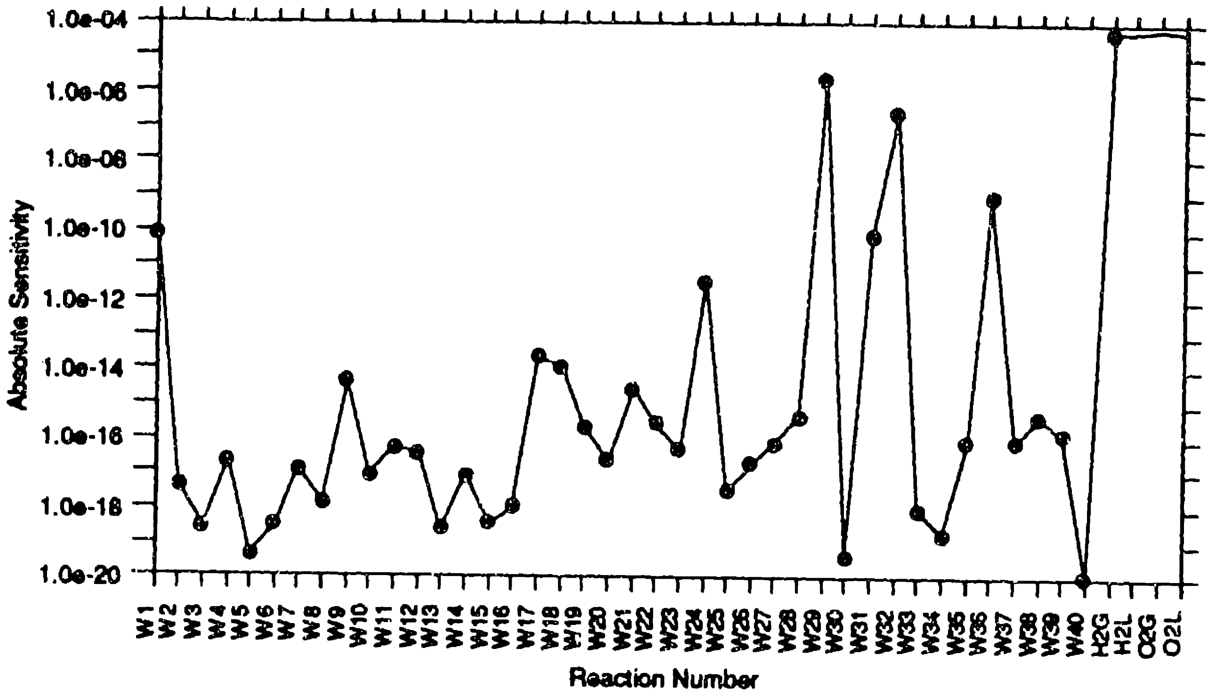


Figure 8-20 Absolute sensitivities of oxygen concentration with respect to reaction rate constants in the core boiling channel under NWC.

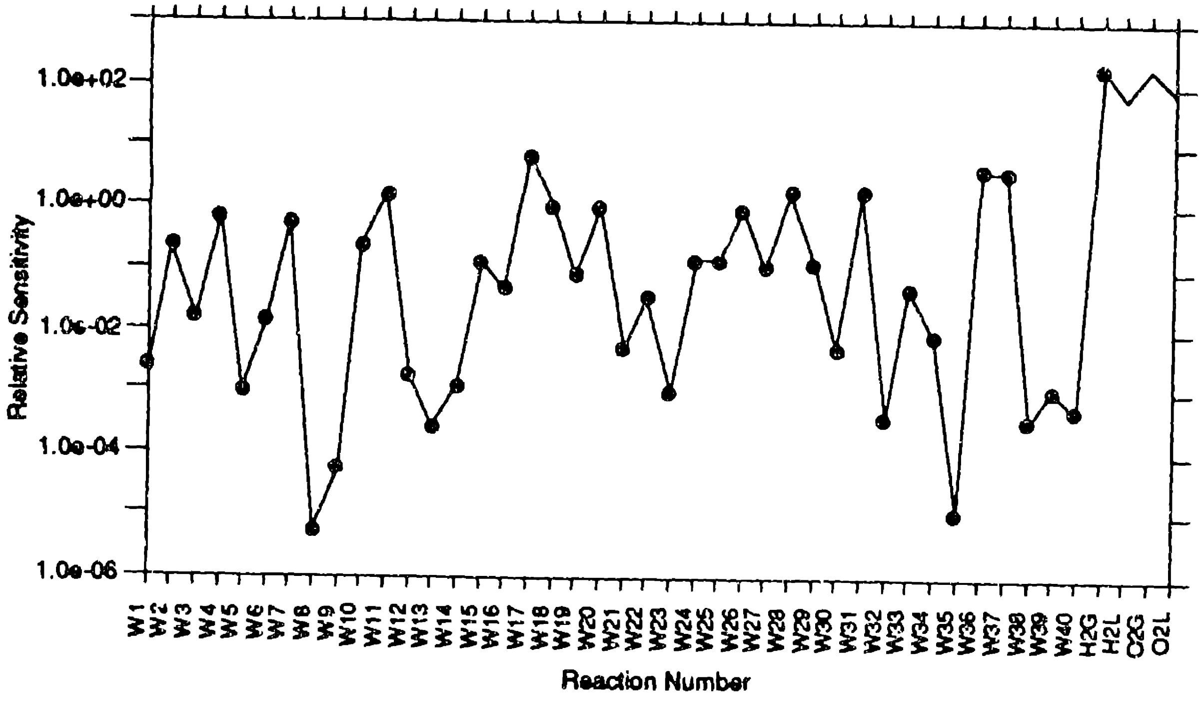


Figure 8-21 Relative sensitivities of oxygen concentration with respect to reaction rate constants in the core boiling channel under NWC.

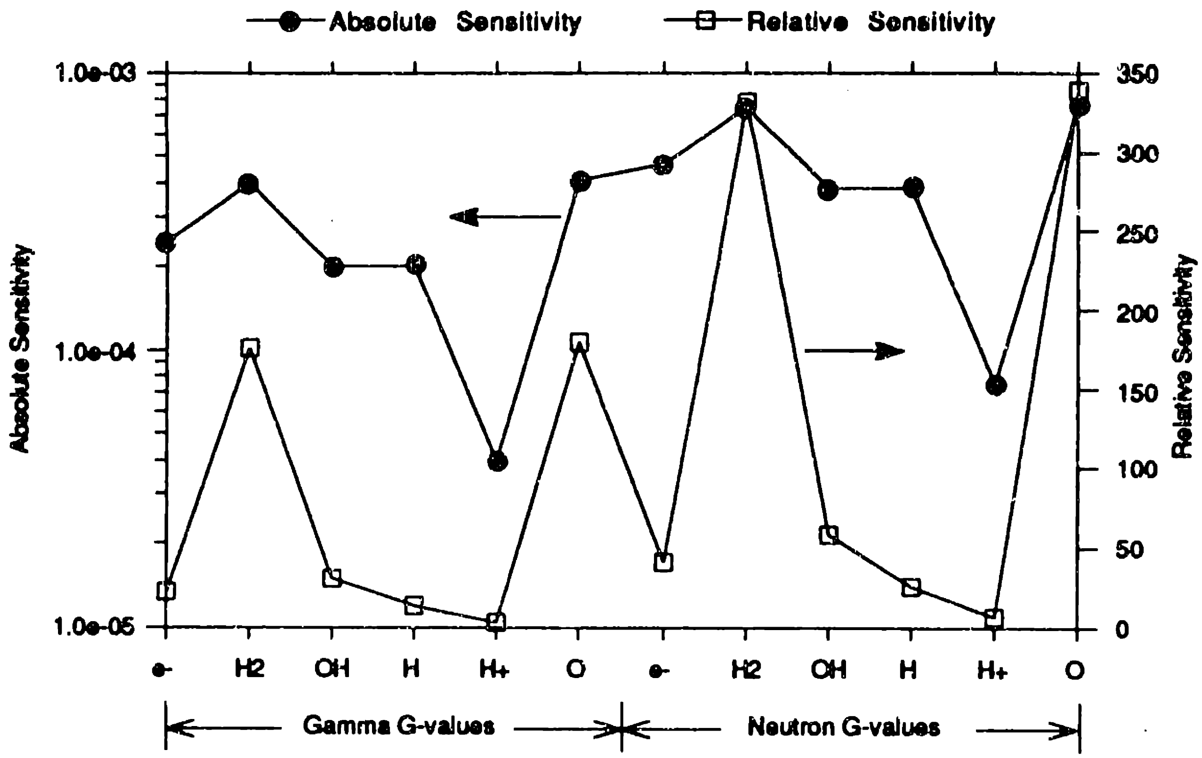


Figure 8-22 Absolute and relative sensitivities of oxygen concentration with respect to g-values in the core boiling channel under NWC.

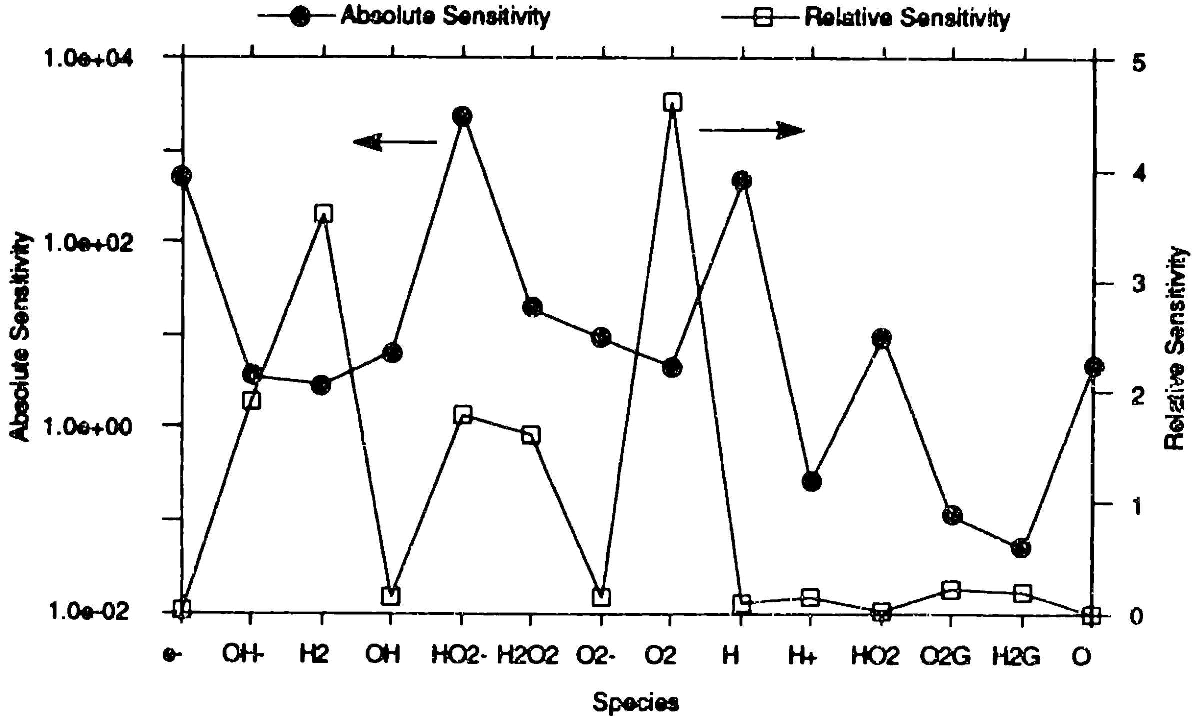


Figure 8-23 Absolute and relative sensitivities of oxygen concentration with respect to inlet concentrations in the core boiling channel under NWC.

Table 8-3 Sensitivity Results For O_2 In the Core Bypass Channel Under NWC.

```
            CORE BYPASS       SENSITIVITY RESULTS FOR O2


             ============= ADJOINT RESULTS =============

  e-        =   -0.451586E+00 **    OH-       =    -0.926972E-01 **
  H2        =   -0.717767E+00 **    OH        =     0.358884E+00 **
  HO2-      =    0.625095E+00 **    H2O2      =     0.717792E+00 **
  O2-       =    0.983995E+00 **    O2        =     0.435577E+00 **
  H         =   -0.358885E+00 **    H+        =     0.926972E-01 **
  HO2       =    0.107669E+01 **    O2G       =     0.000000E+00 **
  H2G       =    0.000000E+00 **    O         =     0.717768E+00 **
  H2O       =   -0.570880E-09 **    2H2O      =    -0.114217E-08 **


                                       ABSOLUTE      RELATIVE
          PARAMETER                   SENSITIVITY   SENSITIVITY
  -------------------------          ------------  ------------

  RATE CONST OF I 1                   0.12599E-05   0.17002E+00
  RATE CONST OF I 2                  -0.12613E-05  -0.17020E+00
  RATE CONST OF W 1                   0.24543E-10   0.56664E-03
  RATE CONST OF W 2                   0.15025E-17   0.52036E-01
  RATE CONST OF W 3                   0.47787E-19   0.16550E-02
  RATE CONST OF W 4                  -0.94932E-17  -0.17808E+00
  RATE CONST OF W 5                   0.56108E-20   0.80964E-04
  RATE CONST OF W 6                  -0.12132E-18  -0.35012E-02
  RATE CONST OF W 7                   0.12588E-17   0.34511E-01
  RATE CONST OF W 8                   0.24603E-18   0.58223E-06
  RATE CONST OF W 9                   0.37317E-15   0.26925E-05
  RATE CONST OF W10                   0.13362E-16   0.23137E+00
  RATE CONST OF W11                   0.84589E-16   0.14647E+01
  RATE CONST OF W12                  -0.12820E-16  -0.36999E-03
  RATE CONST OF W13                   0.39792E-19   0.25839E-04
  RATE CONST OF W14                  -0.36043E-17  -0.32766E-03
  RATE CONST OF W15                  -0.57349E-18  -0.11899E+00
  RATE CONST OF W16                   0.12224E-17   0.35278E-01
  RATE CONST OF W17                  -0.30779E-13  -0.53240E+01
  RATE CONST OF W18                   0.17042E-13   0.89707E+00
  RATE CONST OF W19                  -0.38581E-15  -0.80105E-01
  RATE CONST OF W20                  -0.64838E-17  -0.17777E+00
  RATE CONST OF W21                  -0.86789E-14  -0.10019E-01
  RATE CONST OF W22                  -0.58420E-15  -0.41351E-01
  RATE CONST OF W23                  -0.87975E-16  -0.11209E-02
  RATE CONST OF W24                  -0.59869E-11  -0.15820E+00
  RATE CONST OF W25                  -0.42808E-17  -0.12354E+00
  RATE CONST OF W26                  -0.27909E-16  -0.80544E+00
  RATE CONST OF W27                  -0.11146E-15  -0.94676E-01
  RATE CONST OF W28                  -0.23420E-13  -0.55257E+02
  RATE CONST OF W29                   0.39478E-05   0.11897E+00
```

```
                                      ABSOLUTE      RELATIVE
         PARAMETER                  SENSITIVITY   SENSITIVITY
-------------------------         ------------  ------------

RATE CONST OF W30                  0.13817E-18   0.99692E-02
RATE CONST OF W31                  0.37486E-08   0.55283E+02
RATE CONST OF W32                 -0.50346E-06  -0.52170E-03
RATE CONST OF W33                  0.12534E-17   0.39790E-01
RATE CONST OF W34                 -0.33066E-19  -0.95430E-03
RATE CONST OF W35                  0.98643E-16   0.77727E-05
RATE CONST OF W36                 -0.10671E-08  -0.29258E+01
RATE CONST OF W37                  0.98853E-16   0.28529E+01
RATE CONST OF W38                 -0.63929E-15  -0.29349E-03
RATE CONST OF W39                  0.23257E-15   0.11172E-02
RATE CONST OF W40                 -0.10423E-19  -0.30082E-03
GAMMA   G-VALUE OF e-             -0.20747E-02  -0.11199E+03
NEUTRON G-VALUE OF e-             -0.35738E-02  -0.19290E+03
GAMMA   G-VALUE OF H2             -0.30746E-02  -0.82978E+03
NEUTRON G-VALUE OF H2             -0.52994E-02  -0.14302E+04
GAMMA   G-VALUE OF OH              0.15396E-02   0.14543E+03
NEUTRON G-VALUE OF OH              0.26538E-02   0.25067E+03
GAMMA   G-VALUE OF H              -0.15421E-02  -0.62426E+02
NEUTRON G-VALUE OF H              -0.26589E-02  -0.10764E+03
GAMMA   G-VALUE OF H+              0.52837E-03   0.28520E+02
NEUTRON G-VALUE OF H+              0.90486E-03   0.48841E+02
GAMMA   G-VALUE OF O               0.30831E-02   0.83208E+03
NEUTRON G-VALUE OF O               0.53148E-02   0.14344E+04
CONCENTRATION OF   e-             -0.16358E+05  -0.13510E+00
CONCENTRATION OF   OH-            -0.17274E+03  -0.55367E+02
CONCENTRATION OF   H2             -0.35647E+01  -0.57198E+01
CONCENTRATION OF   OH              0.19146E+03   0.12183E+01
CONCENTRATION OF   HO2-            0.45703E+05   0.57136E+02
CONCENTRATION OF   H2O2           -0.42100E+03  -0.56957E+02
CONCENTRATION OF   O2-             0.69637E+02   0.12360E+01
CONCENTRATION OF   O2              0.38900E+01   0.38908E+01
CONCENTRATION OF   H              -0.14974E+05  -0.11289E+01
CONCENTRATION OF   H+              0.39731E+00   0.13490E+00
CONCENTRATION OF   HO2             0.72047E+02   0.20194E+00
CONCENTRATION OF   O               0.53496E+02   0.60850E-02
CONCENTRATION OF   H2O             0.99540E-05   0.55265E+02
CONCENTRATION OF   2H2O           -0.74168E-08  -0.16961E+01
```

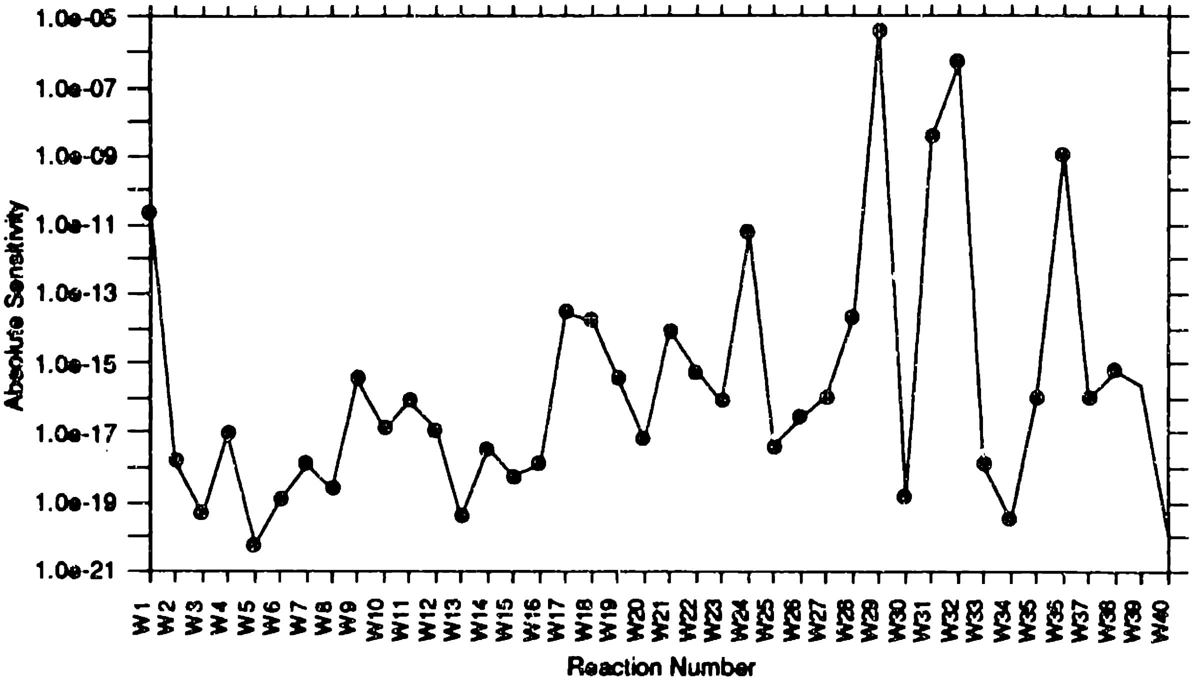


Figure 8-24 Absolute sensitivities of oxygen concentration with respect to reaction rate constants in the core bypass channel under NWC.

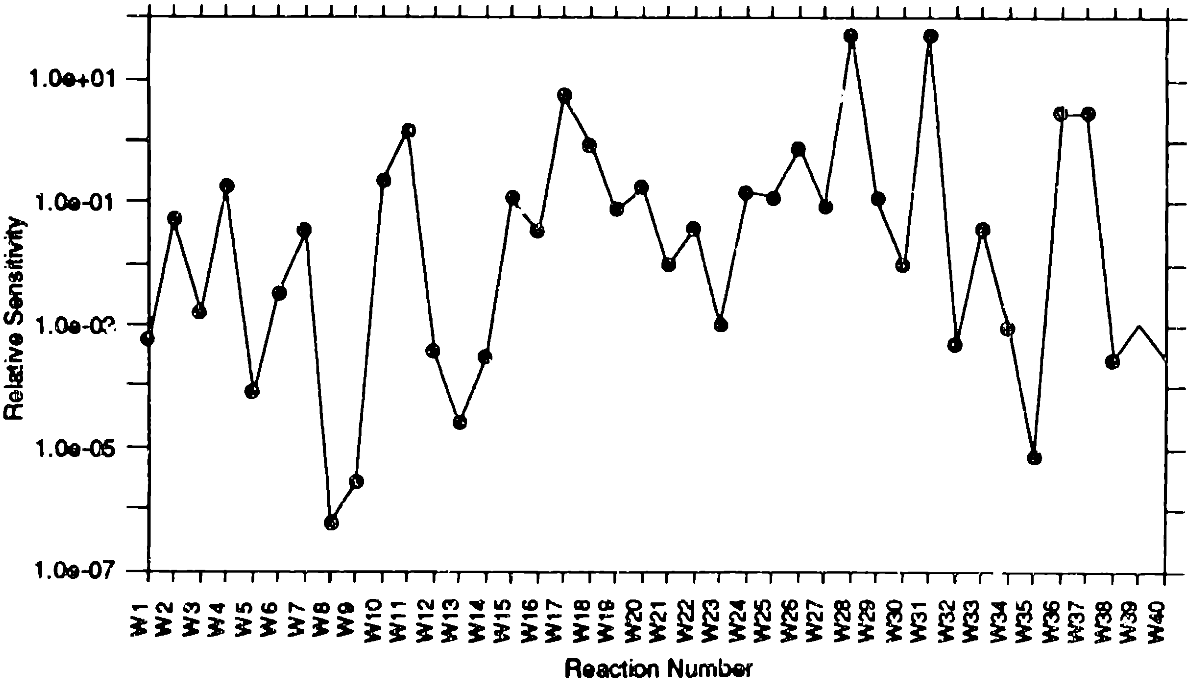


Figure 8-25 Relative sensitivities of oxygen concentration with respect to reaction rate constants in the core bypass channel under NWC.

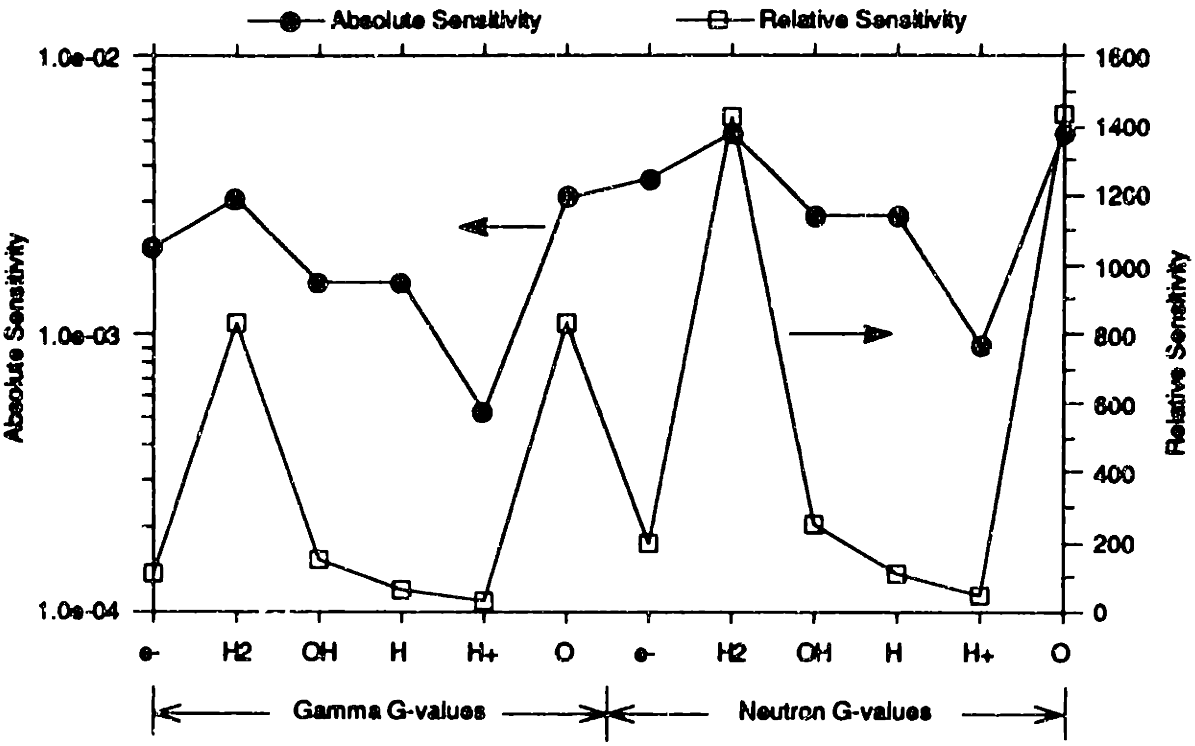


Figure 8-26 Absolute and relative sensitivities of oxygen concentration with respect to g-values in the core bypass channel under NWC.

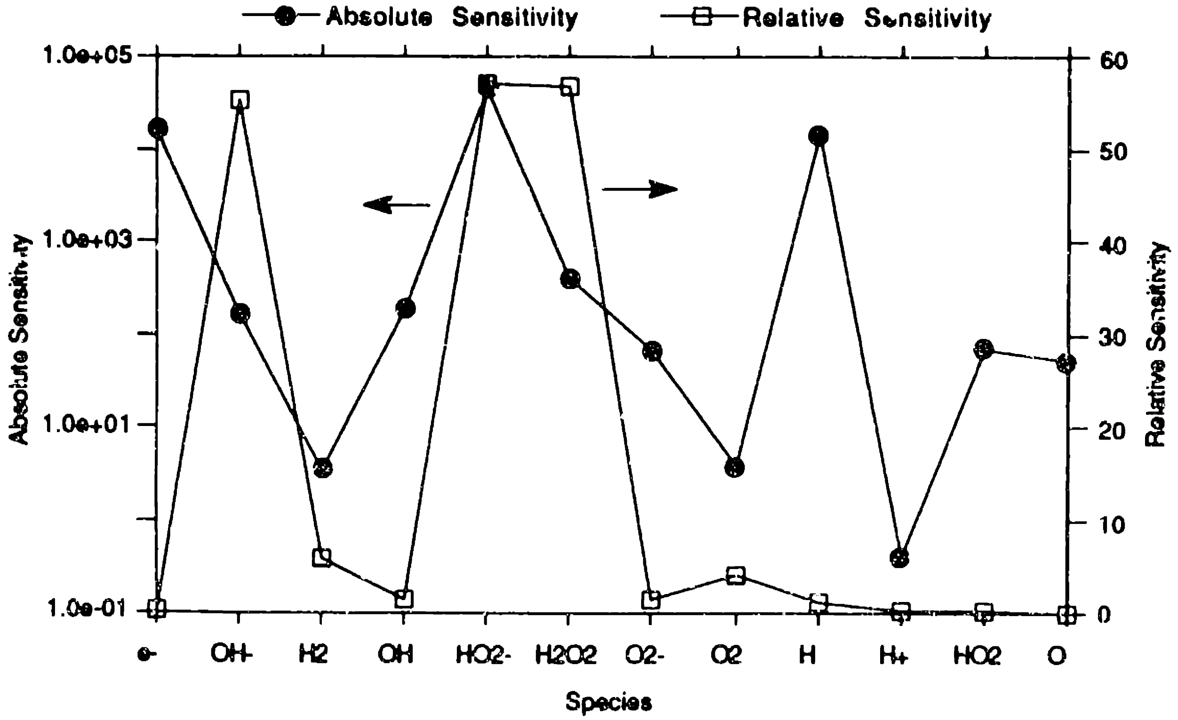


Figure 8-27 Absolute and relative sensitivities of oxygen concentration with respect to inlet concentrations in the core bypass channel under NWC.

Table 8-4 Sensitivity Results For O_2 In the Recirculation Line Under NWC

```
-----------------------------------------------------------------------------

          RECIRC            SENSITIVITY RESULTS FOR O2

-----------------------------------------------------------------------------

              ============ ADJOINT RESULTS ============

   e-        =   -0.384494E+00 **    OH-       =    0.397681E-05 **
   H2        =   -0.394347E-02 **    OH        =   -0.400419E-01 **
   HO2-      =   -0.128414E-01 **    H2O2      =   -0.128454E-01 **
   O2-       =    0.565971E+00 **    O2        =   -0.185274E-04 **
   H         =   -0.433945E+00 **    H+        =   -0.397719E-05 **
   HO2       =    0.565967E+00 **    O2G       =    0.000000E+00 **
   H2G       =    0.000000E+00 **    O         =   -0.795751E-01 **
   H2O       =   -0.717518E-12 **    2H2O      =   -0.119067E-11 **


                                        ABSOLUTE      RELATIVE
            PARAMETER                  SENSITIVITY   SENSITIVITY
   -------------------------          ------------  ------------

   RATE CONST OF I 1                  -0.28840E-10  -0.92307E-05
   RATE CONST OF I 2                   0.28850E-10   0.92337E-05
   RATE CONST OF W 1                  -0.12358E-14  -0.65708E-07
   RATE CONST OF W 2                  -0.73902E-22  -0.58940E-05
   RATE CONST OF W 3                   0.76803E-25   0.61253E-08
   RATE CONST OF W 4                   0.28045E-21   0.12115E-04
   RATE CONST OF W 5                   0.22224E-25   0.73854E-09
   RATE CONST OF W 6                  -0.30461E-24  -0.20245E-07
   RATE CONST OF W 7                  -0.95110E-22  -0.60051E-05
   RATE CONST OF W 8                   0.13361E-24   0.72813E-12
   RATE CONST OF W 9                   0.50919E-22   0.84605E-12
   RATE CONST OF W10                   0.94411E-20   0.37648E-03
   RATE CONST OF W11                   0.61556E-19   0.24546E-02
   RATE CONST OF W12                   0.75864E-20   0.50420E-06
   RATE CONST OF W13                   0.51381E-25   0.76835E-10
   RATE CONST OF W14                   0.10739E-21   0.22482E-07
   RATE CONST OF W15                  -0.57360E-18  -0.27406E+00
   RATE CONST OF W16                   0.12224E-17   0.81242E-01
   RATE CONST OF W17                  -0.30780E-13  -0.12070E+02
   RATE CONST OF W18                   0.17042E-13   0.20582E+01
   RATE CONST OF W19                  -0.38596E-15  -0.18184E+00
   RATE CONST OF W20                  -0.64828E-17  -0.40931E+00
   RATE CONST OF W21                  -0.86638E-14  -0.23033E-01
   RATE CONST OF W22                  -0.58340E-15  -0.93703E-01
   RATE CONST OF W23                  -0.87853E-16  -0.25399E-02
   RATE CONST OF W24                  -0.59780E-11  -0.35846E+00
   RATE CONST OF W25                  -0.42808E-17  -0.28451E+00
   RATE CONST OF W26                  -0.27908E-16  -0.18548E+01
   RATE CONST OF W27                  -0.11146E-15  -0.21483E+00
   RATE CONST OF W28                  -0.26810E-13  -0.14354E+03
   RATE CONST OF W29                   0.39486E-05   0.27403E+00
```

```
                                    ABSOLUTE       RELATIVE
          PARAMETER               SENSITIVITY    SENSITIVITY
 -------------------------       ------------   ------------

 RATE CONST OF W30                 0.13793E-18    0.22918E-01
 RATE CONST OF W31                 0.42831E-08    0.14546E+03
 RATE CONST OF W32                -0.63169E-05   -0.15263E-01
 RATE CONST OF W33                 0.12534E-17    0.91631E-01
 RATE CONST OF W34                -0.33066E-19   -0.21976E-02
 RATE CONST OF W35                 0.98643E-16    0.15625E-04
 RATE CONST OF W36                -0.10671E-08   -0.67377E+01
 RATE CONST OF W37                 0.98853E-16    0.65699E+01
 RATE CONST OF W38                -0.63929E-15   -0.64147E-03
 RATE CONST OF W39                 0.23257E-15    0.25429E-02
 RATE CONST OF W40                -0.10423E-19   -0.69275E-03
 GAMMA    G-VALUE OF e-           -0.20747E-02   -0.26562E+03
 NEUTRON  G-VALUE OF e-           -0.35738E-02   -0.45754E+03
 GAMMA    G-VALUE OF H2           -0.30746E-02   -0.19682E+04
 NEUTRON  G-VALUE OF H2           -0.52994E-02   -0.33923E+04
 GAMMA    G-VALUE OF OH            0.15396E-02    0.34493E+03
 NEUTRON  G-VALUE OF OH            0.26538E-02    0.59457E+03
 GAMMA    G-VALUE OF H            -0.15421E-02   -0.14807E+03
 NEUTRON  G-VALUE OF H            -0.26589E-02   -0.25531E+03
 GAMMA    G-VALUE OF H+            0.52837E-03    0.67645E+02
 NEUTRON  G-VALUE OF H+            0.90486E-03    0.11585E+03
 GAMMA    G-VALUE OF O             0.30831E-02    0.19736E+04
 NEUTRON  G-VALUE OF O             0.53148E-02    0.34021E+04
 CONCENTRATION OF    e-           -0.17227E+05   -0.50078E-07
 CONCENTRATION OF    OH-          -0.19605E+03   -0.15268E+03
 CONCENTRATION OF    H2           -0.35650E+01   -0.42786E+01
 CONCENTRATION OF    OH            0.19243E+03    0.21035E-03
 CONCENTRATION OF    HO2-          0.50415E+05    0.19423E+03
 CONCENTRATION OF    H2O2         -0.46507E+03   -0.19169E+03
 CONCENTRATION OF    O2-           0.70620E+02    0.98686E-01
 CONCENTRATION OF    O2            0.38909E+01    0.38909E+01
 CONCENTRATION OF    H            -0.15642E+05   -0.12680E-03
 CONCENTRATION OF    H+            0.39721E+00    0.31143E+00
 CONCENTRATION OF    HO2           0.73026E+02    0.15624E-01
 CONCENTRATION OF    O             0.55104E+02    0.36396E-16
 CONCENTRATION OF    H2O           0.11336E-04    0.14889E+03
 CONCENTRATION OF    2H2O         -0.74143E-08   -0.40218E+01
```

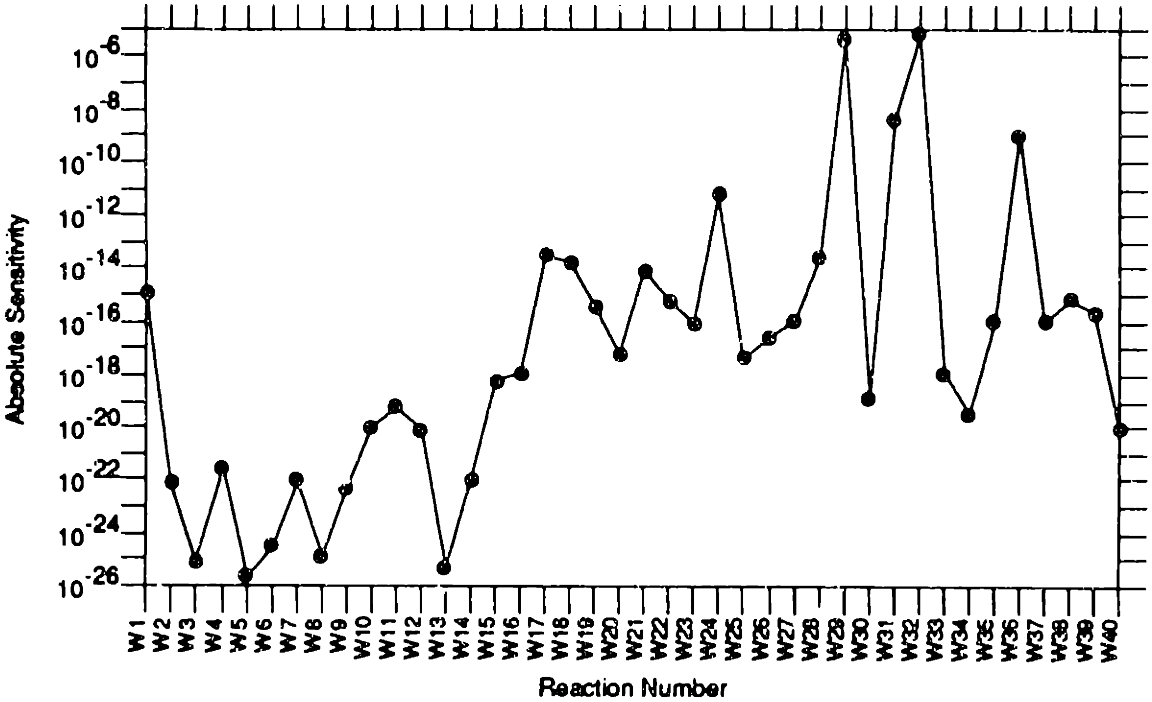


Figure 8-28 Absolute sensitivities of oxygen concentration with respect to reaction rate constants in the recirculation line under NWC.

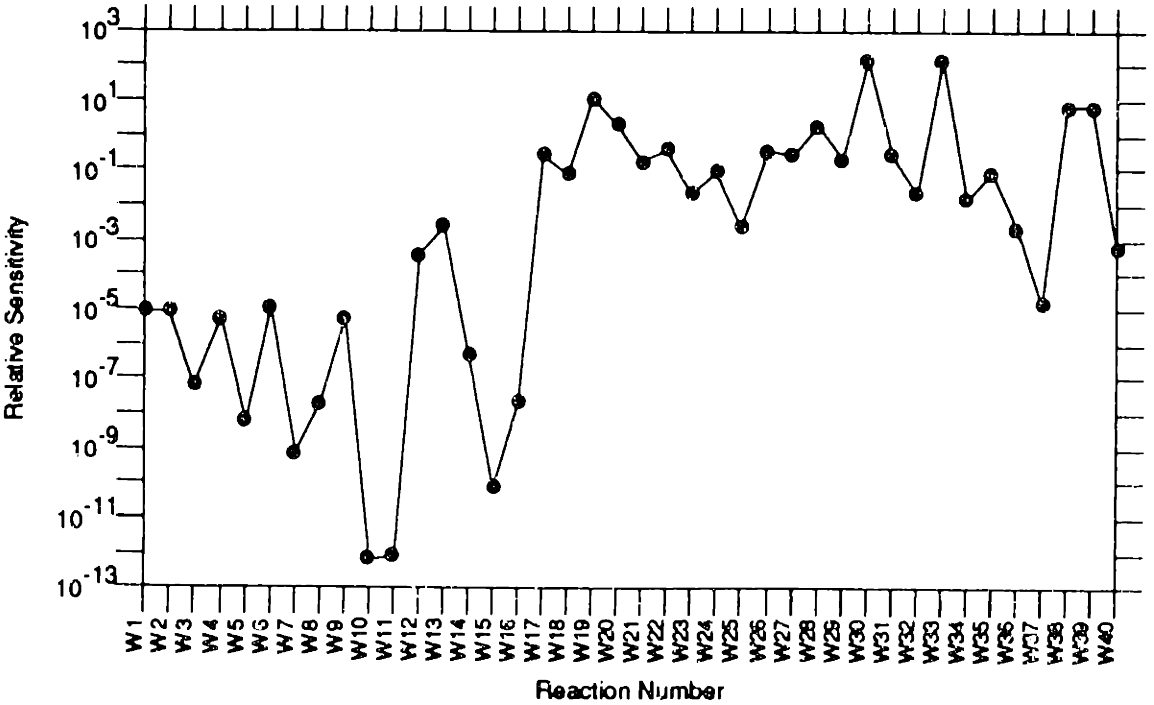


Figure 8-29 Relative sensitivities of oxygen concentration with respect to reaction rate constants in the recirculation line under NWC.

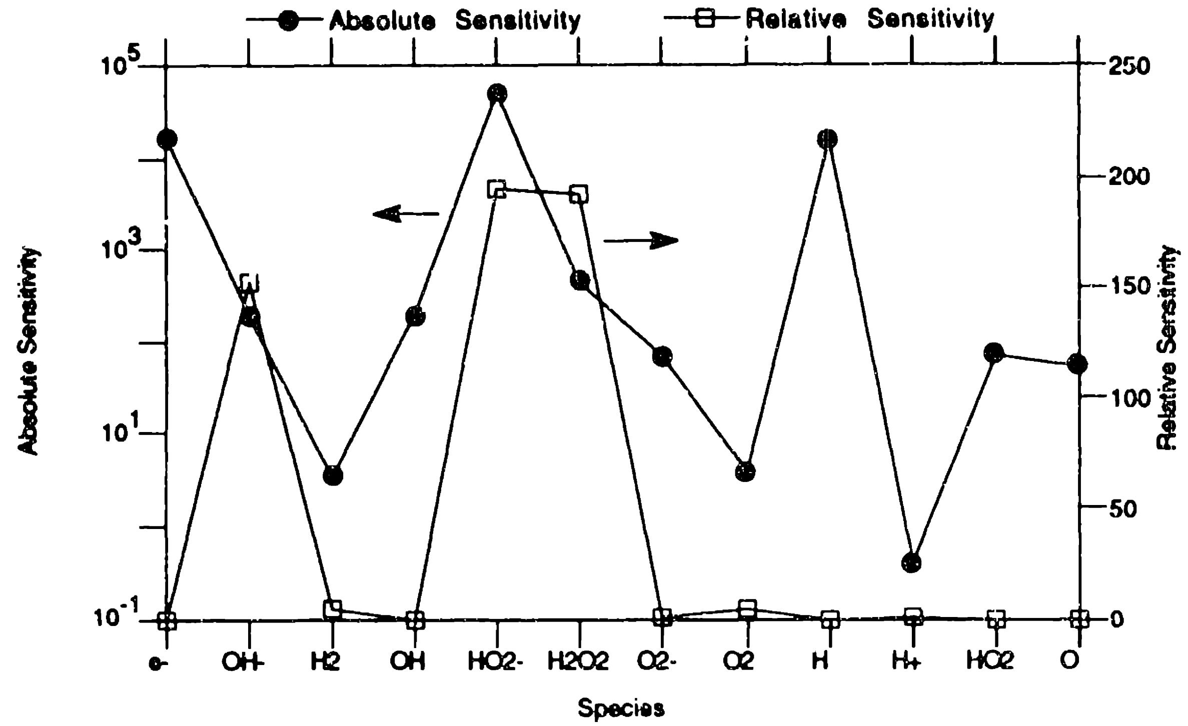


Figure 8-30 Absolute and relative sensitivities of oxygen concentration with respect to inlet concentrations in the recirculation line under NWC.

CHAPTER • 9

Conclusions

A water chemistry simulator for BWRs, RADICAL, has been successfully developed and applied to the Dresden-2 nuclear reactor. This accomplished the objective of this project: developing an in-house water chemistry simulator that is capable of predicting the corrosion environment of BWR components.

In this chapter, the significance of the simulation results is summarized and recommendations for future work are suggested.

I. Significance of Results

The most important result of the simulation performed on Dresden-2 unit using RADICAL is that the oxygen concentration in the recirculation line can be suppressed below the IGSCC threshold level of 20 ppb by injecting 300 ppb of hydrogen in the feedwater line. The simulation confirms the theory and experiments on hydrogen water chemistry and proves one more time that HWC is an effective method of mitigating IGSCC in existing BWR power plants with little modification to the power plant piping. Suppression of oxygen by HWC is less effective in the core boiling region where the dissolved hydrogen is stripped to the vapor phase, lessening the hydrogen concentration in the liquid phase.

The results of this simulation, however, should be interpreted only qualitatively since the model does not completely account for all significant effects. For instance, the simulation results show that the oxygen level in the recirculation line is completely suppressed by injecting 2 ppm of hydrogen, whereas measurements show that oxygen is still present in such a case. Also the presence of impurities in the coolant may affect the results; only pure H_2O coolant has been considered in this thesis.

The sensitivity results revealed that certain parameters that are not intuitively obvious affect the oxygen concentration significantly. The results also showed that the mechanism of oxygen suppression is different in single-phase liquid flow and two-phase flow. The general qualitative shapes of sensitivity plots were quite similar in all regions, which proved that certain important parameters are important in all regions.

The sensitivity results showed that g-values affect the oxygen concentration most significantly. This suggests that careful evaluation of g-values should be performed for accurate simulation results. The simulation results, along with the sensitivity results, should provide a useful guide to experiments which should be performed.

II. Future Work

RADICAL 1.0 is only a beginning step in a long-term goal of better understanding and controlling BWR corrosion, thus extending plant life and availability. The models used in RADICAL are mostly first-order and some, such as the mass transfer between liquid and gas phases, are, in effect, zeroth order approximations. There are many parameters used in RADICAL and many of them are also quite doubtful; the gas release and absorption coefficients, for instance, have been empirically estimated to reproduce observed values.

Careful evaluations of g-values, reaction rate constants, gas release and absorption coefficients, gamma and neutron doserates and the heterogeneous decomposition of H_2O_2 may prove to be a necessary step in bringing the simulator closer to reality. The selection of important parameters can be aided by the sensitivity routine built into RADICAL. Inclusion of metal impurity effects may also become important in certain parts of a BWR, as suggested by Ruiz, et. al. [1989]. This may be achieved by including reaction sets for the metal ions in the water reaction set presently used. Better representation of the steam separation region, with its swirling flow and large wetted surface area, should also be investigated.

Incorporation of nitrogen reactions will make the code more useful, particularly for evaluation of N-16 carryover effects. The additional computed vs. measured data made possible in this augmentation will also help validate code modelling.

The simple two-phase model may also be improved for more accurate simulations. Mason used a plug flow model to better approximate the slow coolant flow in the upper plenum [1990]. The present model is one dimensional, which does not consider the radial concentration gradient. This may not pose a great problem where the coolant velocity is significant in the axial direction, such as the boiling channel, but this may have to be reconsidered in slow regions such as the upper and lower plena.

RADICAL is expected to be incorporated as a part of the code package which is to evolve as a comprehensive corrosion simulator; the code developed by Psaila-Dombrowski [1990] which simulates crack-tip chemistry will be a part of this development.

RADICAL, in its present form, performs chemistry analyses which have not been possible before; its unique incorporation of the sensitivity routine represents significant progress over earlier simulators. RADICAL is capable of simulating other power plants and experimental loops with little modification of the Dresden-2 input file provide in this thesis. The simulator has proved itself as a helpful tool in chemistry studies here at MIT on a number of preliminary applications; RADICAL should also prove to be an indispensable tool elsewhere through further modification and improvements.

APPENDIX • A

RADICAL - User's Manual

This User's Manual contains a tutorial on how to use RADICAL 1.0. This includes preparing an input file, compiling and running the code, and interpreting the output files. The Dresden-2 simulation is used as an example. It is assumed that the code is run on the MicroVAX-II system with MicroVMS 5.0 and VAX FORTRAN 4.2 on which RADICAL was originally developed. The user should be familiar with the operating system and file handling procedures. The code should run on other computer systems with little modification and, in such cases, this User's Manual should provide the necessary guidelines to operate the code.

In the examples that follow, the following notation conventions are used: Helvetica (i.e., san serif font) is used to denote computer responses; Courier bold typeface shows user keyboard input; Times is used to flag explanations. For example, consider the sequence

```
$ RUN  RADICAL                    this runs RADICAL.
```

The computer displays $ on the screen and the user types **`RUN  RADICAL`**. The comment 'this runs RADICAL' explains the action taken. Courier is a monospaced font, and is used here to clearly denote blank spaces; the same font is used for program listing and input/output files.

I. Overview of RADICAL

RADICAL (Radiation Chemistry Analysis Loop code) is a general purpose computer code which is designed to simulate the chemistry of flow channels under irradiation. The primary purpose of RADICAL is to simulate the coolant chemistry of boiling water reactors (BWRs) but it is versatile enough to be used with a wide variety of reactors and test loops.

In the heart of the code are radiolysis equations which are a set of spatial differential equations describing species balances, under chemical, radiolytic, mass transfer and convection effects, of a control volume in a two-phase flow system. This set of differential equations is fed into a differential equation solver subroutine LSODE along with such parameters as the boundary conditions describing concentrations, radiation fields and thermalhydraulic conditions. This stepwise solution is repeated over each component of the loop until the code goes through the specified number of cycles around the entire loop.

A loop is broken down into components which are the building blocks of the loop. Each component has a set of input parameters unique to the component. For instance, the primary region of a BWR is divided into the core, upper plenum, downcomer, etc. Once all components are defined and the input parameters are prepared, the components are connected in series and parallel connections similar to the way an electrical circuit is composed of series and parallel combinations of resistors, capacitors, etc. In this process a node number is specified where two or more components join together. If necessary a component in a loop may be subdivided into a number of parallel and series components to better model the actual component. For instance, Ibe subdivided the downcomer region into four sections to better approximate the γ dose rates [Ibe 1986].

Concentration calculations start at the inlet node of a component specified by the user. Initial concentrations are specified for this component. Once the calculation of the first component is completed, the code proceeds to the next component as specified by the node information in the input file. This next component may be in either series or parallel connection with the first component; RADICAL knows this from the inlet and outlet nodes specified for the component. Keeping track of whether components are in series or parallel connections becomes important in calculating the initial concentrations for the next component from the concentrations of the previous component. For a series connection, it is obvious that the initial concentrations of the next component should be the final concentrations of the previous component. For a number of parallel components connected to a single component, the effective initial concentrations of the single component should be the flowrate-weighed average of the concentration of the parallel components. This automatic calculation of initial concentrations may be overridden by specifying the initial concentrations for a component. In the Dresden-2 input file, the initial concentrations of the component Feedwater have been specified in this way.

One cycle of calculation is completed when RADICAL goes through the entire loop and comes back to the first component it began with. RADICAL also allows multiple cycles through the loop. This is especially useful when the initial concentrations of the first component are not well known, and must be guessed. By running RADICAL a number of cycles, the user can see how good the guesses are by comparing the guessed values to the final concentrations of the last component. Many cycles can be repeated to converge upon a steady-state solution, if such exists. In the Dresden-2 example, two successive cycles were examined.

After familiarization with the code by running a sample, the details of the code operation will be considered.

II. Compiling RADICAL

The RADICAL code package consists of three parts: RADICAL.FOR, RADICAL.BLK, LSODE.FOR. RADICAL.FOR is the source code of RADICAL and RADICAL.BLK is a small text file containing global constant and variable declarations.

LSODE.FOR is the source code of the differential equation solver used in RADICAL.FOR. These files are available from the author on Vax 5 1/4", tape, Apple Macintosh 700 K disk, or IBM-PC diskettes of any kind: John H. Chun, Nuclear Reactor Laboratory, Massachusetts Institute of Technology, 138 Albany Street Rm. NW13-239, Cambridge, MA 02139, (617) 253-5368.

RADICAL runs on double precision, and the source files should be so compiled. First, make a subdirectory called RADICAL and copy all three of the above-named files. Compile and link them as follows:

```
$ for/g  radical,  lsode              compile with double precision option (/g)
$ lin  radical,  lsode
```

III. Input/Output File

In the distribution disk, a sample input file called Dresden0.In is included. This is the input file for Dresden-2 simulation with normal water chemistry. Copy this file to the subdirectory RADICAL and run RADICAL as follows:

```
$ r  radical
INPUT FILE: dresden0.in
```

The code should start execution and messages will be displayed on the terminal screen. It takes approximately 30 minutes on a MicroVAX-II to complete execution.

Once the execution is completed, there should be three output files produced: DRESDEN0.OUT, DRESDEN0.PLOT, DRESDEN0.SENS. DRESDEN0.OUT contains all input parameters and calculated results for all species and operating conditions. DRESDEN0.PLOT contains concentrations of all species for the last cycle, i.e., second cycle in this example. This file is used by RS/1 to plot graphs of concentrations. DRESDEN0.SENS is similar to DRESDEN0.OUT but contains sensitivity results for all species and parameters. This file is also used by RS/1 or similar plotting software to produce graphs.

These text files may be viewed on the screen, printed on the printer, or edited in a text editor. To view the input file, type

```
$ ty  dresden0.in
```

This displays DRESDEN0.IN on the screen without pause. Scrolling may be paused by depressing the Hold Screen button or Ctrl-S (i.e. depress the CONTROL key and the S key on the keyboard simultaneously). The pause can be cancelled by depressing the Hold Screen once more or Ctrl-Q.

A file can be printed by

```
$ pr  dresden0.in
```

or edited using the EDT text editor by

```
$ e  dresden0.in
```

The input file DRESDEN0.IN may be easily changed to simulate hydrogen water chemistry (HWC) by changing the initial hydrogen concentration in the feedwater. Fig. A-1 shows the feedwater portion of the input file. Here the bold-faced 0.0 under $INITIALCONC may be changed to appropriate values to simulate HWC: 1.1115D-4 for 0.3 PPM H_2; 1.8525D-4 for 0.5 PPM H_2; 2.9640D-4 for 0.8 PPM H_2; 7.7805D-4 for 2.1 PPM H_2. The input file format should not be disturbed when modifying input files; pay particular attention to delimiters such as spaces and commas - when in doubt, follow the sample input file exactly. Comments may be freely added to an input file in between blocks of data.

The output results may be plotted using RS/1 on MicroVAX, or similar software. The output file DRESDEN0.PLOT is used for this purpose. The plot file contains one column of numbers for distances and concentrations. The RS/1 procedure RADPLOT (see the listing in Appendix C) may be used within RS/1 to automatically plot simulation results. The user is recommended to import/compile/run the procedure within RS/1 and customize to personal taste. The procedure should be easy to run with the step-by-step instructions given here. The plot file may also be read by other software to produce graphs. For the plots in this thesis, the plot files were converted to multiple columnar format (see

```
**********************************************************************
 @FEEDWATER

 $POSITION
 XLENGTH  =     1.0000000000000      ,
 XBOIL    =  9999.0,
 $END

 $STATE
 VELINLET =     1.0D6,
 FLOWRATE =     0.125,
 $END

 $DOSESHAPE $
 $VOIDFRACTION $

 $INITIALCONC
 CONC =    2*0.D0,0.0,2*0.D0,
          2*0.D0,8.1047D-7,2*0.D0,
          4*0.D0,41.1666666667,
          1694.7
 $END
 0.3 PPM H2 = 1.1115D-4
 0.5 PPM H2 = 1.8525D-4
 0.8 PPM H2 = 2.9640D-4
 2.1 PPM H2 = 7.7805D-4

 $FLAG $
 $SENSITIVITY $

 @END OF FEEDWATER
**********************************************************************
```

Figure A-1 Feedwater portion of the DRESDEN0.IN input file.

DRESDEN0.MAC in **Appendix C**) and transferred to a Macintosh, where Kaleidagraph 2.0 was used to produce the graphs.

IV. Input Parameters

In this section the input parameters for RADICAL are described in detail. In the beginning of the code, RADICAL reads information pertinent to the entire loop. These are divided into several groups and read one group at a time using the **NAMELIST** input method of VAX FORTRAN. This is a non-standard input method employed by VAX FORTRAN and used here for its convenience and compactness.

```
 $SIZE
 NSPECIES  =        16,
 NRX       =        47,
 NSURFRX   =         1,
 NCOMP     =        17,
 NNODE     =         9,
 NCYCLE    =         2,
 $END
```

this line starts at SECOND column.
parameter name = parameter value,
comma is optional but better have it.

a group ends with this line.

Figure A-2 Example of NAMELIST.

NAMELIST works this way: First, a set of parameters is defined under a group name; In the input file, a group name is followed by the dollar sign ('$') which is placed at the *second* column of the input file. No space is allowed between the dollar sign and the group name; the parameter list begins one line below the group name and the parameter is followed by the parameter name and the equal sign ('='); Parameters may be in any order; Not all parameters should be declared. If a parameter is not declared, it defaults to the previous value. This is a convenient way of not having to re-input the parameter. Once all parameters have been declared, the group is followed by '$end' which also starts at the second column of the last line of the group. NAMELIST is insensitive to upper/lower cases.

For each component, there are seven such NAMELIST groups. All group names must be present for each component even if no parameters are explicitly declared, in which case the group name is immediately followed by a space and the dollar sign (see `$DOSESHAPE $` in Fig A-1). Most parameters default to the previously declared values unless explicitly assigned. Exceptions are:

`XInitial` - set to the previous `XFinal`
`TempIn` - set to the previous `TempOut`
`VelInlet` - adjusted to diameter

When in doubt, declare all parameters explicitly.

An example of NAMELIST is illustrated in Fig. A-2.

The groups and the parameters in the input file are:

Group Name : **FileName**

`OutFile` : Output file name

`PlotFile` : Plot data file name
`SensFile` : Sensitivity plot data file name

Group Name : **SIZE**

`NSpecies` : Number of species to be considered
`NRx` : Number of chemical reactions to be evaluated
`NSurfRx` : Number of surface decomposition reaction included in the reactions
`NComp` : Number of components to be evaluated
`NNode` : Number of nodes connecting components

Group Name : **CONTROL**

`NodeStart` : Node number at which evaluation is to begin
`TempRef` : Reference temperature at which reaction constants are given (kelvin)
`PlotOut` : Flag used to control plot file.
= .T. create plot file to be read by RS/1 (default)
= .F. don't create plot file
`LinLin` : Method flag used to control plot data format.
= .T. write linear concentration and linear position (default)
= .F. write log concentration and linear position
`SENS` : Flag used to control sensitivity analysis routine for entire loop.
= .T. evaluate sensitivity of selected components
= .F. don't evaluate sensitivity at all
(each component has its own flag to indicate if sensitivity is to be evaluated for that component. This is accomplished by turning on and off the flag `CalcSens`).
`DEBUG` : Flag used to control debug routines of the code. There are a number of them built into the code and each one should be turned on separately. Default is .False.
`Normalize` : Flag used to control normalization of concentrations output with respect to density.
= .T. normalize concentrations
= .F. don't normalize concentrations (default)
`PPBOUT` : Flag used to control the value of concentrations output.
= .T. convert concentrations to ppb
= .F. leave concentrations in mol/liter (default)

The next group is **LSODEData** and is used to control LSODE. A more detailed explanation of these items is found in the LSODE writeup.which is listed in Appendix C.

`ITASK` : See writeup
`RTOL` : Relative tolerance
`ITOL` : See writeup
`ATOL` : Absolute tolerance
`RWORK` : See writeup
`IWORK` : See writeup
`MF` : Method flag

The next two groups **ADJDATA** and **RESDATA** are identical to **LSODEData** but used for adjoint and response routines. The parameters for the adjoint calculation have the prefix

ADJ in front of the names and the parameters for the response calculation have the prefix RES in front of the names.

Next, g-values for both gamma and neutron radiation and the molecular weight of each species are read in **GVALUE**. Then names of species enclosed in single quotes are read in **NAMES**. Following this, the reaction matrix which contains reaction name (3 characters long), reactants (up to 3 species), products (up to 4 species), rate constants, and activation energies (kJ/mol-kelvin) are read in **REACTION**. Gas reactions are input with mass transfer coefficients in the place of rate constants and the activation energies are set to -1. The last input item is the node information for each component read in **COMPONENTS**. This includes the inlet and outlet nodes defined by the coolant flow direction. The third column is used to indicate if initial concentrations for the component are given.

Once all of the above information is read in, RADICAL starts calculation by reading parameters specific to each component. The input method is similar to the loop information input.

Group Name : **POSITION**

`XInitial` : Initial position of the component (cm).
`XFinal` : Final position of the component (cm). XLength may replace XFinal.
`XLength` : Length of the component (cm). If XInitial and XFinal are given XLength is calculated internally.
`XStep` : Step size at which to print concentration output (cm).
`XBoil` : Position at which boiling occurs (cm). If no boiling occurs within the component, give it a very large number such as 99999 cm.
`XBoilOffset` : Offset used to avoid singularity at XBoil. The default value is 1E-10

Group Name : **STATE**

`TempIn` : Inlet temperature (kelvin).
`TempOut` : Outlet temperature (kelvin). Temperature gradient is calculated assuming linear profile using TempIn and TempOut. But in case boiling occurs within the component, TempOut is maintained from the point of boiling to the exit.
`GammaRate` : Dose rate of gamma radiation (Rad/s).
`NeutRate` : Dose rate of neutron radiation (Rad/s).
`VelInlet` : Liquid velocity at inlet (cm/s).

`Diameter`	: Diameter of the flow channel (cm). This is used to scale decomposition rate and velocity change.
`DensLiq`	: Liquid density (g/cc).
`DensGas`	: Vapor density (g/cc).
`Pressure`	: System pressure (atm).
`FlowRate`	: Mass flowrate (g/s).
`Surface`	: Wall material to be used in decomposition calculation. Should be the same name given as the reaction name.

Next, coefficients of dose shape functions for gamma and neutron radiation are read in **DoseShape**. Flux shapes are fit by a polynomial whose order is given by MAXORDERD and each of the coefficients is input through GAMMAC and NEUTRONC. In similar fashion, void fraction is read in **VoidFraction** through VOIDC. The order of the void fraction polynomial is given by MAXORDERV. Then initial concentrations at XInitial are read in **InitialConc** into the concentration array Conc. Flags are read next in **FLAG**, which includes:

`CalcSurf` = .T. Calculate surface decomposition in this component.
= .F. Don't calculate surface decomposition (default).
`VoidFlag` = .T. Coefficients read in **VoidFraction** are for void fraction (default).
= .F. Coefficients read in **VoidFraction** are for quality.
`CalcSens` = .T. Calculate sensitivity for this component.
= .F. Don't calculate sensitivity for this component (default).
`WriteRx` = .T. Write temperature scaled reaction matrix.
= .F. Don't write it (default).
`WritePara` = .T. Write parameters at each XStep.
= .F. Don't write them (default).

The last input information is pertinent to sensitivity routines and are read only if CalcSens is true. These entries are

`SensStep`	: Number of steps to divide XStep by where concentration profile and adjoint profile are stored. Leave blank for default value of maximum.
`NSens`	: Number of species the sensitivity results are to be calculated for.
`SensSpecies`	: Species for which sensitivity is to be calculated.

To see how these parameters are actually declared and used, see Appendix D for the input file DRESDEN0.IN.

APPENDIX • B

RADICAL - Programmer's Manual

This manual is written for the experienced users of RADICAL who wish to modify the code. RADICAL was originally developed in VAX FORTRAN 4.2 on the MicroVAX-II under MicroVMS 5.0. VAX FORTRAN is very similar to the ANSI standard FORTRAN-77 but includes more advanced functions. Careful attention has been given to avoid any non-standard usage of commands and functions as the code was developed, but for the sake of optimization, a minimum number of non-standard functions were used. These non-standard functions, however, may be translated or rewritten without much difficulty.

I. Code Structure

The RADICAL code was written with a careful attention to its structure and readability; abundant comments and indentations were used. The code is also broken down into a number of nested logical blocks in the form of subroutines and functions which are self-explanatory. Once the global code structure is understood, modifying the code should be a straight-forward task.

There are three files in RADICAL: the first is the main code RADICAL.FOR and the second is the global-variable block RADICAL.BLK which contains global constants, variable declarations, and common variable declarations. The third is LSODE.FOR which is a numerical solver for a system of nonlinear differential equations. LSODE was devel-

```
RADICAL.BLK

        DOUBLE PRECISION DECLARATION

        CONSTANT VARIABLE DECLARATION

        INTEGER VARIABLE DECLARATION

        REAL VARIABLE DECLARATION

        CHARACTER VARIABLE DECLARATION

        BOOLEAN VARIABLE DECLARATION

        COMMON BLOCK DECLARATION
```

Figure B-1 RADICAL.BLK structure

oped at the Lawrence Livermore National Laboratory by Alan C. Hindmarsh. As for RADICAL, LSODE is used as a black box which takes parameters and returns the solutions. RADICAL.BLK is inserted in each subroutine of RADICAL.FOR by a non-standard statement INCLUDE so that global variables do not have to be declared in each subroutine. This reduces the code size substantially. All three files are text files which may be transferred from one computer to another. RADICAL should run on a number of computer systems with little modification. No attempt is made to explain in detail what LSODE does, except a text file LSODE.WRITEUP is included in this thesis and on the distribution disk. Further details of LSODE may be found in the references given at the end of the thesis.

The structure of RADICALBLK is outlined in Fig. B-1. RADICAL.BLK declares all global constants, variables, and common blocks. All global variables are necessarily common to all subroutines to reflect a change of a variable within a subroutine in the rest of the code. A more detailed description of variables will be discussed in section II.

The flowchart of RADICAL is illustrated in Fig. B-2. The flowcharts for the subroutines INITIALIZE and CalcLoop are depicted in Figs. B-3 and B-4. The structure of the main code RADICAL.FOR is given in Fig. B-5. The code is composed of a number of nested subroutines to provide an easy mental visualization of the code flow. The subroutines and functions called within a subroutine are indented for better visualization.

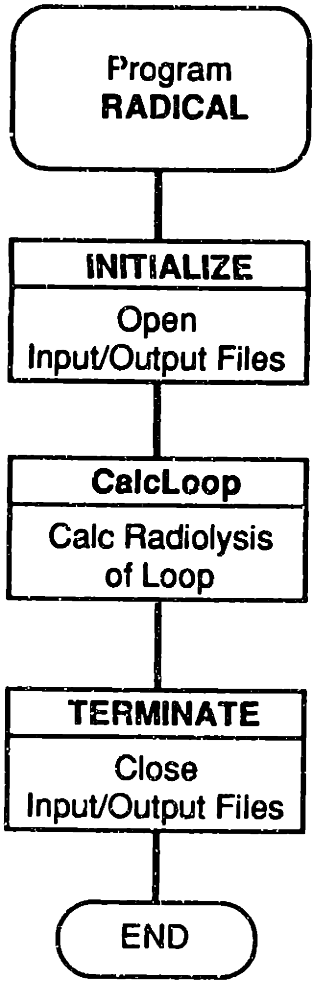


Figure B-2 Flowchart of RADICAL.FOR main subroutines.

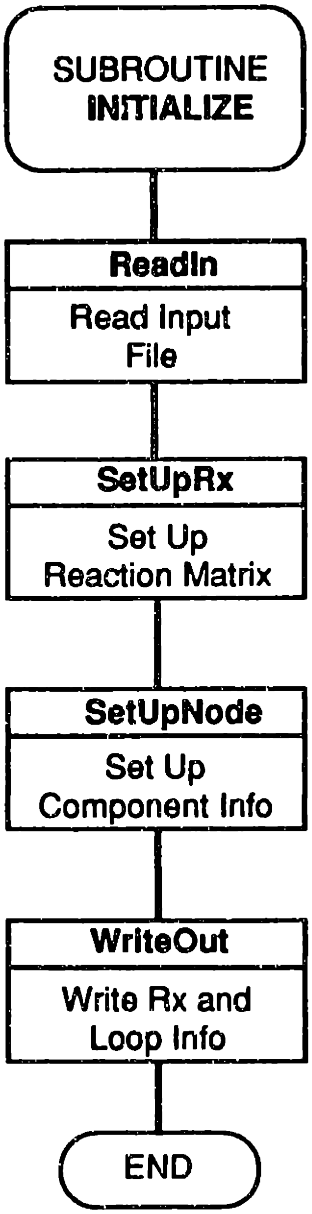


Figure B-3 Flowchart of the subroutine INITIALIZE.

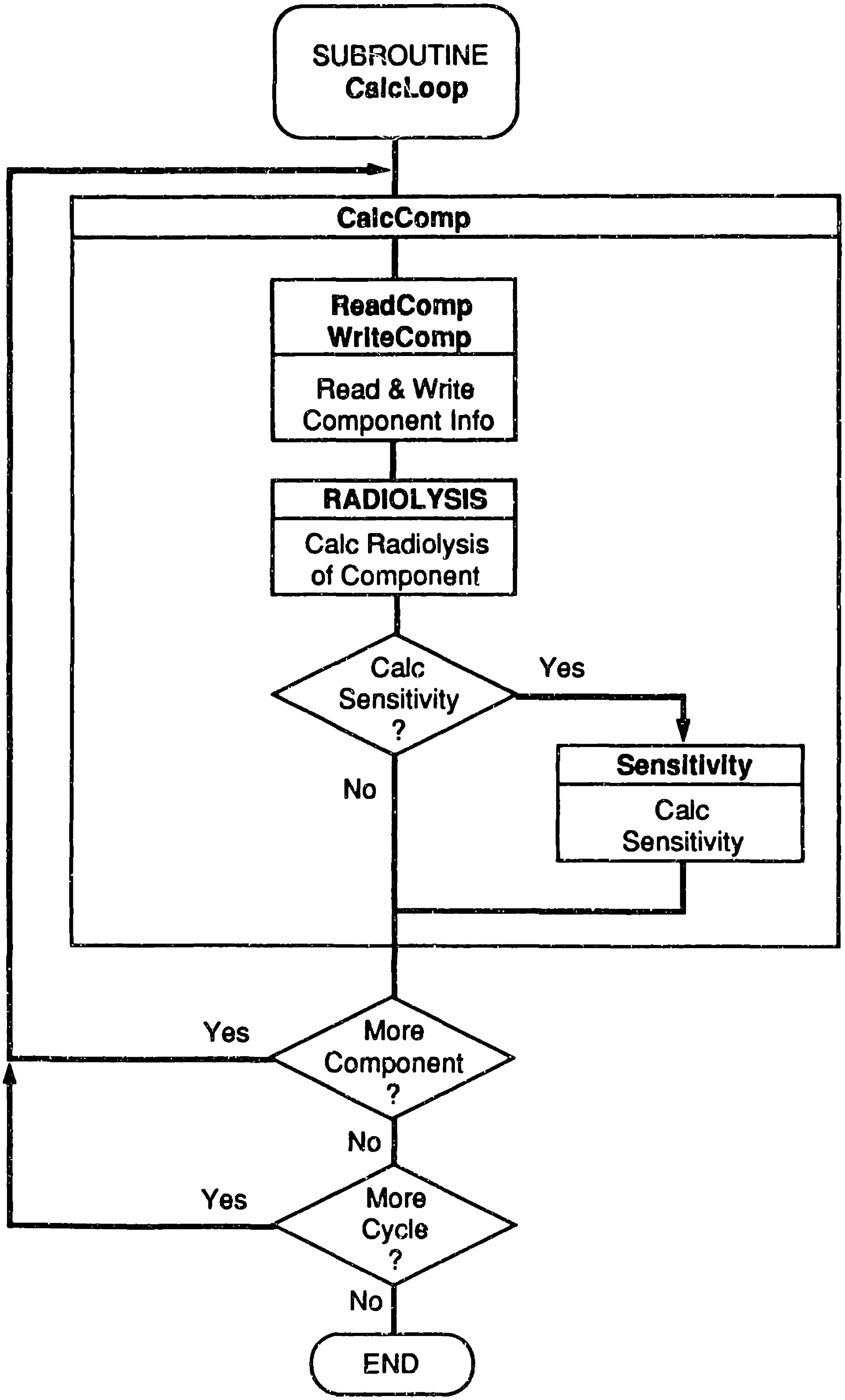


Figure B-4 Flowchart of the subroutine **CalcLoop**.

```
PROGRAM RADICAL

    INITIALIZE
        SECNDS (VAX FORTRAN intrinsic function)
        ReadIn
            FindLine
        SetUpRx
        SetUpNode
        WriteOut
            DATE (VAX FORTRAN intrinsic function)
            TIME (VAX FORTRAN intrinsic function)
    CalcLoop
        CalcComp
            SECNDS
            ReadComp
                FindLine
            ADJUST
            WriteComp
                ARRHNIUS
            RADIOLYSIS
                CONCENTRATION
                    LSODE
                        FRO
                            DoseShape
                            TwoPhase
                            ARRHENIUS
                        JACOB
                WriteConc
            WriteStat
            Sensitivity
                SECNDS
                ADJOINT
                    LSODE
                        AdjFRO
                            INTERPOLATE
                            TwoPhase
                            JACOB
                        AdjJacob
                            INTERPOLATE
                            TwoPhase
                            JACOB
                RESPONSE
                    LSODE
                        ResFRO
                            INTERPOLATE
                            TwoPhase
                            DoseShape
                        ResJacob
                WriteSens
                    SECNDS
        AverageFlow
        PUSH
        PULL
    TERMINATE
        SECNDS
```

Figure B-5 RADICAL.FOR code structure.

The structure of LSODE.FOR is not discussed in this manual. Although LSODE is used as a blackbox in RADICAL, a few points are worth mentioning at this point. A brief description and an example is found in the beginning of LSODE.WRITEUP. The WRITEUP gives a more detailed description in its second half. In RADICAL, LSODE is called three times; first in the subroutine CONCENTRATION where, as the name implies, the concentration profile as a function of position is evaluated. Once the entire concentration profile is evaluated, LSODE is called upon the second time in the subroutine ADJOINT where the adjoint of the concentration profile is evaluated. In this case the adjoint is evaluated backward in space, evaluating from the final position to the initial position. Lastly, LSODE is called in the subroutine RESPONSE where the response of the concentration profile with respect to a number of parameters is evaluated. If the sensitivity analysis is not requested, LSODE is called only once in the subroutine CONCENTRATION.

Each time LSODE is called, LSODE needs two user-supplied subroutines to proceed with the calculation: The first is generically named F, which contains the differential equations to be solved; The second is generically named JAC, which contains the Jacobian of the differential equations given in F. JAC is optional; LSODE can evaluate the Jacobian internally, but slowly. For each of the three calls to LSODE, a set of F and JAC should be provided. In the subroutine CONCENTRATION, FRO and JACOB correspond to F and JAC. FRO contains a set of differential equations, dC/dx, which describes the change of chemical species concentration with respect to position as the coolant flows through a pipe. JACOB contains the Jacobian of the differential equations in FRO. In the subroutine ADJOINT, AdjFRO and AdjJACOB correspond to F and JAC. AdjFRO contains the adjoint of the concentration equation and AdjJACOB contains the Jacobian of the adjoint. This Jacobian turns out to be the transpose of the Jacobian evaluated in JACOB, so AdjJACOB calls JACOB to obtain the Jacobian which is transposed to get the Jacobian for the adjoint. In the subroutine RESPONSE, ResFRO and ResJACOB correspond to F and

JAC. ResFRO contains the response function of the concentration profile and ResJACOB contains the jacobian of the response function, which is zero in all cases.

Once LSODE is fed with F and JAC along with controlling parameters and initial conditions, it evaluates the differential equations using Gear's method. The functions used in RADICAL are generally stiff, *ie.*, change wildly along the integration path. LSODE is geared with routines that handles stiff problems rather well. LSODE is originally written as an initial-value time-dependent solver, but in RADICAL, the equations are converted to depend on position. This is not a major problem since, in principle, the two variables are interchangeable through the velocity.

II. Global and Local Variables

All global variables are declared in RADICAL.BLK and explained briefly in the beginning part of RADICAL.FOR. Local variables are declared in subroutines and also explained within each subroutine where local variables are declared.

Variable names are mostly self-explanatory. The variable names used in the input file are the same as the names used in the program. The reader is recommended to read the variable explanations in the source listing.

APPENDIX • C

RADICAL - Source Listing

This appendix contains the complete listing of RADICAL source code. There are two parts in the source listing: RADICAL.BLK which contains all global variables and RADICAL.FOR which is the FORTRAN-77 code of RADICAL. RADICAL.BLK is called by each subroutine of RADICAL.FOR to establish access to global variables and is primarily used for convenience and compactness of coding.

RADICAL has been developed on the MicroVAX-II computer system with MICROVMS 5.0 and VAX FORTRAN 4.2. VAX FORTRAN is an extension of ANSI FORTRAN-77 and RADICAL.FOR should compile on other computer systems equipped with a FORTRAN-77 compiler. Any deviation from standard FORTRAN-77 syntax has been documented within the code for easy modification.

I. RADICAL.BLK

RADICAL.BLK declares all global constants and variables. This file is made into a separate external file for the convenience of not having to declare global variables in each subroutine. This file also provides ready access to code capacity modifications. For instance, if more than the default number of 50 reactions is used in a simulation, the parameter IRX may be changed in this file to any size desired. The beginning of RADICAL.BLK is made up of such size parameters (i.e., constants). When the code application extends beyond the default capacity, these parameters should be changed and the code recompiled.

Following the size parameters are variable type declarations. All real variables are implicitly declared as double precision (8 bytes on the MicroVAX) and integers default to 4 bytes.

The directive COMMON provides a common ground for such declared variables. This is an easy way to declare global variables (global variables are those variables whose changes in a subroutine are reflected in the rest of the code). The global variables are grouped under appropriate group names.

```
C  RADICAL.BLK
C
C  THIS MODULE IS INCLUDED IN RADICAL AS A COMMON VARIABLE BLOCK
C  USED BY SUBROUTINES.
C
C  VERSION: 1.0         19 MARCH 1990
C
C  CODE CUSTODIAN: JOHN H. CHUN
C                  MASSACHUSETTS INSTITUTE OF TECHNOLOGY
C                  138 ALBANY STREET RM NW13-239
C                  CAMBRIDGE, MA 02139
C                  (617) 253-5368
C
C     IRX=REACTION ARRAY, ISP=SPECIES ARRAY, ICO=COMPONENT ARRAY,
C     INO=NODE ARRAY, IST=INTERPOLATE DATA POINTS ARRAY,
C     IRE=ARRAY OF THE NUMBER OF RESPONSE PARAMETERS,
C     ICY=ARRAY OF THE NUMBER OF CYCLES
C     IDE=ARRAY OF DEBUG FLAGS
C     IPO=ARRAY OF THE ORDER OF POLYNOMAL COEFFICIENTS
C     LRW=LIW=LSODE WORK ARRAY CALCULATED AS GIVEN IN LSODE WRITEUP.
C     ADJUST THESE FOR SPECIFIC APPLICATIONS.
C
      IMPLICIT DOUBLE PRECISION (A-H, O-Z)
      PARAMETER (IRX=50,ISP=30,ICO=30,INO=30,IST=1000,IRE=IRX+3*ISP,
     +           ICY=100,IDE=10,IPO=10,LRW=22+9*IRE+IRE*IRE,LIW=20+IRE)
      PARAMETER GasConst=8.314D-3
C
      INTEGER*4 CompNode(ICO,3),ResITASK,ResITOL,ResMF,
     +          AdjITASK,AdjITOL,AdjMF,SensStep,AdjIWORK(10),
     +          RESIWORK(10),ADJIOPT,RESIOPT
      REAL*4 TIME1,TIME2
      REAL*8 NeutRate,NEUTRON,NEUTRONC(0:IPO),MOLWT(ISP)
      CHARACTER*3 RxName(IRX),SURFACE
      CHARACTER*8 SpeciesName(ISP+1),SensSpecies(ISP)
      CHARACTER*16 CompName(ICO)
      CHARACTER*35 InFile,OutFile,PlotFile,SensFile
      CHARACTER*80 TitleLine
      LOGICAL*1 CalcSurf,PlotOut,LinLin,VoidFlag,CalcSens,SENS,WriteRX,
     +          WRITEPARA,DEBUG(IDE),NORMALIZE,PPBOUT,CycleOut(ICY)
C
      COMMON /FileName/ InFile,OutFile,PlotFile,SensFile,TitleLine
      COMMON /SIZE/ NSpecies,NRx,NSurfRx,NComp,NNode,NCycle,ITER
      COMMON /NAMES/ SpeciesName,RxName
      COMMON /POSITION/ XInitial,XFinal,XLength,XStep,XBoil,XBoilOffset
      COMMON /CYCLE/ ICycle,MaxNode,CycleOut
      COMMON /STATE/ TempIn,TempOut,TempRef,GammaRate,NeutRate,
     +               VelInlet,DIAMETER,TEMP,VelLiq,VelGas,
     +               PRESSURE,DensLiq,DensGas,FlowRate,FlowPara,
     +               SURFACE
      COMMON /LOOPFLAGS/ PlotOut,LinLin,SENS,IGFLAG,DEBUG,NORMALIZE,
     +                   PPBOUT
      COMMON /LSODEData/ IOPT,ITASK,RTOL,ITOL,ATOL,RWORK(LRW),
     +                   IWORK(LIW),ISTATE,MF
      COMMON /AdjLSODEData/ AdjRTOL,AdjITOL,AdjATOL,AdjMF,AdjITASK,
     +                      ADJIOPT,ADJRWORK(10),ADJIWORK
      COMMON /ResLSODEData/ ResRTOL,ResITOL,ResATOL,ResMF,ResITASK,
     +                      RESIOPT,RESRWORK(10),RESIWORK
      COMMON /GValues/ GGamma0(ISP),Gneut0(ISP),GConvert,
```

```
     +                 GGamma(ISP),GNeut(ISP),MOLWT
      COMMON /DoseShape/ MAXORDERD,GAMMAC(0:IPO),NEUTRONC,GAMMA,NEUTRON
      COMMON /VoidFraction/ VOID,VOIDC(0:IPO),MAXORDERV,QUALITY
      COMMON /DERIVATIVE/ DVFDX,DVLDX,DVGDX
      COMMON /CONCENTRATIONS/ CONC(ISP+1),ConcFinal(ICO,ISP),
     +                        ConcNode(INO,ISP)
      COMMON /REACTIONS/ IR(IRX,3),IP(IRX,4),RCInit(IRX),RCSurf(IRX),
     +                   RateConst(IRX),EA(IRX),KOEF(IRX,ISP)
      COMMON /TIME/ TIME1,TIME2
      COMMON /COMPONENT/ CompName,CompNode,NodeCount(INO,2),IComp,
     +                   NodeInfo(INO,2,ICO),CompFlowL(ICO),
     +                   CompFlowG(ICO),NodeStart,SUMFLOWRATEL,
     +                   SUMFLOWRATEG
      COMMON /COMPFLAGS/ CalcSurf,VoidFlag,CalcSens,WriteRX,WRITEPARA
C
      COMMON /CURVE/ MAXITER,ConcCurve(IST+1,ISP),AdjCurve(IST+1,ISP)
      COMMON /RESPONSE/ ResConc(IRE)
      COMMON /ADJOINT/ AdjConc(ISP),AdjET
      COMMON /SENSITIVITY/ SensStep,NSens,SensSpecies,ISens
```

II. RADICAL.FOR

RADICAL.FOR is the main code of RADICAL. The code is written in MicroVAX FORTRAN which is an extension of ANSI FORTRAN-77. Any deviation from the standard syntax has been internally documented and the code should compile on other compilers with little modification.

The code is designed top-down with many subroutines and comments and should be easy to follow. The code structure and variables are documented within the code for ready access. Each subroutine also has a brief section describing its function, other subroutines involved and important local variables used.

```
      PROGRAM RADICAL
C
C***********************************************************************
C                             RADICAL CODE PACKAGE
C                  RADIation Chemistry Analysis Loop code
C***********************************************************************
C
C     VERSION: 1.0                          19 MARCH 1990
C
C     LAST MODIFIED:                        14  JUNE 1990
C
C     DEVELOPMENT STAGE (IN REVERSE TIME)
C
C   1.BORN AGAIN FROM MITIRAD VERSION 7.0
C   2.SENSITIVITY ANALYSIS EXTENSION TO MITIRAD VERSION 6.0
C   3.MULTIPLE-COMPONENT EXTENSION TO MITIRAD VERSION 5.0
C   4.TWO-PHASE FLOW EXTENSION (VERSION MITIRAD 5.0)
C
C     CODE CUSTODIAN:   JOHN H. CHUN
C                       MASSACHUSETTS INSTITUTE OF TECHNOLOGY
C                       138 ALBANY ST. Rm NW13-239
C                       CAMBRIDGE, MA 02139
C                       (617) 253-5368
C
C     SOME IDEAS ADAPTED FROM S. A. SIMONSON'S BWRMIT, 8/05/88
C
C     OPERATING SYSTEM: MICROVMS VERSION 5.0
C                       VAX FORTRAN COMPILER VERSION 4.2
C
C***********************************************************************
C
C     RADICAL 1.0 NOTE
C
C       RADICAL CALCULATES CHEMICAL SPECIES CONCENTRATIONS OF COOLANT AS
C     A FUNCTION OF POSITION ALONG THE FLOW PATH WITH SUCH EFFECTS AS:
C
C            CHEMICAL REACTION
C            RADIOLYSIS
C            CONVECTION
C            MASS TRANSFER BETWEEN LIQUID AND GAS
C            SURFACE DECOMPOSITION OF H2O2
C
C       A LOOP SUCH AS BWR COOLANT LOOP IS DIVIDED INTO A NUMBER OF
C     COMPONENTS WHICH ARE CONNENCTED THROUGH A COMBINATION OF SERIES
C     AND PARALLEL FLOW PATHS.  PARAMETERS FOR EACH COMPONENT IS
C     INPUT THROUGH AN INPUT FILE WHICH CONTAINS SUCH INFORMATION AS:
C       TEMPERATURE, PRESSURE, VOIDFRACTION OR QUALITY, RADIATION DOSE,
C       INITIAL CONCENTRATIONS, FLOW VELOCITY, HYDRAULIC DIAMETER, LENGTH,
C       FLOWRATE, DENSITY, WALL MATERIAL, ETC.
C     CODE STARTS CALCULATION AT THE FIRST COMPONENT AND CONTINUES
C     CALCULATION ALONG THE FLOW PATH.  A COMPONENT WITH, FOR INSTANCE,
C     RADIAL GRADIENT OF RADIATION FIELD SUCH AS DOWNCOMER, MAY BE
C     SUBDIVIDED INTO A NUMBER OF PARALLEL SUB-COMPONENTS TO INCREASE
C     ACCURACY OF THE OUTPUT.
C
C       SENSITIVITY EVALUATOR IS ALSO INCLUDED IN THE CODE TO GET
C     QUANTITATIVE MEASURE OF HOW MUCH INPUT PARAMETERS SUCH AS RATE
C     CONSTANTS AND G-VALUES AFFECT CONCENTRATION OUTPUT.  FOR EXAMPLE
```

```
C     THE CODE CAN EVALUATE THE SENSITIVITY OF H2O2 WITH RESPECT TO
C     RATE CONSTANTS, MASS TRANSFER COEFFICIENT, AND G-VALUES AT EACH
C     COMPONENT.
C
C       THIS IS THE FIRST PUBLISHED VERSION OF RADICAL AFTER A SERIES OF
C     DEBUGGING AND MODIFICATION OF MITIRAD 7.0.  MITIRAD 1.0 IS A CODE
C     PACKAGE DEVELOPED BY SCOTT SIMONSON IN 1988 AT MIT WHICH WAS USED
C     TO ASSESS RADIOACTIVE WASTE IN UNDERGROUND DEPOSITORY.  A MAJOR
C     MODIFICATION TO THE CODE WAS DONE BY JOHN CHUN TO INCLUDE CORRECT
C     REACTION EQUATIONS AND EXTEND IT TO CALCULATE MULTIPLE-COMPONENT
C     SYSTEM.  ROUTINES FOR SENSITIVITY ANALYSIS INCLUDING ADJOINT AND
C     RESPONSE EVALUATOR WERE DEVELOPED AFRESH AND INCLUDED IN THIS
C     VERSION OF RADICAL.
C
C  PROGRAM ELEMENTS:
C
C     RADICAL.BLK IS USED TO DECLARE GLOBAL VARIABLES AND COMMON BLOCKS
C                 IN EACH SUBROUTINE.  INSTEAD OF WRITING THIS IN EACH
C                 SUBROUTINE, AN EXTERNAL FILE 'RADICAL.BLK' IS USED.
C     INITIALIZE: CALLS SUBROUTINE ReadIn, SetUp, WriteComp.
C     ReadIn:     READS REACTION INFORMATION FROM INPUT FILE.
C     FindLine:   POSITIONS INPUT POINTER AT A SPECIFIC LOCATION.
C     SetUpRX:    SETS UP REACTION MATRIX FOR RADIOLYSIS CALCULATION.
C     SetUpNODE:  SETS UP LOOP NODE INFORMATION ARRAY.
C     WriteOut:   PRINTS REACTION INFORMATION TO OUTPUT FILE.
C     CalcLoop:   EVALUATES RADIOLYSIS OF THE ENTIRE ASSEMBLY OF COMPONENTS
C                 BY ADVANCING A NODE AT A TIME AND CALLING 'CalcComp'.
C     CalcComp:   EVALUATES RADIOLYSIS OF A COMPONENT BY CALLING
C                 'RADIOLYSIS'.
C     PUSH:       PUSHES NODE NUMBER INTO STACK. USED FOR RECURSSIVE
C                 EVALUATION OF MULTIPLE PARALLEL-SERIES COMPONENTS.
C     PULL:       PULLS NODE NUMBER FROM STACK.
C     SumFlow:    SUMS VOLUMETRIC FLOWRATES OF ALL COMPONENTS AT NODE.
C     AverageFlow:AVERGES CONCENTRATION AT NODE BY WEIGHING DENSITY AND
C                 FLOWRATE.
C     ReadComp:   READS COMPONENT INPUT PARAMETERS.
C     ADJUST:     ADJUSTS INPUT PARAMETERS FOR 'RADIOLYSIS'.
C     WriteComp:  PRINTS EACH COMPONENT DATA.
C     RADIOLYSIS: CALLS CONCENTRATION WHICH IN TURN CALLS LSODE TO
C                 EVALUATE RADIOLYSIS.
C     CONCENTRATION:CALLS LSODE WHICH IN TURN CALLS FRO AND JACOB WHICH
C                 EVALUATES SPATIAL CONCENTRATION PROFILE.
C     LSODE:      LIVERMORE SOLVER OF ORDINARY DIFFERENTIAL
C                 EQUATIONS -  A SET OF SUBROUTINES
C                 PROVIDED BY ALAN HINDMARSH OF LLNL
C                 WHICH SOLVES A GENERAL SET OF ORDINARY
C                 DIFFERENTIAL EQUATIONS USING GEARS METHOD FOR
C                 STIFF NONLINEAR DIFFERENTIAL EQUATIONS THE CURRENT
C                 VERSION MAY HAVE BEEN MODIFIED TO ONLY INCLUDE THE
C                 STIFF OPTION TO SAVE ON SPACE.
C     FRO:        SETS UP THE CONCENTRATION DIFFERENTIAL EQUATION
C                 TO BE SOLVED BY LSODE.
C     JACOB:      CONTAINS THE JACOBIAN OF THE DIFFERENTIAL EQUATION
C                 IN FRO.
C     DoseShape:  EVALUATES DOSE SHAPE AS A FUNCTION OF POSITION.
C     TwoPhase:   EVALUATES TWO PHASE PARAMETERS.
C     ARRHENIUS:  ADJUSTS RATE CONSTANTS TO TEMPERATURE CHANGES.
C     WriteConc:  WRITES CONCENTRATION OUTPUT TO FILES.
```

```
C     WriteStat:  WRITES RADIOLYSIS RUN STATISTICS TO OUTPUT FILE.
C     SENSITIVITY:CALLS ADJOINT AND RESPONSE TO EVALUATE SENSITIVITY.
C     ADJOINT:    EVALUATES ADJOINT OF THE RADIOLYSIS OUTPUT.
C     ADJFRO:     d(Adjoint)/dx EVALUATOR FOR LSODE.
C     ADJJACOB:   JACOBIAN EVALUATOR FOR ADJOINT.
C     INTERPOLATE:INTERPOLATE RADIOLYSIS AND ADJOINT CURVE OUTPUTS.
C     RESPONSE:   EVALUATES RESPONSE OF ADJOINT.
C     RESFRO:     d(Response)/dx EVALUATOR FOR LSODE.
C     RESJACOB:   JACOBIAN EVALUATOR FOR RESPONSE.
C     WrietSens:  WRITES SENSITIVITY OUTPUT TO FILES.
C     TERMINATE:  TERMINATES PROGRAM BY CLOSING FILES.
C
C  GLOBAL CONSTANTS:
C
C     ICO:       DIMENSION OF COMPONENT ARRAY.
C     INO:       DIMENSION OF NODE ARRAY.
C     IRX:       DIMENSION OF REACTION ARRAY.
C     ISP:       DIMENSION OF SPECIES ARRAY.
C     IST:       DIMENSION OF RADIOLYSIS AND ADJOINT CURVE OUTPUT FOR
C                INTERPOLATION IN ADJFRO AND RESFRO.
C     GASCONST:  UNIVERSAL GAS CONSTANT.
C     LIW:       SIZE OF LSODE INTEGER WORKING ARRAY.
C     LRW:       SIZE OF LSODE REAL WORKING ARRAY.
C
C  GLOBAL VARIABLES:
C
C     AdjCurve:  ADJOINT PROFILE CURVE USED IN INTERPOLATION.
C     AdjXXXXX:  VARIABLE XXXXX USED FOR ADJOINT CALCULATION.
C     CalcSens:  FLAG USED FOR COMPONENT SENSITIVITY ANALYSIS.
C     CalcSurf:  FLAG USED FOR HYDROGEN PEROXIDE SURFACE DECOMPOSITION.
C                TRUE(DEFAULT)=CONSIDER SURFACE EFFECT,
C                FALSE=DISREGARD SURFACE EFFECT
C     CompFlowX: FlowRate OF COMPONENT FOR EITHER LIQUID OR GAS.
C     CompName:  NAME OF COMPONENT.
C     CompNode:  COMPONENT NODE INFORMATION ARRAY.
C     CONC:      SPECIES CONCENTRATION VECTOR (MOLES/L).
C     ConcCurve: CONCENTRATION PROFILE CURVE USED IN INTERPOLATION.
C     ConcFinal: FINAL CONCENTRATION ARRAY OF A COMPONENT (MOLES/L).
C     ConcNode:  AVERAGED CONCENTRATION AT EACH NODE.
C     CycleOut:  FLAG USED TO CONTROL OUTPUT AT EACH CYCLE.
C     DEBUG:     FLAG TO PRINT DIAGNOSTIC MESSAGES ON OUTPUT.
C     DensGas:   DENSITY OF VAPOR (g/cc).
C     DensLiq:   DENSITY OF LIQUID (g/cc).
C     DIAMETER:  EFFECTIVE HYDRAULIC DIAMETER OF THE FLOW CHANNEL (cm).
C     DVFDX:     d(VOID FRACTION)/dx.
C     DVGDX:     d(VAPOR VELOCITY)/dx.
C     DVLDX:     d(LIQUID VELOCITY)/dx.
C     EA:        ACTIVATION ENERGY (KJ/MOLE-K).
C     FlowPara:  FLOW PARAMETER USED IN BANKOFF'S EQUATION.
C     FlowRate:  MASS FlowRate (g/sec).
C     GAMMAC:    COEFFICIENT ARRAY FOR GAMMA DOSE SHAPE POLYNOMIAL.
C     GammaRate: GAMMA DOSE RATE (RAD/S).
C     GasConst:  UNIVERSAL GAS CONSTANT (ATM*LITER/MOL-KELVIN).
C     GConvert:  CONVERSION FACTOR FROM # SPECIES/100 eV TO MOL/L-RAD.
C     GGamma:    ADJUSTED GAMMA G-VALUE (# SPECIES/100 eV) FOR DENSITY.
C     GGamma0:   ORIGINAL GAMMA G-VALUE (# SPECIES/100 eV).
C     GNeut:     ADJUSTED NEUTRON G-VALUE (# SPECIES/100 eV) FOR DENSITY.
C     GNeut0:    ORIGINAL NEUTRON G-VALUE (# SPECIES/100 eV).
```

```
C      ICOMP:     COMPONENT NUMBER UNDER EVALUATION.
C      ICycle:    CYCLE COUNTER.
C      ID1:       REACTION ARRAY SIZING PARAMETER.
C      ID2        REACTANT ARRAY SIZING PARAMETER.
C      INn:       n=1 TO 3; INDICIES ARRAYS FOR CHEMICAL REACTION EVALUATION.
C      InFile:    INPUT DATA FILE.
C      IP:        PRODUCT ARRAY.
C      IR:        REACTANT ARRAY.
C      ISENS:     SENSITIVITY SPECIES NUMBER UNDER EVALUATION.
C      ITER:      ITERATION PERFORMED FOR CURVE DATA POINTS USED TO
C                 INTERPOLATE.
C      KOEF:      REACTION COEFFICIENT; + FOR PRODUCT, - FOR REACTANT.
C                                     1 FOR FIRST ORDER, 2 FOR SECOND ORDER.
C      LinLin:    FLAG FOR PlotFile OUTPUT FORMAT.
C                 TRUE(DEFAULT)=LIN CONC, LIN X; FALSE=LOG CONC, LIN X.
C      MaxIter:   TOTAL ITERATION OF THE CONCENTRATION AND ADJOINT ARRAYS.
C      MaxOrderD: MAXIMUM ORDER OF DOSE SHAPE FUNCTION POLYNOMIAL.
C      MaxOrderV: MAXIMUM ORDER OF VOID FRACTION SHAPE FUNCTION POLYNOMIAL.
C      NComp:     NUMBER OF COMPONENTS IN THE LOOP.
C      NCycle:    NUMBER OF CYCLES TO GO THROUGH THE ENTIRE LOOP.
C      NEUTRONC:  COEFFICIENTS FOR NEUTRON DOSE SHAPE POLYNOMIAL.
C      NeutRate:  NEUTRON DOSE RATE (RAD/S).
C      NNode:     NUMBER OF NODES IN THE LOOP.
C      NodeCount: NUMBER OF BEGINNING AND ENDING COMPONENTS AT EACH NODE.
C      NodeInfo:  LIST OF BEGINNING AND ENDING COMPONENTS AT EACH NODE.
C      NodeStart: NODE AT WHICH EVALUATION BEGINS. INITIAL CONCENTRATIONS
C                 MUST BE GIVEN AT THIS NODE.
C      NRx:       NUMBER OF CHEMCAL REACTIONS.
C      NSens:     NUMBER OF SENSITIVITY SPECIES.
C      NSpecies:  NUMBER OF CHEMICAL SPECIES INCLUDING GAS SPECIES
C      NSurfRx:   NUMBER OF SURFACE REACTIONS IN THE REACTION MATRIX.
C                 SURFACE REACTION MUST BE AT THE END OF THE MATRIX.
C      OutFile:   OUTPUT FILE.
C      PDJ:       COLUMN VECTOR FOR JACOBIAN MATRIX.
C      PlotFile:  PLOT DATA FILE TO BE READ BY RS/1.
C      PlotOut:   FLAG FOR PlotFile OUTPUT TO BE READ BY RS1.
C                 TRUE(DEFAULT)=GENERATE PLOT FILE,FALSE=NO PLOT FILE
C      PPBOUT:    FLAG USED FOR OUTPUT IN PPB INSTEAD OF MOL/LITER.
C      PRESSURE:  SYSTEM PRESSURE (atm).
C      RateConst: RATE CONSTANT AT SYSTEM TEMPERATURE (MOL/L-S IN GENERAL).
C      RCInit:    RATE CONSTANT AT REFERENCE TEMPERATURE (MOL/L-S IN GENERAL).
C      RCSurf:    RATE CONSTANT OF SURFACE DECOMPOSITION (MOL/L-S IN GENERAL).
C      ResXXXXX:  VARIABLE XXXXX FOR RESPONSE CALCULATION.
C      RxName:    ARRAY OF REACTION NAMES.
C      Sens:      FLAG USED FOR SENSITIVITY ANALYSIS. IF SENS IS FALSE,
C                 CALCSENS IS OVERRIDDEN AND NO SENSITIVITY WILL BE CARRIED OUT
C                 AT ALL IN ANY OF THE COMPONENTS.
C      SensFile:  PLOT OUTPUT FILE FOR SENSITIVITY RESULTS.
C      SensSpecies:SENSITIVITY SPECIES NAME ARRAY.
C      SensStep:  dx USED IN SENSITIVITY EVALUATION.
C      SpeciesName:ARRAY OF SPECIES NAMES.
C      SURFACE:   SURFACE MATERIAL OF FLOW PATH.
C      TEMP:      TEMPERATURE ALONG THE FLOW CHANNEL (kelvin).
C      TempIn:    INLET TEMPERATURE (kelvin).
C      TempOut:   OUTLET TEMPERATURE (kelvin).
C      TempRef:   REFERENCE TEMPERATURE TO BASE ARRHENIUS' LAW UPON (kelvin).
C      TIMEx:     SYSTEM TIME USED IN CALCULATING EXECUTION TIME.
C      TitleLine: FIRST LINE OF INPUT FILE WHICH CONTAINS FILE INFORMATION.
```

```
C     VelGas:    VAPOR VELOCITY ALONG THE CHANNEL (cm/s).
C     VelInlet:  INLET LIQUID VELOCITY (cm/s).
C     VelLiq:    LIQUID VELOCITY ALONG THE CHANNEL (cm/s).
C     VOIDC:     COEFFICIENTS FOR VOID FRACTION SHAPE POLYNOMIAL.
C     VoidFlag:  FLAG TO INDICATE WHETHER TO USE VOID FRACTION OR QUALITY.
C                TRUE(DEFAULT)=VOID FRACTION, FALSE=QUALITY.
C     WriteOut:  FLAG INDICATING WHETHER ADJUSTED REACTION MATRIX IS TO
C                BE PRINTED FOR A COMPONENT.
C     WritePara: FLAG FOR PRINTING PARAMETERS WITH EACH CONCENTRATION OUTPUT
C     XBoil:     POSITION OF ONSET OF BOILING IN TWO PHASE FLOW (cm).
C     XFinal:    FINAL POSITION TO EVALUATE RADIOLYSIS (cm).
C     XInitial:  INITIAL POSITION OF CHANNEL (cm).
C     XStep:     POSITION STEP TO BE TAKEN IN OUTPUT (cm).
C
C     LSODE VARIABLES ARE DEFINED IN THE LSODE WRITE-UP
C
C  NON-STANDARD VAX FORTRAN FUNCTIONS CALLED:
C
C     DATE:      RETURNS TODAY'S DATE AS FOUND IN THE SYSTEM
C     INCLUDE:   INCLUDES AN EXTERNAL TEXT FILE AS A PART OF THE SOURCE.
C                'RADICAL.BLK' IS USED TO DECLARE GLOBAL VARIABLES.
C     NAMELIST : COMPACT WAY OF ReadInG INPUT DATA.  THIS MAY BE REWRITTEN
C                TO READ INPUT PARAMETERS ONE BY ONE IN STANDARD WAY.
C     SECNDS:    PASSES SYSTEM CLOCK IN SECONDS TO REAL*4 VARIABLE.
C                THIS FUNCTION MAY BE OMITTED WITHOUT AFFECTING
C                THE ESSENTIAL PART OF THE CODE.
C     TIME:      RETURNS CURRENT TIME AS FOUND IN THE SYSTEM
C
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      CALL INITIALIZE    !READS INPUT PARAMETERS AND PREPARE THEM
      CALL CalcLoop      !EVALUATE LOOP RADIOLYSIS
      CALL TERMINATE     !WRITES RUN STATISTICS AND FINISH JOB
C
      STOP
      END   ! OF RADICAL
```

```
      SUBROUTINE INITIALIZE
C
C**********************************************************************
C     VERSION:          RADICAL 1.0                  19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C**********************************************************************
C     CALLED BY RADICAL
C     CALLS ReadIn, SetUpRX, SetUpNODE, WriteOut
C
C     OPENS INPUT AND OUTPUT FILES AND READS INPUT DATA.
C     PREPARES INPUT DATA FOR RADIOLYSIS AND PRINTS THEM IN OUTPUT FILE.
C**********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      TIME1=SECNDS(0.0) !START CLOCK TO MEASURE TOTAL EXECUTION TIME
C
      TYPE 1            !GET INPUT FILE NAME FROM TERMINAL
1     FORMAT(' INPUT FILE: '$)
      ACCEPT 2,InFile
2     FORMAT(A)
      OPEN (5,FILE=InFile,STATUS='OLD') !OPEN INPUT DATA FILE
C
      CALL ReadIn !READS PLANT INFO
      CALL SetUpRX      !PREPARE REACTIONS FOR RADIOLYSIS CALC
      CALL SetUpNODE    !PREPARE NODE INFORMATION FOR CalcLoop
      OPEN (6,FILE=OutFile,STATUS='NEW')  !CUTPUT FILE
      IF (PlotOut) OPEN (7,FILE=PlotFile,STATUS='NEW')      !PLOT FILE
      IF (SENS)    OPEN (8,FILE=SensFile,STATUS='NEW')      !Sens FILE
      CALL WriteOut     !WRITES TITLE AND RX TO OUTPUT FILE
C
      RETURN
      END   ! OF INITIALIZE
```

```
      SUBROUTINE ReadIn
C
C**********************************************************************
C     VERSION:         RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C**********************************************************************
C     CALLED BY INITIALIZE
C
C     READS THE REACTION MATRIX AND REACTION RATE CONSTANTS.
C**********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      CHARACTER*16 TheName
C
      NAMELIST /FileName/ OutFile,PlotFile,SensFile
      NAMELIST /SIZE/ NSpecies,NRx,NSurfRx,NComp,NNode,NCycle
      NAMELIST /CONTROL/ NodeStart,TempRef,PlotOut,LinLin,SENS,
     +                   DEBUG,NORMALIZE,PPBOUT,CycleOut
      NAMELIST /NAME/ SpeciesName
C
C     ASSIGN DEFAULT VALUES
C
      DATA OUTFILE/'RADICAL.OUT'/,PLOTFILE/'RADICAL.PLOT'/,
     +     SENSFILE/'RADICAL.SENS'/
      DATA NSpecies/1/,NRx/1/,NSurfRx/0/,NComp/1/,NNode/1/,NCycle/1/
      DATA NodeStart/1/,TempRef/298.D0/
      DATA PlotOut/.TRUE./,LinLin/.TRUE./,Sens/.FALSE./,
     +     DEBUG/IDE*.FALSE./,NORMALIZE/.FALSE./,PPBOUT/.FALSE./,
     +     CycleOut/ICY*.FALSE./
C
C     FLAGS USED IN FindLine
C
      NZero=0                  !PRINT MESSAGE AND STOP IF TheName NOT FOUND
      IGFLAG=1                 !NOTIFY CALLER IF TheName NOT FOUND.
C
      READ (5,110) TitleLine
110   FORMAT (A80)
      REWIND (5)
      READ (5,NML=FileName)    !READ OutFile, PlotFile NAMES
      REWIND (5)
      READ (5,NML=SIZE)        !READ NSpecies,NRx
      REWIND (5)
      READ (5,NML=CONTROL,END=109)
      CycleOut(NCycle)=.TRUE. !DEFAULT OUTPUT AT NCYCLE
C
109   REWIND (5)
      TheName='$GVALUE'
      CALL FindLine(TheName,IGFLAG)
      IF ((IGFLAG.LT.0).AND.(.NOT.PPBOUT)) GOTO 114
      READ (5,220) (GGamma0(I),GNeut0(I),MOLWT(I),I=1,NSpecies)
220   FORMAT(9X,D10.3,/9X,D10.3,/9X,D10.3)
C
114   REWIND (5)
      READ (5,NML=NAME)        !READ THE SPECIES NAMES
C
      TheName='$REACTION'      !READ REACTION INFORMATION
      CALL FindLine(TheName,NZero)
      DO 140 I=1,NRx
```

```
        READ(5,100) RxName(I),(IR(I,K),K=1,3),(IP(I,K),K=1,4)
     +             ,RCInit(I),EA(I)
        RCSurf(I)=RCInit(I)
140   CONTINUE
100   FORMAT(X,A3,3X,7I3,D18.8,D18.8)
C
      TheName='$COMPONENT'     !READ LOCP INFO
      CALL FindLine(TheName,NZERO)
      DO 120 I=1,NComp
        READ (5,130) CompName(I),(CompNode(I,J),J=1,3)
120   CONTINUE
130   FORMAT(X,A16,X,3(I4))
C
      RETURN
      END    !OF ReadIn
```

```
      SUBROUTINE FindLine(TheName,LFLAG)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0              19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY MANY SUBROUTINES
C
C     SCANS INPUT FILE AND LOOKS FOR 'TheName'.  ONCE IT FINDS THE TEXT,
C     THE INPUT POINTER POINTS TO THE NEXT LINE.
C
C     LFLAG IS USED TO NOTIFY ERROR CONDITION AND TO TRANSFER CONTROL.
C     IF LFLAG=0 UPON CALL AND TheName IS NOT FOUND, PROGRAM STOPS.
C     IF LFLAG=1 UPON CALL AND TheName IS NOT FOUND, SUBROUTINE RETURNS
C     TO THE CALLER WITH LFLAG=-1 TO NOTIFY THE ERROR.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      CHARACTER*16 AName,TheName
C
      KOUNT=0                   !USED TO SEE IF ENTIRE FILE HAS BEEN SCANNED
100   READ (5,110,END=120) AName    !LOOK FOR TheName
      IF (AName.EQ.TheName) GO TO 130
      GO TO 100
120   IF (KOUNT.EQ.0) THEN    !SCAN ONLY ONCE THROUGH
        KOUNT=1
        REWIND 5         !RESET INPUT POINTER TO THE TOP
        GO TO 100        !AND SCAN ONLY ONE MORE TIME.
      ELSE IF (LFLAG.EQ.0) THEN     !CALLER CHOSE TO STOP IF TheName NOT FOUND
        PRINT 10,TheName,InFile
        WRITE(6,10) TheName,InFile
        STOP
      ELSE
        LFLAG=-1         !NOTIFY THE CALLER
      ENDIF
110   FORMAT(X,A16)
10    FORMAT (' ',A16,' IS NOT FOUND IN THE INPUT FILE ',A35,
     +       /'PROGRAM ABORTED AT SUBROUTINE FINDLINE!')
C
130   RETURN
      END   !OF FindLine
```

```
      SUBROUTINE SetUpRX
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY INITIALIZE
C
C     SETS UP CHEMICAL REACTION EQUATIONS FOR RADIOLYSIS CALCULATION.
C     DEFINES dC/dx WITH ALL APPROPRIATE REACTIONS CONSIDERING WHETHER
C     THE SPECIES IS PRODUCED OR CONSUMED, FIRST OR SECOND ORDER.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION KO(IRX,ISP)
C
C     SET UP THE COEFFICIENT MATRICIES(KOEF) FOR FRO
C
      DO 140 I=1,NRx
C
C       CHECK FOR SECOND ORDER REACTANTS
C
        IF(((IR(I,1).EQ.IR(I,2)).OR.(IR(I,2).EQ.IR(I,3)))
     +     .AND.(IR(I,2).NE.0))THEN
          KOEF(I,IR(I,2))=-2
          KO(I,IR(I,2))=-2
        ENDIF
C
C       CHECK FOR FIRST ORDER REACTANTS
C
        DO 120 K=1,3
          IF((IR(I,K).NE.0).AND.(KOEF(I,IR(I,K)).NE.-2))THEN
            KOEF(I,IR(I,K))=-1
            KO(I,IR(I,K))=-1
          ENDIF
120     CONTINUE
C
C       CHECK FOR SECOND ORDER PRODUCTS
C
        IF(((IP(I,1).EQ.IP(I,2)).OR.(IP(I,2).EQ.IP(I,3)))
     +     .AND.(IP(I,2).NE.0))THEN
          KOEF(I,IP(I,2))=2
        ENDIF
        IF(((IP(I,2).EQ.IP(I,3)).OR.(IP(I,3).EQ.IP(I,4)))
     +     .AND.(IP(I,3).NE.0))THEN
          KOEF(I,IP(I,3))=2
        ENDIF
C
C       FILL UP THE PRODUCTS MATRIX FOR FIRST ORDER PRODUCTS
C
        DO 130 K=1,4
          IF((IP(I,K).NE.0).AND.(KOEF(I,IP(I,K)).NE.2))THEN
            KOEF(I,IP(I,K))=1
          ENDIF
130     CONTINUE
140   CONTINUE
C
C     REMOVE CATALYTIC REACTANTS AND PRODUCTS
```

```
C
      DO 150 K=1,NSPECIES
        DO 151 I=1,NRX
          IF ((KOEF(I,K).NE.KO(I,K)).AND.(KO(I,K).NE.0))
     +       KOEF(I,K)=KOEF(I,K)+KO(I,K)
151     CONTINUE
150   CONTINUE
C
C     ASSIGN ZERO-ORDER RX
C
      DO 180 I=1,NRx
        DO 152 K=1,4             !SET TO BLANK IF ZERO
          IF ((K.LE.3).AND.(IR(I,K).EQ.0)) IR(I,K)=NSpecies+1
          IF (IP(I,K).EQ.0) IP(I,K)=NSpecies+1
152     CONTINUE
180   CONTINUE
C
      RETURN
      END   !OF SetUpRX
```

```
      SUBROUTINE SetUpNode
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY INITIALIZE
C
C     SETS UP NODE INFORMATION ARRAY TO BE USED BY CalcLoop.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
C     FIND THE LARGEST NODE NUMBER
C
      DO 100 J=1,NComp
        DO 110 K=1,2
          MaxNode=MAX(CompNode(J,K),MaxNode)
110     CONTINUE
100   CONTINUE
      PRINT *,'LARGEST NODE NUMBER =',MAXNODE   !TMP
C
C     VECTORIZE NODE INFORMATION
C
      DO 200 I=1,MaxNode
        NodeCount(I,1)=0
        NodeCount(I,2)=0
        DO 210 J=1,NComp
          IF (CompNode(J,1).EQ.I) THEN
            NodeCount(I,1)=NodeCount(I,1)+1
            NodeInfo(I,1,NodeCount(I,1))=J
          ELSE IF (CompNode(J,2).EQ.I) THEN
            NodeCount(I,2)=NodeCount(I,2)+1
            NodeInfo(I,2,NodeCount(I,2))=J
          ENDIF
210     CONTINUE
200   CONTINUE
C
      RETURN
      END   !OF SetUpNODE
```

```
      SUBROUTINE WriteOut
C
C************************************************************************
C     VERSION:        RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C************************************************************************
C     CALLED BY INITIALIZE
C
C     WRITES TITLE, SOME INPUT INFO AND RX MATRIX.
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
      CHARACTER*9 TODAY,NOW
C
      CALL DATE(TODAY)          !VAX FUNCTION
      CALL TIME(NOW)
      WRITE (6,120) TODAY,NOW
120   FORMAT(
     + 12X,    '_______________________________________________________'
     +,/ ,12X,'|                                                     |'
     +,/ ,12X,'|             RADICAL CODE PACKAGE OUTPUT             |'
     +,/ ,12X,'|                    VERSION: 1.0                     |'
     +,/ ,12X,'|                                                     |'
     +,/ ,12X,'|',17X,A9,2X,A9,16X,'|'
     +,/ ,12X,'_______________________________________________________')
      WRITE (6,140)
      WRITE (6,150)
      WRITE (6,140)
      WRITE (6,134) TitleLine
      WRITE (6,135) InFile, OutFile
      IF (PlotOut) WRITE (6,136) PlotFile
      IF (SENS)    WRITE (6,137) SensFile
      WRITE (6,130) NSpecies,NRx,NSurfRx,NComp,NNode,NCycle
140   FORMAT(/80(1H_)/)
150   FORMAT(/37X,'INPUT')
134   FORMAT(A80/)
135   FORMAT(   5X,36H  INPUT FILE NAME                     = ,A35,/
     +          5X,36H  OUTPUT FILE NAME                    = ,A35)
136   FORMAT(   5X,36H  PLOT FILE NAME                      = ,A35)
137   FORMAT(   5X,36H  SENSITIVITY FILE NAME               = ,A35)
130   FORMAT ( /5X,36H  NUMBER OF SPECIES EVALUATED         = ,I8/,
     +          5X,36H  NUMBER OF CHEMICAL REACTIONS        = ,I8/
     +          5X,36H  NUMBER OF SURFACE REACTIONS         = ,I8/
     +          5X,36H  NUMBER OF COMPONENTS                = ,I8/
     +          5X,36H  NUMBER OF NODES                     = ,I8/
     +          5X,36H  NUMBER OF CYCLES                    = ,I8/)
C
      WRITE(6,110) NodeStart,TempRef
110   FORMAT(5X,36H  STARTING NODE                      = ,I8/
     +       5X,36H  REFERENCE TEMPERATURE              = ,F14.5' Kelvin'/)
C
      WRITE (6,256) PlotOut,LinLin,Sens,NORMALIZE,PPBOUT
256   FORMAT( 5X,36H  PlotOut                             = ,L8,
     +       /5X,36H  LinLin                              = ,L8,
     +       /5X,36H  SENS                                = ,L8,
     +       /5X,36H  NORMALIZE                           = ,L8,
     +       /5X,36H  PPBOUT                              = ,L8//)
C
```

```
      WRITE(6,191)
191   FORMAT(7X,19X,'FLOW-IN',4X,'FLOW-OUT',3X,'INITIAL'
     +      /7X,'COMPONENT NAME',7X,'NODE',7X,'NODE',7X,'CONC'
     +      /7X,'----------------',3(3X,'--------'))
      DO 196 I=1,NComp
        WRITE (6,195) CompName(I),(CompNode(I,J),J=1,3)
196   CONTINUE
195   FORMAT(7X,A16,4X,I4,7X,I4,6X,I4)
C
      IF ((IGFLAG.EQ.-1).AND.(.NOT.PPBOUT)) GOTO 211
      WRITE (6,190)
190   FORMAT(//18X,7H GAMMA ,4X,8HNEUTRON ,3X,9HMOLECULAR,
     + /        15X,3X,8HG-VALUES,3X,8HG-VALUES,4X,6HWEIGHT,
     + /        7X,'SPECIES',4X,'(#/100eV)',2X,'(#/100eV)',2X,'(g/mole)',
     + /        7X,'-------- ',3(2X,'-------- '))
      DO 200 I=1,NSpecies
        WRITE (6,210) SpeciesName(I),GGamma0(I),GNeut0(I),MOLWT(I)
200   CONTINUE
210   FORMAT (7X,A8,3(2X,D9.2))
C
211   WRITE (6,292)
      WRITE (6,10)
      WRITE (6,140)
      WRITE (6,11)
292   FORMAT ('1',80(1H_),/)
10    FORMAT (/10X,
     +59HCHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES)
11    FORMAT (/
     +26X,'REACTIONS',30X,'RATE',2X,'ACTIVATION',/63X,'CONSTANT',2X,
     +'ENERGIES'/62X,'           (KJ/MOL-K)'/)
C
      SpeciesName(NSPECIES+1)='        '
      DO 160 I=1,NRx
        WRITE(6,111) RxName(I),(SpeciesName(IR(I,K)),K=1,3),
     +               (SpeciesName(IP(I,K)),K=1,4),RCInit(I),EA(I)
160   CONTINUE
111   FORMAT(1X,A3,1X,3A8,'>',4A8,D9.2,1X,D9.2)
C
C     WRITE SPECIES NAMES TO PLOT FILE AND SENS FILE
C
      IF (PlotOut) THEN               !WRITE CONCENTRATION RESULTS
        WRITE (7,430) TITLELINE
        WRITE (7,420) LinLin
        WRITE (7,420) NSpecies
        WRITE (7,432) (SpeciesName(I),I=1,NSpecies)
      ENDIF
420   FORMAT (1X,I5)
430   FORMAT (1X,A80)
431   FORMAT (1X,A16)
432   FORMAT (1X,A8)
C
      IF (SENS) THEN                  !WRITE SENSITIVITY RESULTS
        WRITE (8,430) TITLELINE
        WRITE (8,420) NSpecies
        WRITE (8,420) NRX
        WRITE (8,432) (SpeciesName(I),I=1,NSpecies)
        WRITE (8,433) (RXNAME(I),I=1,NRX)
      ENDIF
```

```
433    FORMAT (1X,A3)
C
       RETURN
       END    !OF WriteOut
```

```
      SUBROUTINE CalcLoop
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY RADICAL
C     CALLS CalcComp, PUSH, PULL, SumFlow, AverageFlow
C
C     ITERATES THROUGH THE ENTIRE LOOP AND EVALUATE RADIOLYSIS COMPONENT
C     BY COMPONENT AT EACH NODE.  TO HANDLE MULTIPLE PARALLEL-SERIES
C     COMBINATION OF COMPONENTS, RECURSSIVE ROUTINE IS USED WHICH
C     UTILIZE A NODE STACK TO KEEP TRACK OF RECURSION INFORMATION.
C
C  LOCAL VARIABLES
C
C     CompEval:      TRUE IF THE COMPONENT HAS BEEN EVALUATED
C                    FALSE IF THE COMPONENT HAS NOT.
C     InitGiven:     1 IF INITIAL CONCENTRATIONS FOR COMPONENT IS GIVEN
C                    0 IF NOT GIVEN.
C     NCompAtNode:   NUMBER OF COMPONENTS AT NODE.
C     NodeEval:      TRUE IF THE NODE HAS BEEN EVALUATED BY EVALUATING
C                    ALL PRECEEDING COMPONENTS.  IF NOT, RECURSIVE ROUTINE
C                    IS CALLED IN TO EVALUATED ALL PRECEEDING COMPONENTS.
C     NodePrev:      NODE NUMBER OF THE PREVIOUS NODE.
C     STACK:         STACK TO HOLD NODE NUMBERS IN RECURSSIVE CALLS.
C     StackPointer:  STACK POINTER.
C     SumFlowRateL:  TOTAL FLOW RATE WEIGHTED BY LIQUID DENSITY.
C     SumFlowRateG:  TOTAL FLOW RATE WEIGHTED BY LIQUID DENSITY.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      INTEGER StackPointer, STACK(INO)
      LOGICAL*1 CompEval(ICO),NodeEval(INO)
      COMMON/STACK/ STACK, StackPointer
C
      ICYCLE=1
      NODE=NodeStart            !BEGIN CALC AT NodeStart
      StackPointer=0            !RESETS THE STACK
      PRINT *,'NUMBER OF CYCLE = ',NCYCLE
C
C**** LOOP WHICH EVALUATES COMPONENTS AT A NODE ONE BY ONE STARTS HERE.
C
100   NODE=CompNode(NodeInfo(NODE,1,1),2)
      PRINT *,'CYCLE =',ICYCLE,' NODE =',NODE   !TMP
      IF (DEBUG(1)) WRITE (6,*) 'CYCLE =',ICYCLE,' NODE = ',NODE
200   SUMFlowRateL=0.D0         !INITIALIZE TOTAL FlowRate AT EACH NODE
      SUMFlowRateG=0.D0
      DO 130 K=1,NSpecies       !INITIALIZE CONCENTRATIONS
        ConcNode(NODE,K)=0.D0
130   CONTINUE
C
      NCompAtNode=NodeCount(NODE,2) !# OF COMPONENTS ENDING AT NODE I
      DO 110 J=1,NCompAtNode
        IComp=NodeInfo(NODE,2,J)     !COMPONENT ENDING AT NODE I
        InitGiven=CompNode(IComp,3)
        NodePrev=CompNode(IComp,1)
        IF ((.NOT.CompEval(IComp)).AND.
```

```
     +     ((InitGiven.EQ.1).OR.(NodeEval(NodePrev)))) THEN
C
C     INITIAL VALUES GIVEN OR EVALUATED AT NODE AND COMPONENT IS NOT
C     COMPUTED YET
C
        PRINT *,'CALCULATE COMPONENT ',IComp,'  ',COMPNAME(ICOMP) !TMP
          IF (DEBUG(1)) WRITE (6,*)
     +       'CALCULATE COMPONENT ',IComp,'  ',COMPNAME(ICOMP)
          CALL CalcComp
          CompEval(IComp)=.TRUE.    !THIS COMPONENT HAS BEEN EVALUATED
C
        ELSE IF ((CompNode(IComp,3).EQ.0).AND.
     +          (.NOT.NodeEval(NodePrev))) THEN
C
C     NO INITIAL VALUE IS GIVEN OR IT'S NOT ALREADY CALCULATED
C
          CALL PUSH(NODE)
          NODE=CompNode(IComp,1)
          PRINT *,'PUSH INTO NODE ',NODE,' POINTER=',StackPointer !TMP
          IF (DEBUG(1)) WRITE(6,*)
     +       'PUSH INTO NODE ',NODE,' POINTER=',StackPointer
          GO TO 200          !RECURSION
        ENDIF
C
      IF (NCompAtNode.GT.1) CALL SUMFLOW(NODE)
C
110   CONTINUE    !THROUGH ALL PARALLEL COMPONENTS ENDING AT THIS NODE
C
      CALL AVERAGEFLOW (NODE,NCompAtNode)
C
      NodeEval(NODE)=.TRUE.   !EVALUATION OF THIS NODE IS COMPLETE.
C
      IF (StackPointer.GT.0) THEN   !PULL AND CALC THE PREVIOUS NODE
        CALL PULL(NODE)
        PRINT *,'PULL STACK NODE =',NODE,' POINTER=',StackPointer !TMP
        IF (DEBUG(1)) WRITE(6,*)
     *     'PULL STACK NODE =',NODE,' POINTER=',StackPointer
        GO TO 200
      ENDIF
C
      IF (NODE.NE.NodeStart) GO TO 100
C
C**** CONTINUE THROUGH ENTIRE LOOP
C
      IF (ICYCLE.LT.NCYCLE) THEN
        ICYCLE=ICYCLE+1
        DO 300 I=1,NComp
          CompEval(I)=.FALSE. !RESET ALL COMPONENT FLAGS TO FALSE
300     CONTINUE
        DO 310 I=1,MaxNode
          NodeEval(I)=.FALSE. !RESET ALL NODE FLAGS TO FALSE
310     CONTINUE
        GOTO 100
      ENDIF
C
C**** CONTINUE THROUGH NCYCLES
C
      RETURN
```

```
END    !OF CalcLoop
```

```
      SUBROUTINE CalcComp
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcLoop
C     CALLS ReadComp, ADJUST, WriteComp, RADIOLYSIS, WriteStat
C
C     EVALUATES RADIOLYSIS OF A COMPONENT.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      TIME2=SECNDS(0.0) !START CLOCK TO MEASURE COMPONENT EXECUTION TIME
C
      IC=INDEX(CompName(IComp),'DUMMY')    !SEE IF DUMMY COMPONENT
C
      IF (IC.NE.0) GO TO 380        !SKIP IF DUMMY COMPONENT
      CALL ReadComp                 !READ COMPONENT PARAMETERS FROM FILE
      CALL ADJUST             !ADJUST INPUT PARAEMTERS
      XFINALHOLD=XFINAL             !SAVE XFINAL
      XSTEPHOLD=XSTEP               !SAVE XSTEP
      IF (XINITIAL.EQ.XFINAL) GO TO 380   !SKIP IF NULL COMPONENT
      CALL WriteComp                !WRITE INPUT PARAMETERS
      CALL RADIOLYSIS               !EVALUATE RADIOLYSIS
      IF (ICYCLE.EQ.1) CALL WriteStat     !WRITE RUN STATISTICS
C
380   DO 390 I=1,NSpecies           !STORE FINAL CONCENTRATIONS
        ConcFinal(IComp,I)=CONC(I)
390   CONTINUE
C
      IF ((SENS.AND.CALCSENS).AND.(IC.EQ.0).AND.(XLENGTH.NE.0.D0)
     +   .AND.(ICYCLE.EQ.NCYCLE)) CALL SENSITIVITY
C
      XSTEP=XSTEPHOLD               !RESTORE XSTEP FOR NEXT COMPONENT
      XFINAL=XFINALHOLD             !RESTORE XFINAL FOR NEXT COMPONENT
C
      RETURN
      END   !OF CalcComp
```

```
      SUBROUTINE PUSH(NODE)
C
C****************************************************************************
C     VERSION:         RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C****************************************************************************
C     CALLED BY CalcLoop
C
C     PUSHES NODE NUMBER INTO THE STACK.
C****************************************************************************
C
      INCLUDE 'RADICAL.BLK'
      INTEGER StackPointer, STACK(INO)
      COMMON/STACK/ STACK, StackPointer
C
      IF (StackPointer.LE.NNode) THEN
        StackPointer=StackPointer+1
        STACK(StackPointer)=NODE
      ELSE                 !STACK PUSHED TOO FAR. SOMETHING'S WRONG!
        PRINT 10
        WRITE(6,10)
        STOP               !TERMINATE PROGRAM
      ENDIF
10    FORMAT (' ','**** INPUT ERROR! - NOT ENOUGH INITIAL ',
     +         'CONCENTRATION VALUES GIVEN.',
     +         /'PROGRAM TERMINATED AT SUBROUTINE PUSH.')
C
      RETURN
      END   !OF PUSH
```

```
      SUBROUTINE PULL(NODE)
C
C****************************************************************************
C     VERSION:         RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C****************************************************************************
C     CALLED BY CalcLoop
C
C     PULLS NODE NUMBER FROM THE STACK.
C****************************************************************************
C
      INCLUDE 'RADICAL.BLK'
      INTEGER StackPointer, STACK(INO)
      COMMON/STACK/ STACK, StackPointer
C
      IF (StackPointer.GE.1) THEN   !PULL STACK
        NODE=STACK(StackPointer)
        StackPointer=StackPointer-1
      ELSE                 !STACK PULLED TOO FAR. SOMETHING'S WRONG!
        PRINT 10
        WRITE(6,10)
        STOP                     !TERMINATE PROGRAM
      ENDIF
10    FORMAT(' ','**** INPUT ERROR! PROGRAM TERMINATED AT',
     +       ' SUBROUTINE PULL.')
C
      RETURN
      END   !OF PULL
```

```
      SUBROUTINE SumFlow(NODE)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcLoop
C
C     SUMS DENSITY WEIGHED FLOWRATES OF ALL COMPONENTS AT A NODE.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      CompFlowL(IComp)=FlowRate/DensLiq
      IF (XFinal.GT.XBoil) CompFlowG(IComp)=FlowRate/DensGas
      SUMFlowRateL=SUMFlowRateL+CompFlowL(IComp)       !LIQUIT
      SUMFlowRateG=SUMFlowRateG+CompFlowG(IComp)       !GAS
      DO 120 K=1,NSpecies          !AVERAGE CONCENTRATION AT NODE
        IC=INDEX(SpeciesName(K),'G')
        IF (IC.EQ.0) THEN          !LIQUID
          ConcNode(NODE,K)=ConcNode(NODE,K)+
     +                    ConcFinal(IComp,K)*CompFlowL(IComp)
        ELSE                       !GAS
          ConcNode(NODE,K)=ConcNode(NODE,K)+
     +                    ConcFinal(IComp,K)*CompFlowG(IComp)
        ENDIF
120   CONTINUE    !THROUGH ALL SPECIES
C
      RETURN
      END   !OF SUMFLOW
```

```
      SUBROUTINE AverageFlow(NODE,NOfComp)
C
C************************************************************************
C     VERSION:         RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C************************************************************************
C     CALLED BY CalcLoop
C
C     AVERAGES CONCENTRATIONS OF ALL PARALLEL COMPONENTS AT A NODE BY
C     WEIGHING VOLUMETRIC FLOWRATES OF ALL COMPONENTS AT THE NODE.
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      IF (NOfComp.EQ.1) GOTO 150    !NO NEED TO AVERAGE IF ONLY ONE COMP
C
      IF (SUMFlowRateL.EQ.0.D0) THEN      !INPUT ERROR CONDITION
        PRINT 10
        WRITE(6,10)
        STOP
      ENDIF
10    FORMAT (' ','**** ERROR IN INPUT NODE INFORMATION.',
     +        ' SUM OF FLOWRATES IS ZERO.',
     +       /'PROGRAM TERMINATED AT SUBROUTINE AVERAGEFLOW.')
C
      DO 140 K=1,NSpecies      !WEIGH BY TOTAL FlowRate
        IC=INDEX(SpeciesName(K),'G')
        IF (IC.EQ.0) THEN      !LIQUID
          ConcNode(NODE,K)=ConcNode(NODE,K)/SUMFlowRateL
        ELSE IF (SUMFLOWRATEG.NE.0.D0) THEN           !GAS
          ConcNode(NODE,K)=ConcNode(NODE,K)/SUMFlowRateG
        ENDIF
140   CONTINUE             !THROUGH ALL SPECIES
      RETURN
C
150   DO 160 K=1,NSpecies
      ConcNode(NODE,K)=ConcFinal(IComp,K)
160   CONTINUE
C
      RETURN
      END    !OF AVERAGEFLOW
```

```
      SUBROUTINE ReadComp
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcComp
C
C     READS COMPONENT INPUT PARAMETERS FROM INPUT FILE.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      NAMELIST /POSITION/ XInitial,XFinal,XLength,XStep,XBoil,
     +                     XBoilOffset
      NAMELIST /STATE/ TempIn,TempOut,GammaRate,NeutRate,
     +                  VelInlet,DIAMETER,DensLiq,DensGas,
     +                  PRESSURE,FlowRate,SURFACE
      NAMELIST /DoseShape/ MAXORDERD,GAMMAC,NEUTRONC
      NAMELIST /VoidFraction/ MAXORDERV,VOIDC
      NAMELIST /InitialConc/ Conc
      NAMELIST /FLAG/ CalcSurf,VoidFlag,CALCSENS,WRITERX,WRITEPARA
      NAMELIST /SENSITIVITY/ SensStep,NSens,SensSpecies
      NAMELIST /LSODEData/ ITASK,RTOL,ITOL,ATOL,RWORK,IWORK,MF
      NAMELIST /ADJDATA/ ADJITASK,ADJRTOL,ADJITOL,ADJATOL,ADJMF,
     +                    ADJIOPT,ADJRWORK,ADJIWORK
      NAMELIST /RESDATA/ ResITASK,RESRTOL,RESITOL,RESATOL,RESMF,
     +                    RESIOPT,RESRWORK,RESIWORK
C
C     FIRST TIME ONLY DEFAULT VALUES
C
      DATA TEMPIN/298.D0/,TEMPOUT/298.D0/,XBOIL/9999.D0/,DIAMETER/1.D0/,
     +     PRESSURE/1.D0/,DENSLIQ/0.741D0/,DENSGAS/0.0362D0/,
     +     XBoilOffset/1.D-10/,SURFACE/'    '/
      DATA CALCSURF/.TRUE./,VOIDFLAG/.TRUE./,CALCSENS/.FALSE./,
     +     WRITERX/.FALSE./,WRITEPARA/.FALSE./
      DATA MAXORDERD/5/,MAXORDERV/5/
      DATA ATOL/1.D-15/,MF/21/,ITOL/1/,ISTATE/1/,ITASK/4/,RTOL/1.D-5/,
     +     IOPT/0/
      DATA ADJATOL/1.D-10/,ADJMF/21/,ADJITOL/1/,ADJITASK/4/,
     +     ADJRTOL/1.D-4/,ADJIOPT/0/
      DATA RESATOL/1.D-15/,RESMF/21/,RESITOL/1/,ResITASK/4/,
     +     RESRTOL/1.D-5/,RESIOPT/0/
C
C     SET DEFAULT VALUES FOR EACH COMPONENT
C
      DO 10 I=1,NSpecies
        Conc(I)=ConcNode(CompNode(IComp,1),I)   !SET TO PREVIOUS NODE'S CONC
10    CONTINUE
C
      XINITIAL=XFINAL
      XLength=-1.D0
      VELINLET=-1.D0
      DIAMETER=-1.D0
      TEMPIN=TEMPOUT
      SensStep=0
      NZero=0
C
```

```
      CALL FindLine('@'//CompName(IComp),NZERO) !POSITION INPUT POINTER
      READ (5,NML=POSITION)
      CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=STATE)
      CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=DoseShape)
      CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=VoidFraction)
C
C     SKIP READING INITIALCONC AT NODESTART IF BEYOND FIRST CYCLE
C
      IF ((ICycle.GT.1).AND.(CompNode(IComp,1).EQ.NodeStart)) GOTO 100
      CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=INITIALCONC)
C
100   CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=FLAG)
C
      CALL FindLine('@'//CompName(IComp),NZERO)
      IF (SENS.AND.CALCSENS) READ (5,NML=SENSITIVITY,END=110)
C
110   CALL FindLine('@'//CompName(IComp),NZERO)
      READ (5,NML=LSODEData,END=111)      !READ LSODE CONTROL VARIABLES
111   CALL FindLine('@'//CompName(IComp),NZERO)
      IF (SENS.AND.CALCSENS) READ (5,NML=ADJDATA,END=112) !ADJOINT LSODE DATA
112   CALL FindLine('@'//CompName(IComp),NZERO)
      IF (SENS.AND.CALCSENS) READ (5,NML=RESDATA,END=113) !RESPONSE LSODE DATA
C
113   RETURN
      END   !OF ReadComp
```

```
      SUBROUTINE ADJUST
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcComp
C
C     ADJUSTS INPUT DATA FOR RADIOLYSIS CALCULATION.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
C     ASSIGN XFINAL AND XLENGTH FROM GIVEN INPUT INFO
C
      IF (XLength.GE.0.D0) THEN
        XFINAL=XINITIAL+XLENGTH
      ELSE
        XLENGTH=XFINAL-XINITIAL
      ENDIF
      IF (XLENGTH.EQ.0.D0) RETURN
C
C     SIMPLE DIAMETER DEPENDENT VELOCITY CALCULATION
C
      IF (VELINLET.GT.0.D0) THEN
        VELLIQ=VELINLET
      ELSE IF (DIAMETER.GT.0.D0) THEN
        AREARATIO=OLDDIAMETER/DIAMETER*OLDDIAMETER/DIAMETER
        VELLIQ=VELLIQ*AREARATIO
        VELGAS=VELGAS*AREARATIO
      ENDIF
      IF (DIAMETER.LT.0.D0) DIAMETER=OLDDIAMETER
      VELINLET=VELLIQ
      OLDDIAMETER=DIAMETER
C
C     AVOID BLOW-UP AT XBOIL
C
      IF (XFINAL.EQ.XBOIL) THEN
        XFINAL=XFINAL-XBoilOffset   !EVALUATE UP TO JUST BEFORE XBOIL
      ENDIF
C
C     INITIALIZE SURFACE DECOMPOSITION REACTION
C
      IF (NSurfRx.EQ.0) GOTO 110
      DO 100 I=NRx-NSurfRx+1,NRx
        IF ((RxName(I).EQ.SURFACE).AND.(CalcSurf)) THEN
          RCInit(I)=RCSurf(I)/DIAMETER  !DIAMETER DEPENDENT
        ELSE
          RCInit(I)=0.D0      !NO SURFACE DECOMPOSTION REACTION
        ENDIF
100   CONTINUE
C
110   GConvert=1.038D-9*DensLiq     !CONVERT FROM #SPECIES/100eV TO MOLES/L-RAD
      DO 200 I=1,NSpecies
        GNeut(I)=GNeut0(I)*GConvert
      GGamma(I)=GGamma0(I)*GConvert
200   CONTINUE
C
```

```
      FlowPara=0.71D0+0.00143D0*PRESSURE  !P IN ATM
C
      IF (SENS.AND.CALCSENS) THEN
        NOFSTEP=XLENGTH/XSTEP*SENSSTEP
        IF ((SensStep.EQ.0).OR.(NOFSTEP.GT.IST))  !MAXIMIZE SensStep
     +      SensStep=IST/XLENGTH*XStep
        IF (NOFSTEP.GT.IST) PRINT *,'**** SensStep TOO LARGE; ',
     +      'ADJUSTED TO',SENSSTEP
      ENDIF
C
      RETURN
      END   !OF ADJUST
```

```
      SUBROUTINE WriteComp
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcComp
C
C     WRITES COMPONENT DATA TO OUTPUT FILE.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      IF (ICYCLE.GT.1) GOTO 999           !WRITE FIRST CYCLE ONLY
C
      WRITE (6,292)
      WRITE (6,291) ICYCLE,CompName(IComp)
      WRITE (6,290)
292   FORMAT ('1',80(1h_),/)
291   FORMAT(/20X,'OUTPUT FOR CYCLE',I5,' AT ',A15)
290   FORMAT (/80(1h_),/)
C
      WRITE(6,105) XInitial,XFinal,XLength,XStep,XBoil
105   FORMAT(/5X,36H  INITIAL POSITION                  = ,F14.5,' cm',
     +       /5X,36H  FINAL POSITION                    = ,F14.5,' cm',
     +       /5X,36H  FLOW LENGTH                       = ,F14.5,' cm',
     +       /5X,36H  POSITION INCREMENT                = ,F14.5,' cm',
     +       /5X,36H  POSITION OF ONSET OF BOILING      = ,F14.5,' cm',/)
C
      WRITE(6,110) TempIn,TempOut
110   FORMAT (5X,36H  INLET TEMPERATURE                 = ,F14.5' Kelvin',
     +       /5X,36H  OUTLET TEMPERATURE                = ,F14.5' Kelvin')
      WRITE(6,106) VelInlet,DIAMETER,DensLiq,DensGas,PRESSURE,FlowRate
106   FORMAT (5X,36H  INLET LIQUID VELOCITY             = ,F14.5,' cm/s',
     +       /5X,36H  PIPE INTERNAL DIAMETER            = ,F14.5,' cm',
     +       /5X,36H  WATER DENSITY                     = ,F14.5,' g/cc',
     +       /5X,36H  VAPOR DENSITY                     = ,F14.5,' g/cc',
     +       /5X,36H  PRESSURE                          = ,F14.5,' atm',
     +       /5X,36H  MASS FlowRate                     = ,D14.5,' g/s'/)
C
      IF (CalcSurf) WRITE(6,107) SURFACE
107   FORMAT (5X,36H  SURFACE MATERIAL                  = ,A3/)
      IF (CALCSens.AND.SENS) THEN
        WRITE(6,108) (I,SensSpecies(I),I=1,NSens)
        WRITE(6,109) SENSSTEP
      ENDIF
108   FORMAT (6X,    ' SENSITIVITY SPECIES ',I3,9X,'= ',A8)
109   FORMAT(/5X,36H  SensStep                          = ,I8/)

C
      WRITE (6,230) GammaRate,NeutRate,GCONVERT
230   FORMAT(5X,36H GAMMA DOSE RATE MULTIPLIER       = ,D14.5,' Rad/s',
     +      /5X,36H NEUTRON DOSE RATE MULTIPLIER     = ,D14.5' Rad/s',
     +      /5X,36H GConvert                         = ,D14.5)
C
      IF (GammaRate.GT.0.D0) THEN
        WRITE (6,300)
        WRITE (6,310) (I,GAMMAC(I),I=0,MAXORDERD)
```

```
      ENDIF
300   FORMAT (/5X,  '  GAMMA DOSE SHAPE FUNCTION COEFFICIENTS')
310   FORMAT (7X,  'GAMMA COEFFICIENT',I3,12X,'= ',D14.5)
C
252   IF (NeutRate.GT.0.D0) THEN
        WRITE (6,320)
        WRITE (6,330) (I,NEUTRONC(I),I=0,MAXORDERD)
      ENDIF
320   FORMAT (/5X,  '  NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS')
330   FORMAT (7X,  'NEUTRON COEFFICIENT',I3,10X,'= ',D14.5)
C
245   IF (XFinal.GT.XBoil) THEN
        WRITE (6,340)
        WRITE (6,350) (I,VOIDC(I),I=0,MAXORDERV)
      ENDIF
340   FORMAT (/5X,  '  VOID FRACTION FUNCTION COEFFICIENTS')
350   FORMAT (7X,  'VOID FRACTION  COEFFICIENT',I3,3X,'= ',D14.5)
C
      WRITE (6,256) CalcSurf,VoidFlag,CALCSENS,WRITERX,WRITEPARA
256   FORMAT(/5X,36H  CalcSurf                         = ,L8,
     +       /5X,36H  VoidFlag                         = ,L8,
     +       /5X,36H  CalcSens                         = ,L8,
     +       /5X,36H  WriteRx                          = ,L8,
     +       /5X,36H  WritePara                        = ,L8)
C
      WRITE (6,250) ATOL,RTOL
      IF (Sens.AND.CALCSENS) WRITE (6,255) AdjATOL,AdjRTOL,ResATOL,
     +                                     ResRTOL
250   FORMAT(/5X,36H  RADIOLYSIS ABSOLUTE TOLERANCE    = ,D14.5,
     +       /5X,36H             RELATIVE TOLERANCE    = ,D14.5)
255   FORMAT (5X,36H  ADJOINT    ABSOLUTE TOLERANCE    = ,D14.5,
     +       /5X,36H             RELATIVE TOLERANCE    = ,D14.5,
     +       /5X,36H  RESPONSE   ABSOLUTE TOLERANCE    = ,D14.5,
     +       /5X,36H             RELATIVE TOLERANCE    = ,D14.5)
C
      IF (WRITERX) THEN
      CALL ARRHENIUS(XINITIAL)
        WRITE (6,292)
        WRITE (6,10) COMPNAME(ICOMP)
        WRITE (6,290)
        WRITE (6,11)
        DO 160 I=1,NRx
          WRITE(6,111) RxName(I),(SpeciesName(IR(I,K)),K=1,3),
     +                 (SpeciesName(IP(I,K)),K=1,4),RateConst(I),EA(I)
160     CONTINUE
      ENDIF
C
10    FORMAT (/19X,'CHEMICAL REACTIONS FOR ',A16)
11    FORMAT (/
     +  26X,'REACTIONS',30X,'RATE',2X,'ACTIVATION',/63X,'CONSTANT',2X,
     +  'ENERGIES'/62X,'          (KJ/MOL-K)'/)
111   FORMAT(1X,A3,1X,3A8,'>',4A8,D9.2,1X,D9.2)
C
      WRITE (6,293)            !PAGE FEED
293   FORMAT ('1')
C
C     WRITE TO PLOT FILE
C
```

```
999   IF (PlotOut.AND.(ICYCLE.EQ.NCYCLE)) THEN
        ITER=IIDINT(XLENGTH/XStep)+1
        REMAINDER=XLENGTH-XSTEP*DINT(XLENGTH/XSTEP)
        IF (REMAINDER.NE.0.D0) ITER=ITER+1
        WRITE (7,410) CompName(IComp),ITER
      ENDIF
410   FORMAT (1X,A16,/1X,I5)
C
      RETURN
      END    !OF WriteComp
```

```
      SUBROUTINE RADIOLYSIS
C
C************************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C************************************************************************
C     CALLED BY CalcComp
C     CALLS CONCENTRATION, WriteConc
C
C     EVALUATES RADIOLYSIS OF A COMPONENT USING LSODE.
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
C     INITIALIZE FOR LSODE
C
      CONC(NSpecies+1)=1.0D0  !ASSIGN ZERO-ORDER RX
      ISTATE= 1
      RWORK(1)=XFinal
      IWORK(11)=0
      IWORK(12)=0
      IWORK(13)=0
      IWORK(17)=0
      IWORK(18)=0
      X      = XInitial
      XOut   = XInitial
C
      IF (SENS.AND.CALCSENS) THEN
        XSTEP =XStep/DFLOTJ(SensStep)
        ITER  = 1
      ENDIF
C
C**** MAIN LOOP OF RADIOLYSIS BEGINS
C
280   CALL CONCENTRATION(X,XOut)
C
      IF (SENS.AND.CALCSENS) THEN
        IARG=JMOD(ITER-1,SensStep)   !WRITE ONLY AT ORIGINAL XSTEP
        IF (((IARG.EQ.0).OR.(X.EQ.XFinal)).AND.CycleOut(ICYCLE))
     +     CALL WriteConc(X)
        DO 281, I=1,NSpecies   !SAVE CONCENTRATION CURVE FOR SENSITIVITY CALC
          ConcCurve(ITER,I)=CONC(I)
281     CONTINUE
        IF (DEBUG(2)) WRITE(6,*) 'X ',X,' ITER',ITER
        ITER=ITER+1
      ELSE
        IF (CycleOut(ICYCLE)) CALL WriteConc(X)
      ENDIF
C
C     EXIT LOOP UPON XFinal OR LSODE ERROR.
C     ADD 1.D-5 TO X TO FIX ROUND OFF ERROR.
C
      IF (((X+1.D-7).GE.XFinal).OR.(ISTATE.LT.0)) GO TO 380
C
C     INCREMENT XOut AND CONTINUE
C
      XOut = XOut + XStep
      IF (XOut.GT.XFinal) XOut=XFinal
```

```
      GO TO 280
C
C**** CONTINUE THROUGH TIME STEPS UNTIL XFINAL
C
380   MAXITER=ITER-1
C
      RETURN
      END    !OF RADIOLYSIS
```

```
      SUBROUTINE CONCENTRATION (X,XOut)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY RADIOLYSIS.
C     CALLS LSODE FOR RADIOLYSIS EVALUATION.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      EXTERNAL FRO,JACOB
C
280   CALL LSODE(FRO,NSpecies,CONC,X,XOut,ITOL,RTOL,ATOL,ITASK,
     +           ISTATE,IOPT,RWORK,LRW,IWORK,LIW,JACOB,MF)
C
      IF (ISTATE.EQ.-1) THEN  !LSODE ERROR - EXCESSIVE WORK DONE
        ISTATE=2
        PRINT *,'**** WORKING HARD AT CONCENTRATION!'
        IF (DEBUG(1)) WRITE (6,*) '**** WORKING HARD AT CONCENTRATION!'
        GO TO 280       !RESET AND TRY AGAIN
      ELSE IF (ISTATE.LT.0) THEN
        PRINT *,'**** LSODE ERROR. ISTATE =',ISTATE
        IF (DEBUG(1)) WRITE (6,*) '**** LSODE ERROR. ISTATE =',ISTATE
      ENDIF
C
      RETURN
      END   !OF CONCENTRATION
```

```
      SUBROUTINE FRO (NSP,X,CONCVEC,DCDX)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C     CALLS DoseShape, TwoPhase, ARRHENIUS
C
C     FRO CALCULATES THE SPATIAL MASS BALANCE DIFFERENTIAL EQUATION:
C     dC/dx = CHEMICAL GENERATION - CHEMICAL ANNIHILATION
C           + GENERATION BY RADIATION + CONVECTION
C           + MASS TRANSFER BETWEEN GAS AND LIQUID
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION CONCVEC(ISP),DCDX(ISP)    !CONCVEC IS EQUIVALENT TO CONC
C
      IF (DEBUG(9)) WRITE(6,*) 'ENTERING FRO AT X =',X
      CALL DoseShape(X,DSR,DHR)     !EVALUATE DOSE RATES ALONG THE PATH
      CALL TwoPhase(X)        !EVALUATE TWO-PHASE PARAMETERS
      CALL ARRHENIUS(X)       !ADJUST RATE CONSTANTS AT TEMP
C
C     EVALUATE dC/dx.
C     OUTER LOOP ITERATES THROUGH ALL OF THE ODES, AND THE INNER
C     LOOP ITERATES OVER THE APPLICABLE REACTIONS FOR EACH ODE.
C
      DO 110 I=1,NSP
        DCDX(I) = 0.0D0             !INITIALIZE TO ZERO
        IC=INDEX(SpeciesName(I),'G')      !SEE IF THE SPECIES IS GAS
        IC1=INDEX(SpeciesName(I),'H2O ')
        IF (IC1.NE.0) GOTO 110            !SKIP H2O AND 2H2O
C
C     CALC CHEMICAL REACTIONS AND MASS TRANSFER BETWEEN LIQUID AND GAS
C
        DO 100 J=1,NRx
          IF (KOEF(J,I).EQ.0) GOTO 100
          IF (EA(J).LT.0.D0) THEN   !ADJUST MASS TRANSFER RATE
            RateConst(J)=RCInit(J)*VOID/(1.D0-VOID)    !LIQUID
            IF ((IC.NE.0).AND.(X.GE.XBOIL)) RateConst(J)=RCInit(J) !GAS
          ENDIF
          DCDX(I)=DCDX(I)+RateConst(J)*DFLOTJ(KOEF(J,I))*
     +            CONCVEC(IR(J,1))*CONCVEC(IR(J,2))*CONCVEC(IR(J,3))
100   CONTINUE
C
C     CALC IRRADIATION AND CONVECTION TERMS
C
        IF (IC.EQ.0) THEN           !LIQUID
          DCDX(I)=(DCDX(I)+GGamma(I)*DSR+GNeut(I)*DHR
     +            -CONCVEC(I)*(DVLDX-VelLiq/(1.D0-VOID)*DVFDX))
     +            /VelLiq
        ELSE IF (VELGAS.GT.0.D0) THEN     !GAS
          DCDX(I)=(DCDX(I)-CONCVEC(I)*(DVGDX+VelGas/VOID*DVFDX))
     +            /VelGas
        ENDIF
        IF (DEBUG(10)) WRITE(6,*) X,' DCDX(',I,') = ',DCDX(I)
110   CONTINUE            !THROUGH ALL SPECIES
C
```

```
RETURN
END     !OF FRO
```

```
      SUBROUTINE DoseShape(X,DSR,DHR)
C
C***************************************************************************
C     VERSION:          RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***************************************************************************
C     CALLED BY FRO
C
C     EVALUATE DOSE RATES AS A FUNCTION OF TRAVEL UP THE CHANNEL
C***************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      GAMMA=GAMMAC(MaxOrderD) !EVALUATE MAXORDERD-TH POLYNOMIAL
      NEUTRON=NEUTRONC(MaxOrderD)
      DO 100 I=MaxOrderD-1,0,-1
        GAMMA=X*GAMMA+GAMMAC(I)
        NEUTRON=X*NEUTRON+NEUTRONC(I)
100   CONTINUE
      IF (GAMMA.LT.0.0D0) GAMMA=0.0D0
      IF (NEUTRON.LT.0.0D0) NEUTRON=0.0D0
      DSR = GammaRate*GAMMA
      DHR = NeutRate*NEUTRON
C
      RETURN
      END   !OF DoseShape
```

```
      SUBROUTINE TwoPhase(X)
C
C************************************************************************
C     VERSION:          RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C************************************************************************
C     CALLED BY FRO
C
C     EVALUATE TWO-PHASE PARAMETERS.
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      IF (X.LT.XBoil) THEN
        VOID=0.D0
        QUALITY=0.D0
        DVFDX=0.D0
        VelLiq=VelInlet
        DVLDX=0.D0
        VelGas=0.D0
        DVGDX=0.D0
        RETURN
      ENDIF
C
      Void=VOIDC(MaxOrderV)    !EVALUATE MAXORDERV-TH POLYNOMIAL OF VOIDF
      DVFDX=DFLOTJ(MAXORDERV)*VOID
      DO 200 I=MaxOrderV-1,0,-1
        Void=X*Void+VOIDC(I)
        IF (I.GT.0) DVFDX=X*DVFDX+DFLOTJ(I)*VOIDC(I)
200   CONTINUE
C
      IF (VOID.LE.0.0D0) THEN !OVERRIDE DIVISION BY ZERO ERROR
        PRINT *, '**** VOID FRACTION IS .LE. ZERO',X,XBOIL
        WRITE (6,*) '**** VOID FRACTION IS .LE. ZERO',X,XBOIL
        VOID=1.0D-99
        DVFDX=0.D0
        GOTO 100  !DON'T EVEN BOTHER QUALITY
      ENDIF
C
C     IF VoidFlag=FALSE THEN QUALITY COEFFICIENTS ARE INPUT
C     INSTEAD OF VOID FRACTION.  SO CONVERT QUALITY TO VOID FRACTION.
C
      IF (.NOT.VoidFlag) THEN        !INPUT IS QUALITY
        QUALITY=VOID                   !SO CONVERT TO VoidFraction
        VOID=FlowPara/(1.D0-DensGas/DensLiq*(1.D0-1.D0/QUALITY))
        DVFDX=VOID*VOID/FlowPara*DensGas/DensLiq/QUALITY/QUALITY
     +          *DVFDX

      ENDIF
C
100   IF (DVFDX.NE.0.D0) THEN        !SKIP IF CONSTANT VOID FRACTION
                                 !TO KEEP VELOCITIES CONSTANT
        SLIPRATIO=(1.D0-VOID)/(FlowPara-VOID)
        VelLiq=VelInlet/(VOID*(DensGas/DensLiq*SLIPRATIO-1.D0)+1.D0)
        VelGas=SLIPRATIO*VelLiq
      ENDIF
      DSRDX=DVFDX/(FlowPara-VOID)*(SLIPRATIO-1.D0)
      DVLDX=-VelLiq*VelLiq/VelInlet
```

```
     +       *(DVFDX*(DensGas/DensLiq*SLIPRATIO-1.D0)
     +       +VOID*DensGas/DensLiq*DSRDX)
      DVGDX=DSRDX*VelLiq+SLIPRATIO*DVLDX
C
      RETURN
      END    !OF TwoPhase
```

```
      SUBROUTINE ARRHENIUS(X)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY FRO
C
C     USE ARRHENIUS LAW TO CORRECT RATE CONSTANTS AT TEMP.
C     TEMPERATURE IS EVALUATED ALONG THE PATH BY INTERPOLATING TINLET
C     AND TOUTLET LINEARLY. BUT TEMPERATURE IS KEPT CONSTANT IN THE
C     BOILING REGION, TEMPERATURE RISING ONLY UP TO THE ONSET OF
C     BOILING TO TOUTLET.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      TEMP=(TempOut-TempIn)/(XFinal-XInitial)*(X-XInitial)+TempIn
      IF ((XBOIL.GE.XINITIAL).AND.(XBOIL.LT.XFINAL)) THEN
        IF (X.LT.XBoil) THEN          !NOT BOILING YET
          TEMP=(TempOut-TempIn)/(XBoil-XInitial)*(X-XInitial)+TempIn
        ELSE                        !STARTED BOILING
          TEMP=TempOut
        ENDIF
      ENDIF
C
      IF (TEMP.NE.TEMPHOLD) THEN
        DO 277 I=1,NRx
          IF (EA(I).GE.0.0D0)
     +      RateConst(I)=RCInit(I)*DEXP(-EA(I)/GASCONST*
     +                   (1.D0/TEMP-1.D0/TempRef))
277     CONTINUE
        TEMPHOLD=TEMP
      ENDIF
C
      RETURN
      END   !OF ARRHENIUS
```

```
      SUBROUTINE JACOB (NSP,X,CONCVEC,ML,MU,PD,NROWPD)
C
C***********************************************************************
C     VERSION:         RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C
C     JACOB CALCULATES THE FULL JACOBIAN MATRIX OF dC/dx.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION PD(NROWPD,ISP),CONCVEC(ISP)     !CONCVEC IS EQUIV TO  CONC
C
      DO 100 J=1,NSP          !NSP IS EQUIVALENT TO NSpecies
C
C       CHEMICAL REACTIONS AND MASS TRANSFER TERMS
C
        DO 101 I=1,NSP
          PD(I,J)=0.0D0
          IC=INDEX(SpeciesName(I),'G')    !SEE IF THE SPECIES IS GAS
          DO 102 K=1,NRx
            IF((KOEF(K,J).GE.0).OR.(KOEF(K,I).EQ.0)) GOTO 102
            IF (EA(K).LT.0.D0) THEN !ADJUST MASS TRANSFER RATE
              RateConst(K)=RCInit(K)*VOID/(1.D0-VOID)
              IF ((IC.NE.0).AND.(X.GE.XBoil)) RateConst(K)=RCInit(K)
            ENDIF
            A = RateConst(K)*DFLOTJ(KOEF(K,I))
C
            IF(KOEF(K,J).EQ.-2)THEN !SECOND ORDER REACTANT
              PD(I,J)=PD(I,J)+2.D0*A*CONCVEC(IR(K,1))*CONCVEC(IR(K,3))
            ELSE IF (IR(K,1).EQ.J) THEN   !FIRST ORDER REACTANT
              PD(I,J)=PD(I,J)+A*CONCVEC(IR(K,2))*CONCVEC(IR(K,3))
            ELSE IF (IR(K,2).EQ.J) THEN
            PD(I,J)=PD(I,J)+A*CONCVEC(IR(K,1))*CONCVEC(IR(K,3))
            ELSE
              PD(I,J)=PD(I,J)+A*CONCVEC(IR(K,1))*CONCVEC(IR(K,2))
          ENDIF
102       CONTINUE
        PD(I,J)=PD(I,J)/VelLiq
101     CONTINUE
C
C       CONVECTION TERMS
C
        IC=INDEX(SpeciesName(J),'G')
        IF (IC.EQ.0) THEN           !LIQUID
          PD(J,J)=PD(J,J)-DVLDX/VelLiq+DVFDX/(1.D0-VOID)
        ELSE IF (VOID.GT.0.D0) THEN !GAS
          PD(J,J)=(PD(J,J)*VelLiq-DVGDX)/VelGas-DVFDX/VOID
        ENDIF
C
100   CONTINUE
C
      RETURN
      END   !OF JACOB
```

```
      SUBROUTINE WriteConc(X)
C
C**************************************************************************
C     VERSION:        RADICAL 1.0              19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C**************************************************************************
C     CALLED BY RADIOLYSIS
C
C     WRITES CONCENTRATIONS AT EACH STEP TO OUTPUT FILE AND PLOT FILE.
C     THE FLAG LinLin CONTROLS OUTPUT FORMAT FOR PLOT FILE
C       LinLin=.TRUE.  ->  LINEAR CONCENTRATION/LINEAR POSITION
C       LinLin=.FALSE. ->  LOG CONCENTRATION/LINEAR POSITION
C**************************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION COEF(ISP)
C
C     WRITE TO OUTPUT FILE
C
      WRITE (6,290)
      DO 100 I=1,NSPECIES
        COEF(I)=1.0D0
        IF (NORMALIZE) THEN           !NORMALIZE TO DENSITY
          COEF(I)=1.0D0/DENSLIQ
        ENDIF
        IF (PPBOUT) THEN              !CONVERT TO PPB
          COEF(I)=MOLWT(I)*1.0D6/DENSLIQ
        ENDIF
100   CONTINUE
C
      WRITE (6,130) ICYCLE,COMPNAME(ICOMP),X-XINITIAL
      IF (PPBOUT) THEN
        WRITE (6,120) X
      ELSE IF (NORMALIZE) THEN
        WRITE (6,110) X
      ELSE
        WRITE (6,310) X
      ENDIF
      WRITE (6,320) (SpeciesName(I),COEF(I)*CONC(I),I=1,NSPECIES)
C
290   FORMAT (80(1h_),/)
310   FORMAT (12X,'CONCENTRATIONS[moles/liter] AT POSITION = ',
     +        F11.4,' cm'/)
110   FORMAT (12X,'  CONCENTRATIONS[moles/kg]  AT POSITION = ',
     +        F11.4,' cm'/)
120   FORMAT (12X,'       CONCENTRATIONS[ppb]  AT POSITION = ',
     +        F11.4,' cm'/)
130   FORMAT (5X,'CYCLE',I5,8X,'POSITION IN '.A16,' = ',F11.4,' cm')
320   FORMAT (2(5X,A8,' = ',D15.6,' **'))
C
      IF (X.GT.XBoil) THEN    !WRITE GAS CONCENTRATION IN ATM
        WRITE (6,*)
        DO 340 I=1,NSpecies
          IC=INDEX(SpeciesName(I),'G')
          IF (IC.NE.0) THEN
            GAS=CONC(I)*0.018D0/DensGas*PRESSURE      !ASSUME IDEAL GAS
            WRITE(6,330) SpeciesName(I),GAS
          ENDIF
```

```
340     CONTINUE
      ENDIF
330   FORMAT(5X,A8,'  = ',D11.3,' ATM')
C
350   IF (WRITEPARA) THEN
      CALL TWOPHASE(X)
        WRITE (6,300) IWORK(11),TEMP,VELLIQ,VELGAS
        IF (VOIDFLAG) THEN
          WRITE (6,301) VOID
        ELSE
          WRITE (6,301) VOID
          WRITE (6,302) QUALITY
        ENDIF
        WRITE (6,303) GAMMA*GAMMARATE,NEUTRON*NEUTRATE
      ENDIF
300   FORMAT (/5X,'NO. STEPS                    = ',I8,
     +        /5X,'TEMPERATURE (K)              = ',F14.5,
     +        /5X,'LIQUID VELOCITY (CM/S)       = ',F14.5,
     +        /5X,'GAS VELOCITY   (CM/S)        = ',F14.5)
301   FORMAT ( 5X,'VOID FRACTION                = ',F14.5)
302   FORMAT ( 5X,'QUALITY                      = ',F14.5)
303   FORMAT ( 5X,'GAMMA DOSE RATE (RAD/S)      = ',D14.5,
     +        /5X,'NEUTRON DOSE RATE (RAD/S)    = ',D14.5)
C
C     WRITE TO PLOT FILE
C
      IF (PlotOut.AND.(ICYCLE.EQ.NCYCLE)) THEN
        WRITE (7,460) X
        DO 500 I=1,NSpecies
          IF (LinLin) THEN                !LINEAR CONC-LINEAR POSITION
            WRITE (7,460) COEF(I)*CONC(I)
          ELSE IF (CONC(I).GT.0.0D0) THEN !LOG CONC-LINEAR POSITION
            WRITE (7,460) DLOG10(COEF(I)*CONC(I))
          ELSE
            WRITE (7,*)   '   '                !WRITE BLANK
          ENDIF
500     CONTINUE
      ENDIF
460   FORMAT (1X,E21.14)
C
      RETURN
      END   !OF WriteConc
```

```
      SUBROUTINE WriteStat
C
C***********************************************************************
C     VERSION:          RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcComp
C
C     WriteStat WRITES COMPONENT-RUN STATISTICS TO THE OUTPUT FILE.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
C     PRINT THE RUN STATISTICS
C
      ET=SECNDS(TIME2)          !ELAPSED TIME
      WRITE (6,290)
      WRITE (6,381) ICYCLE,COMPNAME(ICOMP)
      WRITE (6,290)
      WRITE (6,390) IWORK(17),IWORK(18),IWORK(11),IWORK(12),IWORK(13),ET
290   FORMAT (/80(1h_),/)
381   FORMAT(/16X,'RUN STATISTICS FOR CYCLE',I5,' AT ',A16)
390   FORMAT(5X,/25H REQUIRED RWORK SIZE   = ,I9,
     +       5X,/25H IWORK SIZE            = ,I9,
     +       5X,/25H NUMBER OF STEPS       = ,I9,
     +       5X,/25H # OF FUNC.- EVALS.    = ,I9,
     +       5X,/25H # OF JACOB.- EVALS    = ,I9,
     +       5X,/25H COMPONENT JOB TIME    = ,F9.2,' seconds')
C
      IF (ISTATE.GT.0) THEN   !SUCCESS
        PRINT 395, COMPNAME(ICOMP)
        WRITE (6,395) CompName(IComp)
      ELSE                !FAILURE
        PRINT 400, ISTATE
        WRITE (6,400) ISTATE
      ENDIF
395   FORMAT (/1X,'CONCENTRATION PROFILE OF ',A16,
     +            ' HAS BEEN EVALUATED SUCCESSFULLY!')
400   FORMAT (/'**** ERROR HALT...ISTATE =',I3)
C
      RETURN
      END   !OF WriteStat
```

```
      SUBROUTINE SENSITIVITY
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY CalcComp
C     CALLS ADJOINT, RESPONSE, WriteSens
C
C     CALCULATES SENSITIVITY WITH RESPECT TO SPECIFIED PARAMETERS.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      ITERHOLD=ITER
      DO 100 I=1,NSens
C
        ISENS=0
        DO 110 J=1,NSpecies    !DETERMINE ISENS
          IF (SensSpecies(I).EQ.SpeciesName(J)) ISens=J
110     CONTINUE
C
        IF (ISENS.EQ.0) THEN  !INPUT ERROR
          PRINT 120
          WRITE (6,120) SENSSPECIES(I)
          GOTO 100
        ENDIF
120     FORMAT ('**** INPUT ERROR **** SensSpecies "',A8,'" NOT FOUND.')
C
        TIME2=SECNDS(0.0)     !START CLOCK TO MEASURE EXECUTION TIME
        ITER=ITERHOLD
        CALL ADJOINT
C
        TIME2=SECNDS(0.0)     !START CLOCK TO MEASURE EXECUTION TIME
        CALL RESPONSE
        CALL WriteSens
C
100   CONTINUE          !THROUGH ALL SENSITIVITY SPECIES
C
      RETURN
      END   !OF SENSITIVITY
```

```
      SUBROUTINE ADJOINT
C
C**********************************************************************
C     VERSION:         RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C**********************************************************************
C     CALLED BY SENSITIVITY
C     CALLS LSODE
C
C     CALCULATES ADJOINT WITH RESPECT TO SPECIFIED PARAMETERS.
C     THE INTEGRAL IS TAKEN BACKWARD ALONG THE FLOW PATH.
C**********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      EXTERNAL ADJFRO,ADJJACOB
C
      PRINT 110, SPECIESNAME(ISENS)
      IF (DEBUG(1)) WRITE (6,110) SPECIESNAME(ISENS)
110   FORMAT (' ENTERING ADJOINT ROUTINE FOR ',A8)
C
C     INITIAL VALUES FOR ADJOINTS ARE ALWAYS ZERO
C
      DO 100, I=1,NSpecies
        AdjConc(I)=0.0D0
100   CONTINUE
C
C     INITIALIZE FOR LSODE
C
      ISTATE= 1
      DO 130 I=1,10
        RWORK(I)=ADJRWORK(I)
        IWORK(I)=ADJIWORK(I)
130   CONTINUE
      RWORK(1)=XInitial
      IWORK(11)=0
      IWORK(12)=0
      IWORK(13)=0
      IWORK(17)=0
      IWORK(18)=0
      X      = XFinal
      XOut   = XFinal
      ITER   = MAXITER          !MAXITER IS PASSED FROM RADIOLYSIS
C
C**** START INTEGRATION LOOP HERE FROM XFinal TO XInitial
C
200   CALL LSODE(ADJFRO,NSpecies,AdjConc,X,XOut,AdjITOL,AdjRTOL,
     +           AdjATOL,AdjITASK,ISTATE,ADJIOPT,RWORK,
     +           LRW,IWORK,LIW,ADJJACOB,AdjMF)
C
      IF (ISTATE.EQ.-1) THEN  !LSODE ERROR - EXCESSIVE WORK DONE
        ISTATE=2
        PRINT 120
        IF (DEBUG(1)) WRITE (6,120)
        GO TO 200         !RESET AND TRY AGAIN
      ENDIF
120   FORMAT ('**** WORKING HARD IN ADJOINT ROUTINE.')
C
      DO 281, I=1,NSpecies    !SAVE ADJOINT CURVE FOR RESPONSE CALC
```

```
        AdjCurve(ITER,I)=AdjConc(I)
281   CONTINUE
C
      IF (DEBUG(2)) WRITE(6,*) 'X',X,' ITER ',ITER
      ITER=ITER-1
C
C     EXIT LOOP UPON XFinal OR LSODE ERROR
C
      IF ((ITER.EQ.0).OR.(X.LE.XInitial).OR.(ISTATE.LT.0)) GOTO 380
C
C     DECREMENT XOut AND CONTINUE
C
      XOut = XOut - XStep
      IF (ISTATE.EQ.1) XOut=DFLOTJ(ITER-1)*XStep+XINITIAL   !ADJUST FINAL dx
      IF (XOut.LT.XInitial) XOut=XInitial
      GO TO 200
C
C**** END OF THE MAIN LOOP
C
380   IF (ISTATE.NE.2) THEN
        PRINT 400, ISTATE
        WRITE (6,400) ISTATE
      ENDIF
400   FORMAT (/'**** ERROR HALT IN ADJOINT EVALUATOR...ISTATE =',I3)
C
      PRINT *,'ADJOINT COMPLETED!'  !TMP
      IF (DEBUG(1)) WRITE (6,*) 'ADJOINT COMPLETED!'
C
      AdjIWORK(1)=IWORK(17)    !SAVE FOR PRINT OUT
      AdjIWORK(2)=IWORK(18)
      AdjIWORK(3)=IWORK(11)
      AdjIWORK(4)=IWORK(12)
      AdjIWORK(5)=IWORK(13)
      AdjET=SECNDS(TIME2)
C
      RETURN
      END   !OF ADJOINT
```

```
      SUBROUTINE ADJFRO (NSP,X,ADJVEC,DADJDX)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C     CALLS INTERPOLATE, TwoPhase, JACOB
C
C     CALCULATES d(ADJOINT)/dx.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION ADJVEC(ISP),DADJDX(ISP),JACOBIAN(ISP,ISP)
      REAL*8 JACOBIAN
C
      CALL INTERPOLATE(X,ConcCurve,CONC)
      CALL TwoPhase(X)
      CALL JACOB(NSP,X,CONC,ML,MU,JACOBIAN,ISP)
      DO 110 I=1,NSP
        DADJDX(I) = -JACOBIAN(ISens,I)
        DO 100 J=1,NSP
          DADJDX(I)=DADJDX(I)-ADJVEC(J)*JACOBIAN(J,I)
100   CONTINUE
110   CONTINUE          !THROUGH ALL SPECIES
C
      IF (DEBUG(3)) WRITE(6,*) 'IN ADJFRO, X=',X
      IF (DEBUG(6)) WRITE(6,210) (SPECIESNAME(I),CONC(I),I=1,NSPECIES)
210   FORMAT(2('CON',2X,A8,' + ',D15.6,' **'))
C
      RETURN
      END   !OF ADJFRO
```

```
      SUBROUTINE ADJJACOB (NSP,X,ADJVEC,ML,MU,ADJPD,NROWPD)
C
C***********************************************************************
C     VERSION:          RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION ADJPD(NROWPD,ISP),ADJVEC(ISP),JACOBIAN(ISP,ISP)
      REAL*8 JACOBIAN
C
      CALL INTERPOLATE(X,ConcCurve,CONC)
      CALL TwoPhase(X)
      CALL JACOB(NSP,X,CONC,ML,MU,JACOBIAN,ISP)
C
      DO 110 J=1,NSP
        DO 100 I=1,NSP
          ADJPD(I,J)=-JACOBIAN(J,I)
100   CONTINUE
110   CONTINUE          !THROUGH ALL SPECIES
C
      RETURN
      END    !OF ADJJACOB
```

```
      SUBROUTINE INTERPOLATE(X,PROFILE,VALUE)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY AdjFRO, ResFRO
C
C     FINDS VALUE AT X FROM PROFILE CURVE ARRAY BY LINEAR INTERPOLATION.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION PROFILE(IST+1,ISP),VALUE(ISP)
C
      XEX=X             !SAVE X AND DON'T MESS WITH IT
      IF (XEX.LT.XInitial) XEX=XInitial   !HANDLE OUT-OF-BOUND CASES
      IF (XEX.GT.XFinal)   XEX=XFinal
C
      DELTAX=XEX-XINITIAL
      ILO =IIDINT(DELTAX/XStep)+1   !INDEX OF LOW-END POINT
      IHI =ILO+1
      REMAINDER=DELTAX-XStep*DINT(DELTAX/XSTEP)
      DX=XStep                !SAVE XSTEP AND DON'T MESS WITH IT
C
C     CORRECT FOR THE LAST INTERVAL OF NON-EVENLY DIVIDED CASE
C
      EVENLENGTH=XSTEP*DINT(XLENGTH/XSTEP)
      FINALDX=XLENGTH-EVENLENGTH
      IF ((FINALDX.NE.0.D0).AND.(XEX.EQ.XFINAL)) THEN
        ILO=ILO+1
        REMAINDER=0.D0
      ENDIF
C
      IF ((FINALDX.NE.0.D0).AND.(XEX.GT.(XFinal-FINALDX)))
     +   DX=FINALDX
C
      DO 100 I=1,NSpecies     !STRAIGHT FORWARD INTERPOLATION
        DY=PROFILE(IHI,I)-PROFILE(ILO,I)
        VALUE(I)=DY/DX*REMAINDER+PROFILE(ILO,I)
100   CONTINUE
C
      IF (DEBUG(4)) WRITE(6,200) X,XSTEP,ILO,REMAINDER,FINALDX
200   FORMAT('X         ',D25.15,' XSTEP  ',D25.15,' ILO',I7,
     +      /'REMAINDER',D25.15,' FINALDX',D25.15)
C
      RETURN
      END   !OF INTERPOLATE
```

```
      SUBROUTINE RESPONSE
C
C***********************************************************************
C     VERSION:         RADICAL 1.0                 19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY SENSITIVITY.
C     CALLS LSODE FOR INTEGRATION.
C
C     CALCULATES RESPONSE WITH RESPECT TO SPECIFIED PARAMETERS.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      EXTERNAL RESFRO,RESJACOB
C
      PRINT *,'ENTERING RESPONSE ROUTINE FOR ',SPECIESNAME(ISENS) !TMP
      IF (DEBUG(1)) WRITE (6,*)
     +   'ENTERING RESPONSE ROUTINE FOR ',SPECIESNAME(ISENS)
C
C     INITIAL VALUES FOR RESPONSE
C
      DO 100, I=1,NSpecies
        ResConc(I)=0.D0
100   CONTINUE
C
C     INITIALIZE FOR LSODE
C
      ISTATE= 1
      DO 110 I=1,10
        RWORK(I)=RESRWORK(I)
        IWORK(I)=RESIWORK(I)
110   CONTINUE
      RWORK(1)=XFinal
      IWORK(11)=0
      IWORK(12)=0
      IWORK(13)=0
      IWORK(17)=0
      IWORK(18)=0
      X=XINITIAL
      XOUT=XFINAL
      NRESPONSE=NRX+3*NSPECIES
C
200   CALL LSODE(RESFRO,NRESPONSE,ResConc,X,XOUT,RESITOL,RESRTOL,
     +           RESATOL,ResITASK,ISTATE,RESIOPT,RWORK,
     +           LRW,IWORK,LIW,RESJACOB,RESMF)
C
      IF (ISTATE.EQ.-1) THEN  !LSODE ERROR - EXCESSIVE WORK DONE
        ISTATE=2
        PRINT 300
        IF (DEBUG(1)) WRITE (6,300)
        GO TO 200       !RESET AND TRY AGAIN
      ENDIF
300   FORMAT ('**** WORKING HARD IN RESPONSE ROUTINE.')
C
      IF (ISTATE.NE.2) THEN
        PRINT 400, ISTATE
        WRITE(6,400) ISTATE
      ENDIF
```

```
400   FORMAT (/'**** ERROR HALT IN RESPONSE EVALUATOR...ISTATE =',I3)
C
      PRINT *,'EXITING RESPONSE ROUTINE.' !TMP
      IF (DEBUG(1)) WRITE (6,*) 'EXITING RESPONSE ROUTINE.'
C
      RETURN
      END    !OF RESPONSE
```

```
      SUBROUTINE RESFRO (NRESP,X,RESVEC,DRDX)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C     CALLS INTERPOLATE, DoseShape
C
C     CALCULATES d(RESPONSE)/dx.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION RESVEC(IRE),DRDX(IRE)  !RESVEC IS SAME AS ResConc
      DIMENSION JACOBIAN(ISP,ISP)
      REAL*8 JACOBIAN
C
      CALL INTERPOLATE(X,ConcCurve,CONC)   !RETURNS CONC(SPECIES) AT X
      CALL INTERPOLATE(X,AdjCurve,AdjConc)       !RETURNS AdjConc(SPECIES) AT X
      CALL TWOPHASE(X)
C
      IF (DEBUG(5)) WRITE(6,*) 'ENTERING RESFRO, X =',X
      IF (DEBUG(7)) WRITE(6,900) (SPECIESNAME(I),CONC(I),I=1,NSPECIES)
      IF (DEBUG(8)) WRITE(6,910)
     +   (SPECIESNAME(I),ADJCONC(I),I=1,NSPECIES)
900   FORMAT (2('CON',2X,A8,' = ',D15.6,' **'))
910   FORMAT (2('ADJ',2X,A8,' = ',D15.6,' **'))
C
      DO 110 I=1,NRX
      CONCEN=CONC(IR(I,1))*CONC(IR(I,2))*CONC(IR(I,3))
        DRDX(I)=DFLOTJ(KOEF(I,ISens))*CONCEN
        IC=INDEX(SpeciesName(ISENS),'G')
        IF (IC.EQ.0) THEN           !LIQUID
          DRDX(I)=DRDX(I)/VELLIQ
          IF ((EA(I).LT.0.D0).AND.(VOID.GT.0.D0))
     +       DRDX(I)=DRDX(I)*(1.D0-VOID)/VOID         !GET MASS TRANSFER RATE
        ELSE IF (VELGAS.GT.0.D0) THEN     !GAS
          DRDX(I)=DRDX(I)/VELGAS
        ENDIF
C
        DO 100 J=1,NSpecies
          A=AdjConc(J)*DFLOTJ(KOEF(I,J))*CONCEN
          IC=INDEX(SpeciesName(J),'G')
          IF (IC.EQ.0) THEN         !LIQUID
            A=A/VELLIQ
            IF ((EA(I).LT.0.D0).AND.(VOID.GT.0.D0))
     +         A=A*(1.D0-VOID)/VOID !GET MASS TRANSER RATE
          ELSE IF (VELGAS.GT.0.D0) THEN   !GAS
            A=A/VELGAS
          ENDIF
          DRDX(I)=DRDX(I)+A
100   CONTINUE
110   CONTINUE          !THROUGH ALL RATE CONSTANTS
C
C     SENSITIVITIES FOR G-VALUES OF GAMMA AND NEUTRON
C
      CALL DoseShape(X,DSR,DHR)     !RETURNS GAMMA AND NEUT DOSE RATE AT X
      DO 200 I=1,NSpecies
```

```
        DRDX(NRX+I)=GCONVERT*DSR*AdjConc(I)        !GAMMA
        IF (I.EQ.ISENS) DRDX(NRX+I)=DRDX(NRX+I)+GCONVERT*DSR
        IF (GGamma(I).EQ.0.D0) DRDX(NRX+I)=0.D0
C
        INEUT=NRX+NSpecies+I                 !NEUTRON
        DRDX(INEUT)=GCONVERT*DHR*ADJCONC(I)
        IF (I.EQ.ISENS) DRDX(INEUT)=DRDX(INEUT)+GCONVERT*DHR
        IF (GNeut(I).EQ.0.D0) DRDX(INEUT)=0.D0
C
        IC=INDEX(SpeciesName(I),'G')
        IF (IC.EQ.0) THEN            !LIQUID
          DRDX(NRX+I)=DRDX(NRX+I)/VELLIQ
          DRDX(INEUT)=DRDX(INEUT)/VELLIQ
        ELSE IF (VELGAS.GT.0.D0) THEN     !GAS
          DRDX(NRX+I)=DRDX(NRX+I)/VELGAS
          DRDX(INEUT)=DRDX(INEUT)/VELGAS
        ENDIF
200   CONTINUE
C
C     SENSITIVITIES WITH RESPECT TO OTHER SPECIES
C
      CALL JACOB(NSpecies,X,CONC,ML,MU,JACOBIAN,ISP)
      DO 300 I=1,NSpecies
        ISPEC=NRX+2*NSPECIES+I
        DRDX(ISPEC) = JACOBIAN(ISens,I)
        DO 310 J=1,NSPECIES
          DRDX(ISPEC)=DRDX(ISPEC)+ADJCONC(J)*JACOBIAN(J,I)
310   CONTINUE
300   CONTINUE          !THROUGH ALL SPECIES
C
      RETURN
      END   !OF RESFRO
```

```
      SUBROUTINE RESJACOB (NRESP,Y,RESVEC,ML,MU,RESPD,NROWPD)
C
C***********************************************************************
C     VERSION:        RADICAL 1.0               19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY LSODE
C
C     JACOBIAN OF RESPONSE FUNCTION IS ZERO
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
      DIMENSION RESPD(NROWPD,IRE),RESVEC(IRE)
C
      RETURN
      END   !OF RESJACOB
```

```
      SUBROUTINE WriteSens
C
C***********************************************************************
C     VERSION:         RADICAL 1.0                  19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C***********************************************************************
C     CALLED BY SENSITIVITY
C
C     WRITES SENSITIVITY RESULTS TO OUTPUT FILE.
C***********************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
C     PRINT SENSITIVITY
C
      WRITE (6,290)
      WRITE (6,100) COMPNAME(ICOMP),SpeciesName(ISens)      !TO PLOT FILE
      WRITE (8,101) COMPNAME(ICOMP),SpeciesName(ISens)      !TO SENS FILE
      WRITE (6,291)
100   FORMAT(/14X,A16,' SENSITIVITY RESULTS FOR ',A8)
101   FORMAT(1X,A16/1X,A8)
C
      WRITE (6,667)
667   FORMAT (/14X,' ============ ADJOINT RESULTS =============='/)
C
      WRITE (6,320) (SpeciesName(I),AdjCurve(1,I),I=1,NSpecies)
320   FORMAT (2(5X,A8,' = ',D15.6,' **'))
C
      WRITE (6,130)             !WRITE RATE CONSTANT SENSITIVITY
130   FORMAT(//36X,'ABSOLUTE',6X,'RELATIVE',
     +      /13X,'PARAMETER',13X,'SENSITIVITY',3X,'SENSITIVITY',
     +      /5X,'-------------------------',2X,2('  ------------')/)
C
      DO 120, I=1,NRx
        RELSENS=ResConc(I)*RateConst(I)/ConcFinal(IComp,ISens)
        IC=INDEX(SPECIESNAME(ISENS),'G')
        IF ((EA(I).LT.0.D0).AND.(IC.EQ.0).AND.(VOID.GT.0.D0))
     +     RELSENS=RELSENS*(1.D0-VOID)/VOID      !MASS TRANSFER RATE
        IF (RELSENS.NE.0.D0) WRITE (6,110)
     +     'RATE CONST OF '//RxName(I)//'          ',ResConc(I),RELSENS
        WRITE (8,460) ResConc(I),RELSENS
120   CONTINUE
C
      DO 140, I=1,NSpecies    !WRITE G-VALUE SENSITIVITY
        RELSENS=ResConc(NRx+I)*GGamma0(I)/ConcFinal(IComp,ISens)
        IF (RELSENS.NE.0.D0) WRITE (6,110)
     +     'GAMMA   G-VALUE OF '//SpeciesName(I),ResConc(NRx+I),RELSENS
        WRITE (8,460) ResConc(NRx+I),RELSENS
C
        IGNeut=NRx+NSpecies+I
        RELSENS=ResConc(IGNeut)*GNeut0(I)/ConcFinal(IComp,ISens)
        IF (RELSENS.NE.0.D0) WRITE (6,110)
     +     'NEUTRON G-VALUE OF '//SpeciesName(I),ResConc(IGNeut),RELSENS
        WRITE (8,460) ResConc(IGNeut),RELSENS
140   CONTINUE
C
      DO 150, I=1,NSpecies    !WRITE SENSITIVITY WRT OTHER SPECIES
        ISPEC=NRx+2*NSpecies+I
```

```
           RELSENS=ResConc(ISPEC)*ConcFinal(IComp,I)
     +            /ConcFinal(IComp,ISens)
           IF (RELSENS.NE.0.D0) WRITE (6,110)
     +        'CONCENTRATION OF   '//SpeciesName(I),ResConc(ISPEC),
     +        RELSENS
           WRITE (8,460) ResConc(ISPEC),RELSENS
150     CONTINUE
C
110     FORMAT(5X,A27,2(D14.5))
460     FORMAT(1X,E21.14)
C
C       PRINT THE RUN STATISTICS
C
        ET=SECNDS(TIME2)          !ELAPSED TIME
        WRITE (6,291)
        WRITE (6,381) COMPNAME(ICOMP)
        WRITE (6,291)
        WRITE (6,385)
        WRITE (6,390) AdjIWORK(1),IWORK(17),AdjIWORK(2),IWORK(18),
     +                AdjIWORK(3),IWORK(11),AdjIWORK(4),IWORK(12),
     +                AdjIWORK(5),IWORK(13),AdjET,ET
290     FORMAT ('1'80(1h_),/)
291     FORMAT (/80(1h_),/)
381     FORMAT(/17X,A16,'SENSITIVITY RUN STATISTICS')
385     FORMAT(/29X,'ADJOINT',21X,'RESPONSE',
     +         /29X,'-------',21X,'--------')
390     FORMAT(5X,/25H REQUIRED RWORK SIZE    = ,I9,20X,I9,
     +         5X,/25H IWORK SIZE             = ,I9,20X,I9,
     +         5X,/25H NUMBER OF STEPS        = ,I9,20X,I9,
     +         5X,/25H # OF FUNC.- EVALS.     = ,I9,20X,I9,
     +         5X,/25H # OF JACOB.- EVALS     = ,I9,20X,I9,
     +         5X,/25H SENSITIVITY JOB TIME   = ,F9.2,' seconds',
     +                                   12X,F9.2,' seconds')
C
        IF (ISTATE.GT.0) THEN   !SUCCESS
          PRINT 395, SPECIESNAME(ISENS),CompName(IComp)
          WRITE (6,395) SPECIESNAME(ISENS),CompName(IComp)
        ELSE                    !FAILURE
          PRINT 400, ISTATE
          WRITE (6,400) ISTATE
        ENDIF
395     FORMAT (/' SENSITIVITY OF ',A8,' IN ',A16,
     +          ' HAS BEEN EVALUATED SUCCESSFULLY!')
400     FORMAT (/' ERROR HALT IN SENSITIVITY ROUTINE...ISTATE =',I3)
C
        RETURN
        END   !OF WriteSens
```

```
      SUBROUTINE TERMINATE
C
C************************************************************************
C     VERSION:         RADICAL 1.0                  19 MARCH 1990
C     CODE CUSTODIAN: JOHN H. CHUN
C************************************************************************
C     CALLED BY RADICAL
C
C     TERMINATE WRITES FINAL RUN STATISTICS TO THE OUTPUT FILE AND
C     CLOSES ALL FILES.
C************************************************************************
C
      INCLUDE 'RADICAL.BLK'
C
      ET=SECNDS(TIME1)        !TOTAL ELAPSED TIME
      WRITE (6,390) ET
390   FORMAT(5X,/25H TOTAL JOB TIME        = ,F9.2,' seconds')
c
      CLOSE (5)   !CLOSE INPUT FILE
      CLOSE (6)   !CLOSE OUTPUT FILE
      IF (PlotOut) CLOSE (7)  !CLOSE PLOT FILE
      IF (SENS)    CLOSE (8)  !CLOSE SENS FILE
C
      RETURN
      END   !OF TERMINATE
```

III. RADPLOT.RS1

RADPLOT.RS1 is a graphics procedure for plotting concentration profiles on the MicroVAX-II system using the RS1 software. The procedure reads in a plot file generated by RADICAL and arranges it into a table which is then plotted on the screen. The plot may be plotted to a plotter or a printer; in this project, the DEC LN03 laser printer was used to produce plots.

For more detail, the reader is referred to RS1 User's Manuals.

```
      PROCEDURE;

      /*
      PROCEDURE RADPLOT

      THIS RS1 PROCEDURE PLOTS CHEMICAL SPECIES CONCENTRATION VS.
      POSITION FROM THE PLOT OUTPUT FILE OF RADICAL.

      MODIFIED BY             : JOHN CHUN     MAR 1990
      ORIGINALLY WRITTEN BY   : SCOTT SIMONSON        1988
      */

      ERASE;
      ANSWER = GETTEXT("CREATE A NEW TABLE OR USE AN OLD ONE? [N/O] ");
      IF (ANSWER = "N") THEN BEGIN;

        /* CREATE TABLE FROM PLOT FILE */

        PLOTFILE = GETTEXT("PLOT FILE TO READ? ");
        PF = INFILE(PLOTFILE);
        TITLELINE=GETLINE(PF);
        LINLIN=DECODE(GETLINE(PF),"I(6)");/* READ LINLIN; LINLIN=-1, LOGLIN=0 */

        NSPECIES=DECODE(GETLINE(PF),"I(6)");    /* READ NSPECIES */
NEWT:   TABLEC = GETTEXT("NEW TABLE NAME('DIR' FOR DIRECTORY) [File Read:"
                    CAT PLOTFILE CAT "] ");
        IF (TABLEC = "DIR") THEN BEGIN;
          DIR;
          GO TO NEWT;
        END;
        NROW=NSPECIES+1;
        ALLOCATE TABLE(TABLEC) NROW ROWS BY 0 COLUMNS;
        SET TITLE OF TABLE(TABLEC) TO TITLELINE;
        TABLEC[0,0]=PLOTFILE;
        TABLEC[1,0]="X (cm)";
        DO I = 1 TO NSPECIES;       /* READ SPECIES NAMES */
          SPECIESNAME = GETLINE(PF);
          N = I + 1;
          TABLEC[N,0]=SPECIESNAME;
        END;

        ICOL=1;
      NEXTCOL=1;
        DO WHILE NOT TESTEND(PF);
          COMPNAME=GETLINE(PF);
          ITER=DECODE(GETLINE(PF),"I(6)");
        STARTCOL=NEXTCOL;
          TABLEC[0,STARTCOL]=COMPNAME;
          STARTCOL1=STARTCOL+1;
          NEXTCOL=STARTCOL+ITER;
          TABLEC[0,STARTCOL1]=NEXTCOL;
          DO I = 1 TO ITER;
            X=DECODE(GETLINE(PF),"E(22,14)");
            TABLEC[1,ICOL]=X;
            DO J = 1 TO NSPECIES;
              CONC=DECODE(GETLINE(PF),"E(22,14)");
              IROW=J+1;
              IF ((CONC<>0)OR(LINLIN=-1)) THEN TABLEC[IROW,ICOL]=CONC;
```

```
            END;
            ICOL=ICOL+1;
          END;
        END;
        CLOSE(PF);
      TABLEC[0,STARTCOL1]=-TABLEC[0,STARTCOL1];
      END;
      ELSE BEGIN; /* READ THE NAME OF AN OLD TABLE */
OLDT:   TABLEC = GETTEXT
                    ("NAME OF THE OLD TABLE('DIR' TO SEE DIRECTORY)? ");
        IF (TABLEC = "DIR") THEN BEGIN;
          DIR;
          GO TO OLDT;
        END;
      END;

      /* BEGIN PLOTTING ROUTINE */

GN:   GRAPHNAME = GETTEXT("NAME OF THE GRAPH FILE('DIR' TO SEE DIRECTORY)? [ "
                  CAT TABLEC CAT "G ] ");
      IF (GRAPHNAME = "DIR") THEN BEGIN;
        DIR;
        GO TO GN;
      END;
      IF (GRAPHNAME = "") THEN GRAPHNAME = TABLEC CAT "G";
      MAKE GRAPH(GRAPHNAME) FROM GRAPH("TEMPLOT");
      SET GRAPHTITLE OF GRAPH(GRAPHNAME) TO
        "Chemical Species Concentration Profile from BWRMIT
        Data From File " CAT TABLEC[0,0];

PL:   STARTCOL=1;
      STARTCOL1=2;
      ERASE;
      TYPE " ";
      TYPE " COLUMN      COMPONENT NAME";
      TYPE " ------    ------------------";
      DO WHILE TABLEC[0,STARTCOL1]>0;
        STARTCOL1=STARTCOL+1;
        IF (STARTCOL<1000) SPACE="     ";
        IF (STARTCOL<100) SPACE="      ";
        IF (STARTCOL<10) SPACE="       ";
        TYPE NOCR "   ", STARTCOL, SPACE, TABLEC[0,STARTCOL];
        TYPE " ";
        STARTCOL=TABLEC[0,STARTCOL1];
      END;
      TYPE " ";
      COMPCOLB = GETNUMBER("COLUMN # OF COMPONENT TO BEGIN WITH(0 IF DONE)? ");
      IF (COMPCOLB=0) GO TO DONE;
      COMPCOLE = GETNUMBER("COLUMN # OF COMPONENT TO END WITH? ");

      ICURVE = 0;
MORE: ICURVE = ICURVE + 1;
      COMPCOLE1=COMPCOLE+1;
      ENDCOL=ABS(TABLEC[0,COMPCOLE1])-1;
      DIS COL 0 OF TABLE(TABLEC) WHERE COL 0 <> "X (cm)";
      DISPLAY GRAPH(GRAPHNAME) AT (0.4,0.);
      SPECIES =
        GETNUMBER("ROW # OF SPECIES TO GRAPH(ENTER 0 TO EXIT)? ");
```

```
        IF (SPECIES = 0) THEN GO TO PL;
        ADD CURVE TO GRAPH(GRAPHNAME) FROM ROW 1 OF TABLE(TABLEC) VS ROW
          SPECIES OF COLUMN COMPCOLB TO ENDCOL OF TABLE(TABLEC);
        SET CONNECTED OF CURVE(ICURVE) OF GRAPH(GRAPHNAME) TO "YES";
        SET LABEL OF CURVE(ICURVE) OF GRAPH(GRAPHNAME) TO TABLEC[SPECIES,0];
        SET LOW OF X AXIS OF GRAPH(GRAPHNAME) TO TABLEC[1,COMPCOLB];
        SET HIGH OF X AXIS OF GRAPH(GRAPHNAME) TO TABLEC[1,ENDCOL];
        GO TO MORE;

DONE:   GRAPHNOTE = GETTEXT("NOTES FOR GRAPH? ");
        IF (GRAPHNOTE <> "") THEN
          SET GRAPHNOTES OF GRAPH(GRAPHNAME) TO GRAPHNOTE;
        IF (YESANSWER("PLOT THE GRAPH? [Y/N]", TRUE) = TRUE) THEN
          PLOT GRAPH(GRAPHNAME) HEIGHT .75 WIDTH .75 AT (.15,.1);

        ERASE;
        TYPE "  END OF RADPLOT";
        TYPE NOCR "  THE FOLLOWING TABLE WAS CREATED:  ",TABLEC;
        TYPE " ";
        TYPE NOCR "  THE FOLLOWING GRAPH WAS CREATED:  ",GRAPHNAME;
        END;
```

IV. LSODE.WRITEUP

This writeup is part of the LSODE code package and has been duplicated from Simonson's thesis. This writeup should provide enough information on the user interface and internal workings of LSODE in case the user wishes to modify RADICAL. The reader is referred to other references listed at the end of this thesis for more detail.

```
C-----------------------------------------------------------------------
C THIS IS THE AUGUST 13, 1981 VERSION OF
C LSODE.. LIVERMORE SOLVER FOR ORDINARY DIFFERENTIAL EQUATIONS.
C THIS VERSION IS IN SINGLE PRECISION.
C
C LSODE SOLVES THE INITIAL VALUE PROBLEM FOR STIFF OR NONSTIFF
C SYSTEMS OF FIRST ORDER ODE-S,
C     DY/DT = F(T,Y) ,  OR, IN COMPONENT FORM,
C     DY(I)/DT = F(I) = F(I,T,Y(1),Y(2),...,Y(NEQ)) (I = 1,...,NEQ).
C LSODE IS A PACKAGE BASED ON THE GEAR AND GEARB PACKAGES, AND ON THE
C OCTOBER 23, 1978 VERSION OF THE TENTATIVE ODEPACK USER INTERFACE
C STANDARD, WITH MINOR MODIFICATIONS.
C-----------------------------------------------------------------------
C REFERENCE..
C     ALAN C. HINDMARSH,  LSODE AND LSODI, TWO NEW INITIAL VALUE
C     ORDINARY DIFFERENTIAL EQUATION SOLVERS,
C     ACM-SIGNUM NEWSLETTER, VOL. 15, NO. 4 (1980), PP. 10-11.
C-----------------------------------------------------------------------
C AUTHOR AND CONTACT.. ALAN C. HINDMARSH,
C                      MATHEMATICS AND STATISTICS DIVISION, L-316
C                      LAWRENCE LIVERMORE NATIONAL LABORATORY
C                      LIVERMORE, CA 94550.
C-----------------------------------------------------------------------
C SUMMARY OF USAGE.
C
C COMMUNICATION BETWEEN THE USER AND THE LSODE PACKAGE, FOR NORMAL
C SITUATIONS, IS SUMMARIZED HERE.  THIS SUMMARY DESCRIBES ONLY A SUBSET
C OF THE FULL SET OF OPTIONS AVAILABLE.  SEE THE FULL DESCRIPTION FOR
C DETAILS, INCLUDING OPTIONAL COMMUNICATION, NONSTANDARD OPTIONS,
C AND INSTRUCTIONS FOR SPECIAL SITUATIONS.  SEE ALSO THE EXAMPLE
C PROBLEM (WITH PROGRAM AND OUTPUT) FOLLOWING THIS SUMMARY.
C
C A. FIRST PROVIDE A SUBROUTINE OF THE FORM..
C               SUBROUTINE F (NEQ, T, Y, YDOT)
C               DIMENSION Y(NEQ), YDOT(NEQ)
C WHICH SUPPLIES THE VECTOR FUNCTION F BY LOADING YDOT(I) WITH F(I).
C
C B. NEXT DETERMINE (OR GUESS) WHETHER OR NOT THE PROBLEM IS STIFF.
C STIFFNESS OCCURS WHEN THE JACOBIAN MATRIX DF/DY HAS AN EIGENVALUE
C WHOSE REAL PART IS NEGATIVE AND LARGE IN MAGNITUDE, COMPARED TO THE
C RECIPROCAL OF THE T SPAN OF INTEREST.  IF THE PROBLEM IS NONSTIFF,
C USE A METHOD FLAG MF = 10.  IF IT IS STIFF, THERE ARE FOUR STANDARD
C CHOICES FOR MF, AND LSODE REQUIRES THE JACOBIAN MATRIX IN SOME FORM.
C THIS MATRIX IS REGARDED EITHER AS FULL (MF = 21 OR 22),
C OR BANDED (MF = 24 OR 25).  IN THE BANDED CASE, LSODE REQUIRES TWO
C HALF-BANDWIDTH PARAMETERS ML AND MU.  THESE ARE, RESPECTIVELY, THE
C WIDTHS OF THE LOWER AND UPPER PARTS OF THE BAND, EXCLUDING THE MAIN
C DIAGONAL.  THUS THE BAND CONSISTS OF THE LOCATIONS (I,J) WITH
C I-ML .LE. J .LE. I+MU, AND THE FULL BANDWIDTH IS ML+MU+1.
C
C C. IF THE PROBLEM IS STIFF, YOU ARE ENCOURAGED TO SUPPLY THE JACOBIAN
C DIRECTLY (MF = 21 OR 24), BUT IF THIS IS NOT FEASIBLE, LSODE WILL
C COMPUTE IT INTERNALLY BY DIFFERENCE QUOTIENTS (MF = 22 OR 25).
C IF YOU ARE SUPPLYING THE JACOBIAN, PROVIDE A SUBROUTINE OF THE FORM..
C               SUBROUTINE JAC (NEQ, T, Y, ML, MU, PD, NROWPD)
C               DIMENSION Y(NEQ), PD(NROWPD,NEQ)
C WHICH SUPPLIES DF/DY BY LOADING PD AS FOLLOWS..
C     FOR A FULL JACOBIAN (MF = 21), LOAD PD(I,J) WITH DF(I)/DY(J),
```

```
C THE PARTIAL DERIVATIVE OF F(I) WITH RESPECT TO Y(J).  (IGNORE THE
C ML AND MU ARGUMENTS IN THIS CASE.)
C     FOR A BANDED JACOBIAN (MF = 24), LOAD PD(I-J+MU+1,J) WITH
C DF(I)/DY(J), I.E. LOAD THE DIAGONAL LINES OF DF/DY INTO THE ROWS OF
C PD FROM THE TOP DOWN.
C     IN EITHER CASE, ONLY NONZERO ELEMENTS NEED BE LOADED.
C
C D. WRITE A MAIN PROGRAM WHICH CALLS SUBROUTINE LSODE ONCE FOR
C EACH POINT AT WHICH ANSWERS ARE DESIRED.  THIS SHOULD ALSO PROVIDE
C FOR POSSIBLE USE OF LOGICAL UNIT 6 FOR OUTPUT OF ERROR MESSAGES
C BY LSODE.  ON THE FIRST CALL TO LSODE, SUPPLY ARGUMENTS AS FOLLOWS..
C F      = NAME OF SUBROUTINE FOR RIGHT-HAND SIDE VECTOR F.
C          THIS NAME MUST BE DECLARED EXTERNAL IN CALLING PROGRAM.
C NEQ    = NUMBER OF FIRST ORDER ODE-S.
C Y      = ARRAY OF INITIAL VALUES, OF LENGTH NEQ.
C T      = THE INITIAL VALUE OF THE INDEPENDENT VARIABLE.
C TOUT   = FIRST POINT WHERE OUTPUT IS DESIRED (.NE. T).
C ITOL   = 1 OR 2 ACCORDING AS ATOL (BELOW) IS A SCALAR OR ARRAY.
C RTOL   = RELATIVE TOLERANCE PARAMETER (SCALAR).
C ATOL   = ABSOLUTE TOLERANCE PARAMETER (SCALAR OR ARRAY).
C          THE ESTIMATED LOCAL ERROR IN Y(I) WILL BE CONTROLLED SO AS
C          TO BE ROUGHLY LESS (IN MAGNITUDE) THAN
C             EWT(I) = RTOL*ABS(Y(I)) + ATOL     IF ITOL = 1, OR
C             EWT(I) = RTOL*ABS(Y(I)) + ATOL(I)  IF ITOL = 2.
C          THUS THE LOCAL ERROR TEST PASSES IF, IN EACH COMPONENT,
C          EITHER THE ABSOLUTE ERROR IS LESS THAN ATOL (OR ATOL(I)),
C          OR THE RELATIVE ERROR IS LESS THAN RTOL.
C          USE RTOL = 0.0 FOR PURE ABSOLUTE ERROR CONTROL, AND
C          USE ATOL = 0.0 (OR ATOL(I) = 0.0) FOR PURE RELATIVE ERROR
C          CONTROL.  CAUTION.. ACTUAL (GLOBAL) ERRORS MAY EXCEED THESE
C          LOCAL TOLERANCES, SO CHOOSE THEM CONSERVATIVELY.
C ITASK  = 1 FOR NORMAL COMPUTATION OF OUTPUT VALUES OF Y AT T = TOUT.
C ISTATE = INTEGER FLAG (INPUT AND OUTPUT).  SET ISTATE = 1.
C IOPT   = 0 TO INDICATE NO OPTIONAL INPUTS USED.
C RWORK  = REAL WORK ARRAY OF LENGTH AT LEAST..
C             20 + 16*NEQ                    FOR MF = 10,
C             22 +  9*NEQ + NEQ**2           FOR MF = 21 OR 22,
C             22 + 10*NEQ + (2*ML + MU)*NEQ  FOR MF = 24 OR 25.
C LRW    = DECLARED LENGTH OF RWORK (IN USER-S DIMENSION).
C IWORK  = INTEGER WORK ARRAY OF LENGTH AT LEAST..
C             20        FOR MF = 10,
C             20 + NEQ  FOR MF = 21, 22, 24, OR 25.
C          IF MF = 24 OR 25, INPUT IN IWORK(1),IWORK(2) THE LOWER
C          AND UPPER HALF-BANDWIDTHS ML,MU.
C LIW    = DECLARED LENGTH OF IWORK (IN USER-S DIMENSION).
C JAC    = NAME OF SUBROUTINE FOR JACOBIAN MATRIX (MF = 21 OR 24).
C          IF USED, THIS NAME MUST BE DECLARED EXTERNAL IN CALLING
C          PROGRAM.  IF NOT USED, PASS A DUMMY NAME.
C MF     = METHOD FLAG.  STANDARD VALUES ARE..
C          10 FOR NONSTIFF (ADAMS) METHOD, NO JACOBIAN USED.
C          21 FOR STIFF (BDF) METHOD, USER-SUPPLIED FULL JACOBIAN.
C          22 FOR STIFF METHOD, INTERNALLY GENERATED FULL JACOBIAN.
C          24 FOR STIFF METHOD, USER-SUPPLIED BANDED JACOBIAN.
C          25 FOR STIFF METHOD, INTERNALLY GENERATED BANDED JACOBIAN.
C NOTE THAT THE MAIN PROGRAM MUST DECLARE ARRAYS Y, RWORK, IWORK,
C AND POSSIBLY ATOL.
C
C E. THE OUTPUT FROM THE FIRST CALL (OR ANY CALL) IS..
```

```
C       Y = ARRAY OF COMPUTED VALUES OF Y(T) VECTOR.
C       T = CORRESPONDING VALUE OF INDEPENDENT VARIABLE (NORMALLY TOUT).
C ISTATE = 2  IF LSODE WAS SUCCESSFUL, NEGATIVE OTHERWISE.
C           -1 MEANS EXCESS WORK DONE ON THIS CALL (PERHAPS WRONG MF).
C           -2 MEANS EXCESS ACCURACY REQUESTED (TOLERANCES TOO SMALL).
C           -3 MEANS ILLEGAL INPUT DETECTED (SEE PRINTED MESSAGE).
C           -4 MEANS REPEATED ERROR TEST FAILURES (CHECK ALL INPUTS).
C           -5 MEANS REPEATED CONVERGENCE FAILURES (PERHAPS BAD JACOBIAN
C              SUPPLIED OR WRONG CHOICE OF MF OR TOLERANCES).
C           -6 MEANS ERROR WEIGHT BECAME ZERO DURING PROBLEM. (SOLUTION
C              COMPONENT I VANISHED, AND ATOL OR ATOL(I) = 0.)
C
C F. TO CONTINUE THE INTEGRATION AFTER A SUCCESSFUL RETURN, SIMPLY
C RESET TOUT AND CALL LSODE AGAIN.  NO OTHER PARAMETERS NEED BE RESET.
C
C-----------------------------------------------------------------------
C EXAMPLE PROBLEM.
C
C THE FOLLOWING IS A SIMPLE EXAMPLE PROBLEM, WITH THE CODING
C NEEDED FOR ITS SOLUTION BY LSODE.  THE PROBLEM IS FROM CHEMICAL
C KINETICS, AND CONSISTS OF THE FOLLOWING THREE RATE EQUATIONS..
C     DY1/DT = -.04*Y1 + 1.E4*Y2*Y3
C     DY2/DT = .04*Y1 - 1.E4*Y2*Y3 - 3.E7*Y2**2
C     DY3/DT = 3.E7*Y2**2
C ON THE INTERVAL FROM T = 0.0 TO T = 4.E10, WITH INITIAL CONDITIONS
C Y1 = 1.0, Y2 = Y3 = 0.  THE PROBLEM IS STIFF.
C
C THE FOLLOWING CODING SOLVES THIS PROBLEM WITH LSODE, USING MF = 21
C AND PRINTING RESULTS AT T = .4, 4., ..., 4.E10.  IT USES
C ITOL = 2 AND ATOL MUCH SMALLER FOR Y2 THAN Y1 OR Y3 BECAUSE
C Y2 HAS MUCH SMALLER VALUES.
C AT THE END OF THE RUN, STATISTICAL QUANTITIES OF INTEREST ARE
C PRINTED (SEE OPTIONAL OUTPUTS IN THE FULL DESCRIPTION BELOW).
C
C     EXTERNAL FEX, JEX
C     DIMENSION Y(3), ATOL(3), RWORK(58), IWORK(23)
C     NEQ = 3
C     Y(1) = 1.
C     Y(2) = 0.
C     Y(3) = 0.
C     T = 0.
C     TOUT = .4
C     ITOL = 2
C     RTOL = 1.E-4
C     ATOL(1) = 1.E-6
C     ATOL(2) = 1.E-10
C     ATOL(3) = 1.E-6
C     ITASK = 1
C     ISTATE = 1
C     IOPT = 0
C     LRW = 58
C     LIW = 23
C     MF = 21
C     DO 40 IOUT = 1,12
C       CALL LSODE(FEX,NEQ,Y,T,TOUT,ITOL,RTOL,ATOL,ITASK,ISTATE,
C    1     IOPT,RWORK,LRW,IWORK,LIW,JEX,MF)
C       WRITE(6,20)T,Y(1),Y(2),Y(3)
C 20    FORMAT(7H AT T =,E12.4,6H   Y =,3E14.6)
```

```
C         IF (ISTATE .LT. 0) GO TO 80
C 40      TOUT = TOUT*10.
C       WRITE(6,60)IWORK(11),IWORK(12),IWORK(13)
C 60    FORMAT(/12H NO. STEPS =,I4,11H  NO. F-S =,I4,11H  NO. J-S =,I4)
C       STOP
C 80    WRITE(6,90)ISTATE
C 90    FORMAT(///22H ERROR HALT.. ISTATE =,I3)
C       STOP
C       END
C
C       SUBROUTINE FEX (NEQ, T, Y, YDOT)
C       DIMENSION Y(3), YDOT(3)
C       YDOT(1) = -.04*Y(1) + 1.E4*Y(2)*Y(3)
C       YDOT(3) = 3.E7*Y(2)*Y(2)
C       YDOT(2) = -YDOT(1) - YDOT(3)
C       RETURN
C       END
C
C       SUBROUTINE JEX (NEQ, T, Y, ML, MU, PD, NRPD)
C       DIMENSION Y(3), PD(NRPD,3)
C       PD(1,1) = -.04
C       PD(1,2) = 1.E4*Y(3)
C       PD(1,3) = 1.E4*Y(2)
C       PD(2,1) = .04
C       PD(2,3) = -PD(1,3)
C       PD(3,2) = 6.E7*Y(2)
C       PD(2,2) = -PD(1,2) - PD(3,2)
C       RETURN
C       END
C
C THE OUTPUT OF THIS PROGRAM (ON A CDC-7600 IN SINGLE PRECISION)
C IS AS FOLLOWS..
C
C   AT T =  4.0000E-01   Y =  9.851726E-01  3.386406E-05  1.479357E-02
C   AT T =  4.0000E+00   Y =  9.055142E-01  2.240418E-05  9.446344E-02
C   AT T =  4.0000E+01   Y =  7.158050E-01  9.184616E-06  2.841858E-01
C   AT T =  4.0000E+02   Y =  4.504846E-01  3.222434E-06  5.495122E-01
C   AT T =  4.0000E+03   Y =  1.831701E-01  8.940379E-07  8.168290E-01
C   AT T =  4.0000E+04   Y =  3.897016E-02  1.621193E-07  9.610297E-01
C   AT T =  4.0000E+05   Y =  4.935213E-03  1.983756E-08  9.950648E-01
C   AT T =  4.0000E+06   Y =  5.159269E-04  2.064759E-09  9.994841E-01
C   AT T =  4.0000E+07   Y =  5.306413E-05  2.122677E-10  9.999469E-01
C   AT T =  4.0000E+08   Y =  5.494529E-06  2.197824E-11  9.999945E-01
C   AT T =  4.0000E+09   Y =  5.129458E-07  2.051784E-12  9.999995E-01
C   AT T =  4.0000E+10   Y = -7.170586E-08 -2.868234E-13  1.000000E+00
C
C   NO. STEPS = 330  NO. F-S = 405  NO. J-S =  69
C----------------------------------------------------------------------
C FULL DESCRIPTION OF USER INTERFACE TO LSODE.
C
C THE USER INTERFACE TO LSODE CONSISTS OF THE FOLLOWING PARTS.
C
C I.   THE CALL SEQUENCE TO SUBROUTINE LSODE, WHICH IS A DRIVER
C      ROUTINE FOR THE SOLVER.  THIS INCLUDES DESCRIPTIONS OF BOTH
C      THE CALL SEQUENCE ARGUMENTS AND OF USER-SUPPLIED ROUTINES.
C      FOLLOWING THESE DESCRIPTIONS IS A DESCRIPTION OF
C      OPTIONAL INPUTS AVAILABLE THROUGH THE CALL SEQUENCE, AND THEN
C      A DESCRIPTION OF OPTIONAL OUTPUTS (IN THE WORK ARRAYS).
```

```
C
C II.  DESCRIPTIONS OF OTHER ROUTINES IN THE LSODE PACKAGE THAT MAY BE
C      (OPTIONALLY) CALLED BY THE USER.  THESE PROVIDE THE ABILITY TO
C      ALTER ERROR MESSAGE HANDLING, SAVE AND RESTORE THE INTERNAL
C      COMMON, AND OBTAIN SPECIFIED DERIVATIVES OF THE SOLUTION Y(T).
C
C III. DESCRIPTIONS OF COMMON BLOCKS TO BE DECLARED IN OVERLAY
C      OR SIMILAR ENVIRONMENTS, OR TO BE SAVED WHEN DOING AN INTERRUPT
C      OF THE PROBLEM AND CONTINUED SOLUTION LATER.
C
C IV.  DESCRIPTION OF TWO SUBROUTINES IN THE LSODE PACKAGE, EITHER OF
C      WHICH THE USER MAY REPLACE WITH HIS OWN VERSION, IF DESIRED.
C      THESE RELATE TO THE MEASUREMENT OF ERRORS.
C
C-----------------------------------------------------------------------
C PART I.  CALL SEQUENCE.
C
C THE CALL SEQUENCE PARAMETERS USED FOR INPUT ONLY ARE
C     F, NEQ, TOUT, ITOL, RTOL, ATOL, ITASK, IOPT, LRW, LIW, JAC, MF,
C AND THOSE USED FOR BOTH INPUT AND OUTPUT ARE
C     Y, T, ISTATE.
C THE WORK ARRAYS RWORK AND IWORK ARE ALSO USED FOR CONDITIONAL AND
C OPTIONAL INPUTS AND OPTIONAL OUTPUTS.  (THE TERM OUTPUT HERE REFERS
C TO THE RETURN FROM SUBROUTINE LSODE TO THE USER-S CALLING PROGRAM.)
C
C THE LEGALITY OF INPUT PARAMETERS WILL BE THOROUGHLY CHECKED ON THE
C INITIAL CALL FOR THE PROBLEM, BUT NOT CHECKED THEREAFTER UNLESS A
C CHANGE IN INPUT PARAMETERS IS FLAGGED BY ISTATE = 3 ON INPUT.
C
C THE DESCRIPTIONS OF THE CALL ARGUMENTS ARE AS FOLLOWS.
C
C F      = THE NAME OF THE USER-SUPPLIED SUBROUTINE DEFINING THE
C          ODE SYSTEM.  THE SYSTEM MUST BE PUT IN THE FIRST-ORDER
C          FORM DY/DT = F(T,Y), WHERE F IS A VECTOR-VALUED FUNCTION
C          OF THE SCALAR T AND THE VECTOR Y.  SUBROUTINE F IS TO
C          COMPUTE THE FUNCTION F.  IT IS TO HAVE THE FORM
C               SUBROUTINE F (NEQ, T, Y, YDOT)
C               DIMENSION Y(1), YDOT(1)
C          WHERE NEQ, T, AND Y ARE INPUT, AND THE ARRAY YDOT = F(T,Y)
C          IS OUTPUT.  Y AND YDOT ARE ARRAYS OF LENGTH NEQ.
C          (IN THE DIMENSION STATEMENT ABOVE, 1 IS A DUMMY
C          DIMENSION.. IT CAN BE REPLACED BY ANY VALUE.)
C          SUBROUTINE F SHOULD NOT ALTER Y(1),...,Y(NEQ).
C          F MUST BE DECLARED EXTERNAL IN THE CALLING PROGRAM.
C
C          SUBROUTINE F MAY ACCESS USER-DEFINED QUANTITIES IN
C          NEQ(2),... AND Y(NEQ(1)+1),... IF NEQ IS AN ARRAY
C          (DIMENSIONED IN F) AND Y HAS LENGTH EXCEEDING NEQ(1).
C          SEE THE DESCRIPTIONS OF NEQ AND Y BELOW.
C
C NEQ    = THE SIZE OF THE ODE SYSTEM (NUMBER OF FIRST ORDER
C          ORDINARY DIFFERENTIAL EQUATIONS).  USED ONLY FOR INPUT.
C          NEQ MAY BE DECREASED, BUT NOT INCREASED, DURING THE PROBLEM.
C          IF NEQ IS DECREASED (WITH ISTATE = 3 ON INPUT), THE
C          REMAINING COMPONENTS OF Y SHOULD BE LEFT UNDISTURBED, IF
C          THESE ARE TO BE ACCESSED IN F AND/OR JAC.
C
C          NORMALLY, NEQ IS A SCALAR, AND IT IS GENERALLY REFERRED TO
```

```
C          AS A SCALAR IN THIS USER INTERFACE DESCRIPTION.  HOWEVER,
C          NEQ MAY BE AN ARRAY, WITH NEQ(1) SET TO THE SYSTEM SIZE.
C          (THE LSODE PACKAGE ACCESSES ONLY NEQ(1).)  IN EITHER CASE,
C          THIS PARAMETER IS PASSED AS THE NEQ ARGUMENT IN ALL CALLS
C          TO F AND JAC.  HENCE, IF IT IS AN ARRAY, LOCATIONS
C          NEQ(2),... MAY BE USED TO STORE OTHER INTEGER DATA AND PASS
C          IT TO F AND/OR JAC.  SUBROUTINES F AND/OR JAC MUST INCLUDE
C          NEQ IN A DIMENSION STATEMENT IN THAT CASE.
C
C Y      = A REAL ARRAY FOR THE VECTOR OF DEPENDENT VARIABLES, OF
C          LENGTH NEQ OR MORE.  USED FOR BOTH INPUT AND OUTPUT ON THE
C          FIRST CALL (ISTATE = 1), AND ONLY FOR OUTPUT ON OTHER CALLS.
C          ON THE FIRST CALL, Y MUST CONTAIN THE VECTOR OF INITIAL
C          VALUES.  ON OUTPUT, Y CONTAINS THE COMPUTED SOLUTION VECTOR,
C          EVALUATED AT T.  IF DESIRED, THE Y ARRAY MAY BE USED
C          FOR OTHER PURPOSES BETWEEN CALLS TO THE SOLVER.
C
C          THIS ARRAY IS PASSED AS THE Y ARGUMENT IN ALL CALLS TO
C          F AND JAC.  HENCE ITS LENGTH MAY EXCEED NEQ, AND LOCATIONS
C          Y(NEQ+1),... MAY BE USED TO STORE OTHER REAL DATA AND
C          PASS IT TO F AND/OR JAC.  (THE LSODE PACKAGE ACCESSES ONLY
C          Y(1),...,Y(NEQ).)
C
C T      = THE INDEPENDENT VARIABLE.  ON INPUT, T IS USED ONLY ON THE
C          FIRST CALL, AS THE INITIAL POINT OF THE INTEGRATION.
C          ON OUTPUT, AFTER EACH CALL, T IS THE VALUE AT WHICH A
C          COMPUTED SOLUTION Y IS EVALUATED (USUALLY THE SAME AS TOUT).
C          ON AN ERROR RETURN, T IS THE FARTHEST POINT REACHED.
C
C TOUT   = THE NEXT VALUE OF T AT WHICH A COMPUTED SOLUTION IS DESIRED.
C          USED ONLY FOR INPUT.
C
C          WHEN STARTING THE PROBLEM (ISTATE = 1), TOUT MAY BE EQUAL
C          TO T FOR ONE CALL, THEN SHOULD .NE. T FOR THE NEXT CALL.
C          FOR THE INITIAL T, AN INPUT VALUE OF TOUT .NE. T IS USED
C          IN ORDER TO DETERMINE THE DIRECTION OF THE INTEGRATION
C          (I.E. THE ALGEBRAIC SIGN OF THE STEP SIZES) AND THE ROUGH
C          SCALE OF THE PROBLEM.  INTEGRATION IN EITHER DIRECTION
C          (FORWARD OR BACKWARD IN T) IS PERMITTED.
C
C          IF ITASK = 2 OR 5 (ONE-STEP MODES), TOUT IS IGNORED AFTER
C          THE FIRST CALL (I.E. THE FIRST CALL WITH TOUT .NE. T).
C          OTHERWISE, TOUT IS REQUIRED ON EVERY CALL.
C
C          IF ITASK = 1, 3, OR 4, THE VALUES OF TOUT NEED NOT BE
C          MONOTONE, BUT A VALUE OF TOUT WHICH BACKS UP IS LIMITED
C          TO THE CURRENT INTERNAL T INTERVAL, WHOSE ENDPOINTS ARE
C          TCUR - HU AND TCUR (SEE OPTIONAL OUTPUTS, BELOW, FOR
C          TCUR AND HU).
C
C ITOL   = AN INDICATOR FOR THE TYPE OF ERROR CONTROL.  SEE
C          DESCRIPTION BELOW UNDER ATOL.  USED ONLY FOR INPUT.
C
C RTOL   = A RELATIVE ERROR TOLERANCE PARAMETER, EITHER A SCALAR OR
C          AN ARRAY OF LENGTH NEQ.  SEE DESCRIPTION BELOW UNDER ATOL.
C          INPUT ONLY.
C
C ATOL   = AN ABSOLUTE ERROR TOLERANCE PARAMETER, EITHER A SCALAR OR
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C          AN ARRAY OF LENGTH NEQ.  INPUT ONLY.
C
C             THE INPUT PARAMETERS ITOL, RTOL, AND ATOL DETERMINE
C          THE ERROR CONTROL PERFORMED BY THE SOLVER.  THE SOLVER WILL
C          CONTROL THE VECTOR E = (E(I)) OF ESTIMATED LOCAL ERRORS
C          IN Y, ACCORDING TO AN INEQUALITY OF THE FORM
C                      RMS-NORM OF ( E(I)/EWT(I) )   .LE.   1,
C          WHERE       EWT(I) = RTOL(I)*ABS(Y(I)) + ATOL(I),
C          AND THE RMS-NORM (ROOT-MEAN-SQUARE NORM) HERE IS
C          RMS-NORM(V) = SQRT(SUM V(I)**2 / NEQ).  HERE EWT = (EWT(I))
C          IS A VECTOR OF WEIGHTS WHICH MUST ALWAYS BE POSITIVE, AND
C          THE VALUES OF RTOL AND ATOL SHOULD ALL BE NON-NEGATIVE.
C          THE FOLLOWING TABLE GIVES THE TYPES (SCALAR/ARRAY) OF
C          RTOL AND ATOL, AND THE CORRESPONDING FORM OF EWT(I).
C
C             ITOL    RTOL       ATOL          EWT(I)
C              1     SCALAR     SCALAR     RTOL*ABS(Y(I)) + ATOL
C              2     SCALAR     ARRAY      RTOL*ABS(Y(I)) + ATOL(I)
C              3     ARRAY      SCALAR     RTOL(I)*ABS(Y(I)) + ATOL
C              4     ARRAY      ARRAY      RTOL(I)*ABS(Y(I)) + ATOL(I)
C
C          WHEN EITHER OF THESE PARAMETERS IS A SCALAR, IT NEED NOT
C          BE DIMENSIONED IN THE USER-S CALLING PROGRAM.
C
C          IF NONE OF THE ABOVE CHOICES (WITH ITOL, RTOL, AND ATOL
C          FIXED THROUGHOUT THE PROBLEM) IS SUITABLE, MORE GENERAL
C          ERROR CONTROLS CAN BE OBTAINED BY SUBSTITUTING
C          USER-SUPPLIED ROUTINES FOR THE SETTING OF EWT AND/OR FOR
C          THE NORM CALCULATION.  SEE PART IV BELOW.
C
C          IF GLOBAL ERRORS ARE TO BE ESTIMATED BY MAKING A REPEATED
C          RUN ON THE SAME PROBLEM WITH SMALLER TOLERANCES, THEN ALL
C          COMPONENTS OF RTOL AND ATOL (I.E. OF EWT) SHOULD BE SCALED
C          DOWN UNIFORMLY.
C
C ITASK  = AN INDEX SPECIFYING THE TASK TO BE PERFORMED.
C          INPUT ONLY.  ITASK HAS THE FOLLOWING VALUES AND MEANINGS.
C          1  MEANS NORMAL COMPUTATION OF OUTPUT VALUES OF Y(T) AT
C             T = TOUT (BY OVERSHOOTING AND INTERPOLATING).
C          2  MEANS TAKE ONE STEP ONLY AND RETURN.
C          3  MEANS STOP AT THE FIRST INTERNAL MESH POINT AT OR
C             BEYOND T = TOUT AND RETURN.
C          4  MEANS NORMAL COMPUTATION OF OUTPUT VALUES OF Y(T) AT
C             T = TOUT BUT WITHOUT OVERSHOOTING T = TCRIT.
C             TCRIT MUST BE INPUT AS RWORK(1).  TCRIT MAY BE EQUAL TO
C             OR BEYOND TOUT, BUT NOT BEHIND IT IN THE DIRECTION OF
C             INTEGRATION.  THIS OPTION IS USEFUL IF THE PROBLEM
C             HAS A SINGULARITY AT OR BEYOND T = TCRIT.
C          5  MEANS TAKE ONE STEP, WITHOUT PASSING TCRIT, AND RETURN.
C             TCRIT MUST BE INPUT AS RWORK(1).
C
C          NOTE..  IF ITASK = 4 OR 5 AND THE SOLVER REACHES TCRIT
C          (WITHIN ROUNDOFF), IT WILL RETURN T = TCRIT (EXACTLY) TO
C          INDICATE THIS (UNLESS ITASK = 4 AND TOUT COMES BEFORE TCRIT,
C          IN WHICH CASE ANSWERS AT T = TOUT ARE RETURNED FIRST).
C
C ISTATE = AN INDEX USED FOR INPUT AND OUTPUT TO SPECIFY THE
C          THE STATE OF THE CALCULATION.
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C
C          ON INPUT, THE VALUES OF ISTATE ARE AS FOLLOWS.
C          1  MEANS THIS IS THE FIRST CALL FOR THE PROBLEM
C             (INITIALIZATIONS WILL BE DONE).  SEE NOTE BELOW.
C          2  MEANS THIS IS NOT THE FIRST CALL, AND THE CALCULATION
C             IS TO CONTINUE NORMALLY, WITH NO CHANGE IN ANY INPUT
C             PARAMETERS EXCEPT POSSIBLY TOUT AND ITASK.
C             (IF ITOL, RTOL, AND/OR ATOL ARE CHANGED BETWEEN CALLS
C             WITH ISTATE = 2, THE NEW VALUES WILL BE USED BUT NOT
C             TESTED FOR LEGALITY.)
C          3  MEANS THIS IS NOT THE FIRST CALL, AND THE
C             CALCULATION IS TO CONTINUE NORMALLY, BUT WITH
C             A CHANGE IN INPUT PARAMETERS OTHER THAN
C             TOUT AND ITASK.  CHANGES ARE ALLOWED IN
C             NEQ, ITOL, RTOL, ATOL, IOPT, LRW, LIW, MF, ML, MU,
C             AND ANY OF THE OPTIONAL INPUTS EXCEPT H0.
C             (SEE IWORK DESCRIPTION FOR ML AND MU.)
C          NOTE..  A PRELIMINARY CALL WITH TOUT = T IS NOT COUNTED
C          AS A FIRST CALL HERE, AS NO INITIALIZATION OR CHECKING OF
C          INPUT IS DONE.  (SUCH A CALL IS SOMETIMES USEFUL FOR THE
C          PURPOSE OF OUTPUTTING THE INITIAL CONDITIONS.)
C          THUS THE FIRST CALL FOR WHICH TOUT .NE. T REQUIRES
C          ISTATE = 1 ON INPUT.
C
C          ON OUTPUT, ISTATE HAS THE FOLLOWING VALUES AND MEANINGS.
C           1  MEANS NOTHING WAS DONE, AS TOUT WAS EQUAL TO T WITH
C              ISTATE = 1 ON INPUT.  (HOWEVER, AN INTERNAL COUNTER WAS
C              SET TO DETECT AND PREVENT REPEATED CALLS OF THIS TYPE.)
C           2  MEANS THE INTEGRATION WAS PERFORMED SUCCESSFULLY.
C          -1  MEANS AN EXCESSIVE AMOUNT OF WORK (MORE THAN MXSTEP
C              STEPS) WAS DONE ON THIS CALL, BEFORE COMPLETING THE
C              REQUESTED TASK, BUT THE INTEGRATION WAS OTHERWISE
C              SUCCESSFUL AS FAR AS T.  (MXSTEP IS AN OPTIONAL INPUT
C              AND IS NORMALLY 500.)  TO CONTINUE, THE USER MAY
C              SIMPLY RESET ISTATE TO A VALUE .GT. 1 AND CALL AGAIN
C              (THE EXCESS WORK STEP COUNTER WILL BE RESET TO 0).
C              IN ADDITION, THE USER MAY INCREASE MXSTEP TO AVOID
C              THIS ERROR RETURN (SEE BELOW ON OPTIONAL INPUTS).
C          -2  MEANS TOO MUCH ACCURACY WAS REQUESTED FOR THE PRECISION
C              OF THE MACHINE BEING USED.  THIS WAS DETECTED BEFORE
C              COMPLETING THE REQUESTED TASK, BUT THE INTEGRATION
C              WAS SUCCESSFUL AS FAR AS T.  TO CONTINUE, THE TOLERANCE
C              PARAMETERS MUST BE RESET, AND ISTATE MUST BE SET
C              TO 3.  THE OPTIONAL OUTPUT TOLSF MAY BE USED FOR THIS
C              PURPOSE.  (NOTE.. IF THIS CONDITION IS DETECTED BEFORE
C              TAKING ANY STEPS, THEN AN ILLEGAL INPUT RETURN
C              (ISTATE = -3) OCCURS INSTEAD.)
C          -3  MEANS ILLEGAL INPUT WAS DETECTED, BEFORE TAKING ANY
C              INTEGRATION STEPS.  SEE WRITTEN MESSAGE FOR DETAILS.
C              NOTE..  IF THE SOLVER DETECTS AN INFINITE LOOP OF CALLS
C              TO THE SOLVER WITH ILLEGAL INPUT, IT WILL CAUSE
C              THE RUN TO STOP.
C          -4  MEANS THERE WERE REPEATED ERROR TEST FAILURES ON
C              ONE ATTEMPTED STEP, BEFORE COMPLETING THE REQUESTED
C              TASK, BUT THE INTEGRATION WAS SUCCESSFUL AS FAR AS T.
C              THE PROBLEM MAY HAVE A SINGULARITY, OR THE INPUT
C              MAY BE INAPPROPRIATE.
C          -5  MEANS THERE WERE REPEATED CONVERGENCE TEST FAILURES ON
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C              ONE ATTEMPTED STEP, BEFORE COMPLETING THE REQUESTED
C              TASK, BUT THE INTEGRATION WAS SUCCESSFUL AS FAR AS T.
C              THIS MAY BE CAUSED BY AN INACCURATE JACOBIAN MATRIX,
C              IF ONE IS BEING USED.
C          -6  MEANS EWT(I) BECAME ZERO FOR SOME I DURING THE
C              INTEGRATION.  PURE RELATIVE ERROR CONTROL (ATOL(I)=0.0)
C              WAS REQUESTED ON A VARIABLE WHICH HAS NOW VANISHED.
C              THE INTEGRATION WAS SUCCESSFUL AS FAR AS T.
C
C          NOTE..  SINCE THE NORMAL OUTPUT VALUE OF ISTATE IS 2,
C          IT DOES NOT NEED TO BE RESET FOR NORMAL CONTINUATION.
C          ALSO, SINCE A NEGATIVE INPUT VALUE OF ISTATE WILL BE
C          REGARDED AS ILLEGAL, A NEGATIVE OUTPUT VALUE REQUIRES THE
C          USER TO CHANGE IT, AND POSSIBLY OTHER INPUTS, BEFORE
C          CALLING THE SOLVER AGAIN.
C
C IOPT   = AN INTEGER FLAG TO SPECIFY WHETHER OR NOT ANY OPTIONAL
C          INPUTS ARE BEING USED ON THIS CALL.  INPUT ONLY.
C          THE OPTIONAL INPUTS ARE LISTED SEPARATELY BELOW.
C          IOPT = 0 MEANS NO OPTIONAL INPUTS ARE BEING USED.
C                   DEFAULT VALUES WILL BE USED IN ALL CASES.
C          IOPT = 1 MEANS ONE OR MORE OPTIONAL INPUTS ARE BEING USED.
C
C RWORK  = A REAL WORKING ARRAY (SINGLE PRECISION).
C          THE LENGTH OF RWORK MUST BE AT LEAST
C             20 + NYH*(MAXORD + 1) + 3*NEQ + LWM    WHERE
C          NYH    = THE INITIAL VALUE OF NEQ,
C          MAXORD = 12 (IF METH = 1) OR 5 (IF METH = 2) (UNLESS A
C                   SMALLER VALUE IS GIVEN AS AN OPTIONAL INPUT),
C          LWM    = 0             IF MITER = 0,
C          LWM    = NEQ**2 + 2    IF MITER IS 1 OR 2,
C          LWM    = NEQ + 2       IF MITER = 3, AND
C          LWM    = (2*ML+MU+1)*NEQ + 2 IF MITER IS 4 OR 5.
C          (SEE THE MF DESCRIPTION FOR METH AND MITER.)
C          THUS IF MAXORD HAS ITS DEFAULT VALUE AND NEQ IS CONSTANT,
C          THIS LENGTH IS..
C             20 + 16*NEQ                    FOR MF = 10,
C             22 + 16*NEQ + NEQ**2           FOR MF = 11 OR 12,
C             22 + 17*NEQ                    FOR MF = 13,
C             22 + 17*NEQ + (2*ML+MU)*NEQ    FOR MF = 14 OR 15,
C             20 +  9*NEQ                    FOR MF = 20,
C             22 +  9*NEQ + NEQ**2           FOR MF = 21 OR 22,
C             22 + 10*NEQ                    FOR MF = 23,
C             22 + 10*NEQ + (2*ML+MU)*NEQ    FOR MF = 24 OR 25.
C          THE FIRST 20 WORDS OF RWORK ARE RESERVED FOR CONDITIONAL
C          AND OPTIONAL INPUTS AND OPTIONAL OUTPUTS.
C
C          THE FOLLOWING WORD IN RWORK IS A CONDITIONAL INPUT..
C            RWORK(1) = TCRIT = CRITICAL VALUE OF T WHICH THE SOLVER
C                       IS NOT TO OVERSHOOT.  REQUIRED IF ITASK IS
C                       4 OR 5, AND IGNORED OTHERWISE.  (SEE ITASK.)
C
C LRW    = THE LENGTH OF THE ARRAY RWORK, AS DECLARED BY THE USER.
C          (THIS WILL BE CHECKED BY THE SOLVER.)
C
C IWORK  = AN INTEGER WORK ARRAY.  THE LENGTH OF IWORK MUST BE AT LEAST
C             20        IF MITER = 0 OR 3 (MF = 10, 13, 20, 23), OR
C             20 + NEQ  OTHERWISE (MF = 11, 12, 14, 15, 21, 22, 24, 25).
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C          THE FIRST FEW WORDS OF IWORK ARE USED FOR CONDITIONAL AND
C          OPTIONAL INPUTS AND OPTIONAL OUTPUTS.
C
C          THE FOLLOWING 2 WORDS IN IWORK ARE CONDITIONAL INPUTS..
C            IWORK(1) = ML     THESE ARE THE LOWER AND UPPER
C            IWORK(2) = MU     HALF-BANDWIDTHS, RESPECTIVELY, OF THE
C                       BANDED JACOBIAN, EXCLUDING THE MAIN DIAGONAL.
C                       THE BAND IS DEFINED BY THE MATRIX LOCATIONS
C                       (I,J) WITH I-ML .LE. J .LE. I+MU.  ML AND MU
C                       MUST SATISFY  0 .LE.  ML,MU  .LE. NEQ-1.
C                       THESE ARE REQUIRED IF MITER IS 4 OR 5, AND
C                       IGNORED OTHERWISE.  ML AND MU MAY IN FACT BE
C                       THE BAND PARAMETERS FOR A MATRIX TO WHICH
C                       DF/DY IS ONLY APPROXIMATELY EQUAL.
C
C LIW    = THE LENGTH OF THE ARRAY IWORK, AS DECLARED BY THE USER.
C          (THIS WILL BE CHECKED BY THE SOLVER.)
C
C NOTE..  THE WORK ARRAYS MUST NOT BE ALTERED BETWEEN CALLS TO LSODE
C FOR THE SAME PROBLEM, EXCEPT POSSIBLY FOR THE CONDITIONAL AND
C OPTIONAL INPUTS, AND EXCEPT FOR THE LAST 3*NEQ WORDS OF RWORK.
C THE LATTER SPACE IS USED FOR INTERNAL SCRATCH SPACE, AND SO IS
C AVAILABLE FOR USE BY THE USER OUTSIDE LSODE BETWEEN CALLS, IF
C DESIRED (BUT NOT FOR USE BY F OR JAC).
C
C JAC    = THE NAME OF THE USER-SUPPLIED ROUTINE (MITER = 1 OR 4) TO
C          COMPUTE THE JACOBIAN MATRIX, DF/DY, AS A FUNCTION OF
C          THE SCALAR T AND THE VECTOR Y.  IT IS TO HAVE THE FORM
C               SUBROUTINE JAC (NEQ, T, Y, ML, MU, PD, NROWPD)
C               DIMENSION Y(1), PD(NROWPD,1)
C          WHERE NEQ, T, Y, ML, MU, AND NROWPD ARE INPUT AND THE ARRAY
C          PD IS TO BE LOADED WITH PARTIAL DERIVATIVES (ELEMENTS OF
C          THE JACOBIAN MATRIX) ON OUTPUT.  PD MUST BE GIVEN A FIRST
C          DIMENSION OF NROWPD.  T AND Y HAVE THE SAME MEANING AS IN
C          SUBROUTINE F.  (IN THE DIMENSION STATEMENT ABOVE, 1 IS A
C          DUMMY DIMENSION.. IT CAN BE REPLACED BY ANY VALUE.)
C               IN THE FULL MATRIX CASE (MITER = 1), ML AND MU ARE
C          IGNORED, AND THE JACOBIAN IS TO BE LOADED INTO PD IN
C          COLUMNWISE MANNER, WITH DF(I)/DY(J) LOADED INTO PD(I,J).
C               IN THE BAND MATRIX CASE (MITER = 4), THE ELEMENTS
C          WITHIN THE BAND ARE TO BE LOADED INTO PD IN COLUMNWISE
C          MANNER, WITH DIAGONAL LINES OF DF/DY LOADED INTO THE ROWS
C          OF PD.  THUS DF(I)/DY(J) IS TO BE LOADED INTO PD(I-J+MU+1,J).
C          ML AND MU ARE THE HALF-BANDWIDTH PARAMETERS (SEE IWORK).
C          THE LOCATIONS IN PD IN THE TWO TRIANGULAR AREAS WHICH
C          CORRESPOND TO NONEXISTENT MATRIX ELEMENTS CAN BE IGNORED
C          OR LOADED ARBITRARILY, AS THEY ARE OVERWRITTEN BY LSODE.
C               JAC NEED NOT PROVIDE DF/DY EXACTLY.  A CRUDE
C          APPROXIMATION (POSSIBLY WITH A SMALLER BANDWIDTH) WILL DO.
C               IN EITHER CASE, PD IS PRESET TO ZERO BY THE SOLVER,
C          SO THAT ONLY THE NONZERO ELEMENTS NEED BE LOADED BY JAC.
C          EACH CALL TO JAC IS PRECEDED BY A CALL TO F WITH THE SAME
C          ARGUMENTS NEQ, T, AND Y.  THUS TO GAIN SOME EFFICIENCY,
C          INTERMEDIATE QUANTITIES SHARED BY BOTH CALCULATIONS MAY BE
C          SAVED IN A USER COMMON BLOCK BY F AND NOT RECOMPUTED BY JAC,
C          IF DESIRED.  ALSO, JAC MAY ALTER THE Y ARRAY, IF DESIRED.
C          JAC MUST BE DECLARED EXTERNAL IN THE CALLING PROGRAM.
C               SUBROUTINE JAC MAY ACCESS USER-DEFINED QUANTITIES IN
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C          NEQ(2),... AND Y(NEQ(1)+1),... IF NEQ IS AN ARRAY
C          (DIMENSIONED IN JAC) AND Y HAS LENGTH EXCEEDING NEQ(1).
C          SEE THE DESCRIPTIONS OF NEQ AND Y ABOVE.
C
C MF     = THE METHOD FLAG.  USED ONLY FOR INPUT.  THE LEGAL VALUES OF
C          MF ARE 10, 11, 12, 13, 14, 15, 20, 21, 22, 23, 24, AND 25.
C          MF HAS DECIMAL DIGITS METH AND MITER.. MF = 10*METH + MITER.
C          METH INDICATES THE BASIC LINEAR MULTISTEP METHOD..
C            METH = 1 MEANS THE IMPLICIT ADAMS METHOD.
C            METH = 2 MEANS THE METHOD BASED ON BACKWARD
C                     DIFFERENTIATION FORMULAS (BDF-S).
C          MITER INDICATES THE CORRECTOR ITERATION METHOD..
C            MITER = 0 MEANS FUNCTIONAL ITERATION (NO JACOBIAN MATRIX
C                      IS INVOLVED).
C            MITER = 1 MEANS CHORD ITERATION WITH A USER-SUPPLIED
C                      FULL (NEQ BY NEQ) JACOBIAN.
C            MITER = 2 MEANS CHORD ITERATION WITH AN INTERNALLY
C                      GENERATED (DIFFERENCE QUOTIENT) FULL JACOBIAN
C                      (USING NEQ EXTRA CALLS TO F PER DF/DY VALUE).
C            MITER = 3 MEANS CHORD ITERATION WITH AN INTERNALLY
C                      GENERATED DIAGONAL JACOBIAN APPROXIMATION.
C                      (USING 1 EXTRA CALL TO F PER DF/DY EVALUATION).
C            MITER = 4 MEANS CHORD ITERATION WITH A USER-SUPPLIED
C                      BANDED JACOBIAN.
C            MITER = 5 MEANS CHORD ITERATION WITH AN INTERNALLY
C                      GENERATED BANDED JACOBIAN (USING ML+MU+1 EXTRA
C                      CALLS TO F PER DF/DY EVALUATION).
C          IF MITER = 1 OR 4, THE USER MUST SUPPLY A SUBROUTINE JAC
C          (THE NAME IS ARBITRARY) AS DESCRIBED ABOVE UNDER JAC.
C          FOR OTHER VALUES OF MITER, A DUMMY ARGUMENT CAN BE USED.
C-----------------------------------------------------------------------
C OPTIONAL INPUTS.
C
C THE FOLLOWING IS A LIST OF THE OPTIONAL INPUTS PROVIDED FOR IN THE
C CALL SEQUENCE.  (SEE ALSO PART II.)  FOR EACH SUCH INPUT VARIABLE,
C THIS TABLE LISTS ITS NAME AS USED IN THIS DOCUMENTATION, ITS
C LOCATION IN THE CALL SEQUENCE, ITS MEANING, AND THE DEFAULT VALUE.
C THE USE OF ANY OF THESE INPUTS REQUIRES IOPT = 1, AND IN THAT
C CASE ALL OF THESE INPUTS ARE EXAMINED.  A VALUE OF ZERO FOR ANY
C OF THESE OPTIONAL INPUTS WILL CAUSE THE DEFAULT VALUE TO BE USED.
C THUS TO USE A SUBSET OF THE OPTIONAL INPUTS, SIMPLY PRELOAD
C LOCATIONS 5 TO 10 IN RWORK AND IWORK TO 0.0 AND 0 RESPECTIVELY, AND
C THEN SET THOSE OF INTEREST TO NONZERO VALUES.
C
C NAME    LOCATION      MEANING AND DEFAULT VALUE
C
C H0      RWORK(5)  THE STEP SIZE TO BE ATTEMPTED ON THE FIRST STEP.
C                   THE DEFAULT VALUE IS DETERMINED BY THE SOLVER.
C
C HMAX    RWORK(6)  THE MAXIMUM ABSOLUTE STEP SIZE ALLOWED.
C                   THE DEFAULT VALUE IS INFINITE.
C
C HMIN    RWORK(7)  THE MINIMUM ABSOLUTE STEP SIZE ALLOWED.
C                   THE DEFAULT VALUE IS 0.  (THIS LOWER BOUND IS NOT
C                   ENFORCED ON THE FINAL STEP BEFORE REACHING TCRIT
C                   WHEN ITASK = 4 OR 5.)
C
C MAXORD  IWORK(5)  THE MAXIMUM ORDER TO BE ALLOWED.  THE DEFAULT
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C                       VALUE IS 12 IF METH = 1, AND 5 IF METH = 2.
C                       IF MAXORD EXCEEDS THE DEFAULT VALUE, IT WILL
C                       BE REDUCED TO THE DEFAULT VALUE.
C                       IF MAXORD IS CHANGED DURING THE PROBLEM, IT MAY
C                       CAUSE THE CURRENT ORDER TO BE REDUCED.
C
C MXSTEP  IWORK(6)   MAXIMUM NUMBER OF (INTERNALLY DEFINED) STEPS
C                       ALLOWED DURING ONE CALL TO THE SOLVER.
C                       THE DEFAULT VALUE IS 500.
C
C MXHNIL  IWORK(7)   MAXIMUM NUMBER OF MESSAGES PRINTED (PER PROBLEM)
C                       WARNING THAT T + H = T ON A STEP (H = STEP SIZE).
C                       THIS MUST BE POSITIVE TO RESULT IN A NON-DEFAULT
C                       VALUE.  THE DEFAULT VALUE IS 10.
C-----------------------------------------------------------------------
C OPTIONAL OUTPUTS.
C
C AS OPTIONAL ADDITIONAL OUTPUT FROM LSODE, THE VARIABLES LISTED
C BELOW ARE QUANTITIES RELATED TO THE PERFORMANCE OF LSODE
C WHICH ARE AVAILABLE TO THE USER.  THESE ARE COMMUNICATED BY WAY OF
C THE WORK ARRAYS, BUT ALSO HAVE INTERNAL MNEMONIC NAMES AS SHOWN.
C EXCEPT WHERE STATED OTHERWISE, ALL OF THESE OUTPUTS ARE DEFINED
C ON ANY SUCCESSFUL RETURN FROM LSODE, AND ON ANY RETURN WITH
C ISTATE = -1, -2, -4, -5, OR -6.  ON AN ILLEGAL INPUT RETURN
C (ISTATE = -3), THEY WILL BE UNCHANGED FROM THEIR EXISTING VALUES
C (IF ANY), EXCEPT POSSIBLY FOR TOLSF, LENRW, AND LENIW.
C ON ANY ERROR RETURN, OUTPUTS RELEVANT TO THE ERROR WILL BE DEFINED,
C AS NOTED BELOW.
C
C NAME    LOCATION      MEANING
C
C HU      RWORK(11)  THE STEP SIZE IN T LAST USED (SUCCESSFULLY).
C
C HCUR    RWORK(12)  THE STEP SIZE TO BE ATTEMPTED ON THE NEXT STEP.
C
C TCUR    RWORK(13)  THE CURRENT VALUE OF THE INDEPENDENT VARIABLE
C                       WHICH THE SOLVER HAS ACTUALLY REACHED, I.E. THE
C                       CURRENT INTERNAL MESH POINT IN T.  ON OUTPUT, TCUR
C                       WILL ALWAYS BE AT LEAST AS FAR AS THE ARGUMENT
C                       T, BUT MAY BE FARTHER (IF INTERPOLATION WAS DONE).
C
C TOLSF   RWORK(14)  A TOLERANCE SCALE FACTOR, GREATER THAN 1.0,
C                       COMPUTED WHEN A REQUEST FOR TOO MUCH ACCURACY WAS
C                       DETECTED (ISTATE = -3 IF DETECTED AT THE START OF
C                       THE PROBLEM, ISTATE = -2 OTHERWISE).  IF ITOL IS
C                       LEFT UNALTERED BUT RTOL AND ATOL ARE UNIFORMLY
C                       SCALED UP BY A FACTOR OF TOLSF FOR THE NEXT CALL,
C                       THEN THE SOLVER IS DEEMED LIKELY TO SUCCEED.
C                       (THE USER MAY ALSO IGNORE TOLSF AND ALTER THE
C                       TOLERANCE PARAMETERS IN ANY OTHER WAY APPROPRIATE.)
C
C NST     IWORK(11)  THE NUMBER OF STEPS TAKEN FOR THE PROBLEM SO FAR.
C
C NFE     IWORK(12)  THE NUMBER OF F EVALUATIONS FOR THE PROBLEM SO FAR.
C
C NJE     IWORK(13)  THE NUMBER OF JACOBIAN EVALUATIONS (AND OF MATRIX
C                       LU DECOMPOSITIONS) FOR THE PROBLEM SO FAR.
C
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C NQU     IWORK(14) THE METHOD ORDER LAST USED (SUCCESSFULLY).
C
C NQCUR   IWORK(15) THE ORDER TO BE ATTEMPTED ON THE NEXT STEP.
C
C IMXER   IWORK(16) THE INDEX OF THE COMPONENT OF LARGEST MAGNITUDE IN
C                   THE WEIGHTED LOCAL ERROR VECTOR ( E(I)/EWT(I) ),
C                   ON AN ERROR RETURN WITH ISTATE = -4 OR -5.
C
C LENRW   IWORK(17) THE LENGTH OF RWORK ACTUALLY REQUIRED.
C                   THIS IS DEFINED ON NORMAL RETURNS AND ON AN ILLEGAL
C                   INPUT RETURN FOR INSUFFICIENT STORAGE.
C
C LENIW   IWORK(18) THE LENGTH OF IWORK ACTUALLY REQUIRED.
C                   THIS IS DEFINED ON NORMAL RETURNS AND ON AN ILLEGAL
C                   INPUT RETURN FOR INSUFFICIENT STORAGE.
C
C THE FOLLOWING TWO ARRAYS ARE SEGMENTS OF THE RWORK ARRAY WHICH
C MAY ALSO BE OF INTEREST TO THE USER AS OPTIONAL OUTPUTS.
C FOR EACH ARRAY, THE TABLE BELOW GIVES ITS INTERNAL NAME,
C ITS BASE ADDRESS IN RWORK, AND ITS DESCRIPTION.
C
C NAME    BASE ADDRESS      DESCRIPTION
C
C YH      21             THE NORDSIECK HISTORY ARRAY, OF SIZE NYH BY
C                        (NQCUR + 1), WHERE NYH IS THE INITIAL VALUE
C                        OF NEQ.  FOR J = 0,1,...,NQCUR, COLUMN J+1
C                        OF YH CONTAINS HCUR**J/FACTORIAL(J) TIMES
C                        THE J-TH DERIVATIVE OF THE INTERPOLATING
C                        POLYNOMIAL CURRENTLY REPRESENTING THE SOLUTION,
C                        EVALUATED AT T = TCUR.
C
C ACOR     LENRW-NEQ+1   ARRAY OF SIZE NEQ USED FOR THE ACCUMULATED
C                        CORRECTIONS ON EACH STEP, SCALED ON OUTPUT
C                        TO REPRESENT THE ESTIMATED LOCAL ERROR IN Y
C                        ON THE LAST STEP.  THIS IS THE VECTOR E IN
C                        THE DESCRIPTION OF THE ERROR CONTROL.  IT IS
C                        DEFINED ONLY ON A SUCCESSFUL RETURN FROM LSODE.
C
C-----------------------------------------------------------------------
C PART II.  OTHER ROUTINES CALLABLE.
C
C THE FOLLOWING ARE OPTIONAL CALLS WHICH THE USER MAY MAKE TO
C GAIN ADDITIONAL CAPABILITIES IN CONJUNCTION WITH LSODE.
C (THE ROUTINES XSETUN AND XSETF ARE DESIGNED TO CONFORM TO THE
C SLATEC ERROR HANDLING PACKAGE.)
C
C     FORM OF CALL                  FUNCTION
C   CALL XSETUN(LUN)           SET THE LOGICAL UNIT NUMBER, LUN, FOR
C                              OUTPUT OF MESSAGES FROM LSODE, IF
C                              THE DEFAULT IS NOT DESIRED.
C                              THE DEFAULT VALUE OF LUN IS 6.
C
C   CALL XSETF(MFLAG)          SET A FLAG TO CONTROL THE PRINTING OF
C                              MESSAGES BY LSODE.
C                              MFLAG = 0 MEANS DO NOT PRINT. (DANGER..
C                              THIS RISKS LOSING VALUABLE INFORMATION.)
C                              MFLAG = 1 MEANS PRINT (THE DEFAULT).
C
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```
C                                 EITHER OF THE ABOVE CALLS MAY BE MADE AT
C                                 ANY TIME AND WILL TAKE EFFECT IMMEDIATELY.
C
C   CALL SVCOM (RSAV, ISAV)       STORE IN RSAV AND ISAV THE CONTENTS
C                                 OF THE INTERNAL COMMON BLOCKS USED BY
C                                 LSODE (SEE PART III BELOW).
C                                 RSAV MUST BE A REAL ARRAY OF LENGTH 219
C                                 OR MORE, AND ISAV MUST BE AN INTEGER
C                                 ARRAY OF LENGTH 41 OR MORE.
C
C   CALL RSCOM (RSAV, ISAV)       RESTORE, FROM RSAV AND ISAV, THE CONTENTS
C                                 OF THE INTERNAL COMMON BLOCKS USED BY
C                                 LSODE.  PRESUMES A PRIOR CALL TO SVCOM
C                                 WITH THE SAME ARGUMENTS.
C
C                                 SVCOM AND RSCOM ARE USEFUL IF
C                                 INTERRUPTING A RUN AND RESTARTING
C                                 LATER, OR ALTERNATING BETWEEN TWO OR
C                                 MORE PROBLEMS SOLVED WITH LSODE.
C
C   CALL INTDY(,,,,,)             PROVIDE DERIVATIVES OF Y, OF VARIOUS
C        (SEE BELOW)              ORDERS, AT A SPECIFIED POINT T, IF
C                                 DESIRED.  IT MAY BE CALLED ONLY AFTER
C                                 A SUCCESSFUL RETURN FROM LSODE.
C
C THE DETAILED INSTRUCTIONS FOR USING INTDY ARE AS FOLLOWS.
C THE FORM OF THE CALL IS..
C
C   CALL INTDY (T, K, RWORK(21), NYH, DKY, IFLAG)
C
C THE INPUT PARAMETERS ARE..
C
C T          = VALUE OF INDEPENDENT VARIABLE WHERE ANSWERS ARE DESIRED
C              (NORMALLY THE SAME AS THE T LAST RETURNED BY LSODE).
C              FOR VALID RESULTS, T MUST LIE BETWEEN TCUR - HU AND TCUR.
C              (SEE OPTIONAL OUTPUTS FOR TCUR AND HU.)
C K          = INTEGER ORDER OF THE DERIVATIVE DESIRED.  K MUST SATISFY
C              0 .LE. K .LE. NQCUR, WHERE NQCUR IS THE CURRENT ORDER
C              (SEE OPTIONAL OUTPUTS).  THE CAPABILITY CORRESPONDING
C              TO K = 0, I.E. COMPUTING Y(T), IS ALREADY PROVIDED
C              BY LSODE DIRECTLY.  SINCE NQCUR .GE. 1, THE FIRST
C              DERIVATIVE DY/DT IS ALWAYS AVAILABLE WITH INTDY.
C RWORK(21)  = THE BASE ADDRESS OF THE HISTORY ARRAY YH.
C NYH        = COLUMN LENGTH OF YH, EQUAL TO THE INITIAL VALUE OF NEQ.
C
C THE OUTPUT PARAMETERS ARE..
C
C DKY        = A REAL ARRAY OF LENGTH NEQ CONTAINING THE COMPUTED VALUE
C              OF THE K-TH DERIVATIVE OF Y(T).
C IFLAG      = INTEGER FLAG, RETURNED AS 0 IF K AND T WERE LEGAL,
C              -1 IF K WAS ILLEGAL, AND -2 IF T WAS ILLEGAL.
C              ON AN ERROR RETURN, A MESSAGE IS ALSO WRITTEN.
C-----------------------------------------------------------------------
C PART III.  COMMON BLOCKS.
C
C IF LSODE IS TO BE USED IN AN OVERLAY SITUATION, THE USER
C MUST DECLARE, IN THE PRIMARY OVERLAY, THE VARIABLES IN..
C   (1) THE CALL SEQUENCE TO LSODE,
```

```
C   (2) THE TWO INTERNAL COMMON BLOCKS
C         /LS0001/  OF LENGTH  258  (219 SINGLE PRECISION WORDS
C                         FOLLOWED BY 39 INTEGER WORDS),
C         /EH0001/  OF LENGTH  2 (INTEGER WORDS).
C
C IF LSODE IS USED ON A SYSTEM IN WHICH THE CONTENTS OF INTERNAL
C COMMON BLOCKS ARE NOT PRESERVED BETWEEN CALLS, THE USER SHOULD
C DECLARE THE ABOVE TWO COMMON BLOCKS IN HIS MAIN PROGRAM TO INSURE
C THAT THEIR CONTENTS ARE PRESERVED.
C
C IF THE SOLUTION OF A GIVEN PROBLEM BY LSODE IS TO BE INTERRUPTED
C AND THEN LATER CONTINUED, SUCH AS WHEN RESTARTING AN INTERRUPTED RUN
C OR ALTERNATING BETWEEN TWO OR MORE PROBLEMS, THE USER SHOULD SAVE,
C FOLLOWING THE RETURN FROM THE LAST LSODE CALL PRIOR TO THE
C INTERRUPTION, THE CONTENTS OF THE CALL SEQUENCE VARIABLES AND THE
C INTERNAL COMMON BLOCKS, AND LATER RESTORE THESE VALUES BEFORE THE
C NEXT LSODE CALL FOR THAT PROBLEM.  TO SAVE AND RESTORE THE COMMON
C BLOCKS, USE SUBROUTINES SVCOM AND RSCOM (SEE PART II ABOVE).
C
C NOTE.. IN THIS VERSION OF LSODE, THERE ARE TWO DATA STATEMENTS,
C IN SUBROUTINES LSODE AND XERRWV, WHICH LOAD VARIABLES INTO THESE
C LABELED COMMON BLOCKS.  ON SOME SYSTEMS, IT MAY BE NECESSARY TO
C MOVE THESE TO A SEPARATE BLOCK DATA SUBPROGRAM.
C
C-----------------------------------------------------------------------
C PART IV.  OPTIONALLY REPLACEABLE SOLVER ROUTINES.
C
C BELOW ARE DESCRIPTIONS OF TWO ROUTINES IN THE LSODE PACKAGE WHICH
C RELATE TO THE MEASUREMENT OF ERRORS.  EITHER ROUTINE CAN BE
C REPLACED BY A USER-SUPPLIED VERSION, IF DESIRED.  HOWEVER, SINCE SUCH
C A REPLACEMENT MAY HAVE A MAJOR IMPACT ON PERFORMANCE, IT SHOULD BE
C DONE ONLY WHEN ABSOLUTELY NECESSARY, AND ONLY WITH GREAT CAUTION.
C (NOTE.. THE MEANS BY WHICH THE PACKAGE VERSION OF A ROUTINE IS
C SUPERSEDED BY THE USER-S VERSION MAY BE SYSTEM-DEPENDENT.)
C
C (A) EWSET.
C THE FOLLOWING SUBROUTINE IS CALLED JUST BEFORE EACH INTERNAL
C INTEGRATION STEP, AND SETS THE ARRAY OF ERROR WEIGHTS, EWT, AS
C DESCRIBED UNDER ITOL/RTOL/ATOL ABOVE..
C     SUBROUTINE EWSET (NEQ, ITOL, RTOL, ATOL, YCUR, EWT)
C WHERE NEQ, ITOL, RTOL, AND ATOL ARE AS IN THE LSODE CALL SEQUENCE,
C YCUR CONTAINS THE CURRENT DEPENDENT VARIABLE VECTOR, AND
C EWT IS THE ARRAY OF WEIGHTS SET BY EWSET.
C
C IF THE USER SUPPLIES THIS SUBROUTINE, IT MUST RETURN IN EWT(I)
C (I = 1,...,NEQ) A POSITIVE QUANTITY SUITABLE FOR COMPARING ERRORS
C IN Y(I) TO.  THE EWT ARRAY RETURNED BY EWSET IS PASSED TO THE
C VNORM ROUTINE (SEE BELOW), AND ALSO USED BY LSODE IN THE COMPUTATION
C OF THE OPTIONAL OUTPUT IMXER, THE DIAGONAL JACOBIAN APPROXIMATION,
C AND THE INCREMENTS FOR DIFFERENCE QUOTIENT JACOBIANS.
C
C IN THE USER-SUPPLIED VERSION OF EWSET, IT MAY BE DESIRABLE TO USE
C THE CURRENT VALUES OF DERIVATIVES OF Y.  DERIVATIVES UP TO ORDER NQ
C ARE AVAILABLE FROM THE HISTORY ARRAY YH, DESCRIBED ABOVE UNDER
C OPTIONAL OUTPUTS.  IN EWSET, YH IS IDENTICAL TO THE YCUR ARRAY,
C EXTENDED TO NQ + 1 COLUMNS WITH A COLUMN LENGTH OF NYH AND SCALE
C FACTORS OF H**J/FACTORIAL(J).  ON THE FIRST CALL FOR THE PROBLEM,
C GIVEN BY NST = 0, NQ IS 1 AND H IS TEMPORARILY SET TO 1.0.
```

```
C THE QUANTITIES NQ, NYH, H, AND NST CAN BE OBTAINED BY INCLUDING
C IN EWSET THE STATEMENTS..
C     COMMON /LS0001/ RLS(219),ILS(39)
C     NQ = ILS(35)
C     NYH = ILS(14)
C     NST = ILS(36)
C     H = RLS(213)
C THUS, FOR EXAMPLE, THE CURRENT VALUE OF DY/DT CAN BE OBTAINED AS
C YCUR(NYH+I)/H  (I=1,...,NEQ)  (AND THE DIVISION BY H IS
C UNNECESSARY WHEN NST = 0).
C
C (B) VNORM.
C THE FOLLOWING IS A REAL FUNCTION ROUTINE WHICH COMPUTES THE WEIGHTED
C ROOT-MEAN-SQUARE NORM OF A VECTOR V..
C     D = VNORM (N, V, W)
C WHERE..
C   N = THE LENGTH OF THE VECTOR,
C   V = REAL ARRAY OF LENGTH N CONTAINING THE VECTOR,
C   W = REAL ARRAY OF LENGTH N CONTAINING WEIGHTS,
C   D = SQRT( (1/N) * SUM(V(I)*W(I))**2 ).
C VNORM IS CALLED WITH N = NEQ AND WITH W(I) = 1.0/EWT(I), WHERE
C EWT IS AS SET BY SUBROUTINE EWSET.
C
C IF THE USER SUPPLIES THIS FUNCTION, IT SHOULD RETURN A NON-NEGATIVE
C VALUE OF VNORM SUITABLE FOR USE IN THE ERROR CONTROL IN LSODE.
C NONE OF THE ARGUMENTS SHOULD BE ALTERED BY VNORM.
C FOR EXAMPLE, A USER-SUPPLIED VNORM ROUTINE MIGHT..
C   -SUBSTITUTE A MAX-NORM OF (V(I)*W(I)) FOR THE RMS-NORM, OR
C   -IGNORE SOME COMPONENTS OF V IN THE NORM, WITH THE EFFECT OF
C    SUPPRESSING THE ERROR CONTROL ON THOSE COMPONENTS OF Y.
C-----------------------------------------------------------------------
C-----------------------------------------------------------------------
C OTHER ROUTINES IN THE LSODE PACKAGE.
C
C IN ADDITION TO SUBROUTINE LSODE, THE LSODE PACKAGE INCLUDES THE
C FOLLOWING SUBROUTINES AND FUNCTION ROUTINES..
C  INTDY    COMPUTES AN INTERPOLATED VALUE OF THE Y VECTOR AT T = TOUT.
C  STODE    IS THE CORE INTEGRATOR, WHICH DOES ONE STEP OF THE
C           INTEGRATION AND THE ASSOCIATED ERROR CONTROL.
C  CFODE    SETS ALL METHOD COEFFICIENTS AND TEST CONSTANTS.
C  PREPJ    COMPUTES AND PREPROCESSES THE JACOBIAN MATRIX J = DF/DY
C           AND THE NEWTON ITERATION MATRIX P = I - H*L0*J.
C  SOLSY    MANAGES SOLUTION OF LINEAR SYSTEM IN CHORD ITERATION.
C  EWSET    SETS THE ERROR WEIGHT VECTOR EWT BEFORE EACH STEP.
C  VNORM    COMPUTES THE WEIGHTED R.M.S. NORM OF A VECTOR.
C  SVCOM AND RSCOM   ARE USER-CALLABLE ROUTINES TO SAVE AND RESTORE,
C           RESPECTIVELY, THE CONTENTS OF THE INTERNAL COMMON BLOCKS.
C  SGEFA AND SGESL   ARE ROUTINES FROM LINPACK FOR SOLVING FULL
C           SYSTEMS OF LINEAR ALGEBRAIC EQUATIONS.
C  SGBFA AND SGBSL   ARE ROUTINES FROM LINPACK FOR SOLVING BANDED
C           LINEAR SYSTEMS.
C  SAXPY, SSCAL, ISAMAX, AND SDOT   ARE BASIC LINEAR ALGEBRA MODULES
C           (BLAS) USED BY THE ABOVE LINPACK ROUTINES.
C  R1MACH   COMPUTES THE UNIT ROUNDOFF IN A MACHINE-INDEPENDENT MANNER.
C  XERRWV, XSETUN, AND XSETF   HANDLE THE PRINTING OF ALL ERROR
C           MESSAGES AND WARNINGS.  XERRWV IS MACHINE-DEPENDENT.
C NOTE..  VNORM, ISAMAX, SDOT, AND R1MACH ARE FUNCTION ROUTINES.
C ALL THE OTHERS ARE SUBROUTINES.
```

```
C
C THE INTRINSIC AND EXTERNAL ROUTINES USED BY LSODE ARE..
C ABS, AMAX1, AMIN1, FLOAT, MAX0, MIN0, MOD, SIGN, SQRT, AND WRITE.
C
C-----------------------------------------------------------------------
C  END OF WRITEUP
```

APPENDIX • D

RADICAL Sample Input/Output Files

The input and output files used for Dresden-2 water chemistry simulations are listed in this appendix as samples. The samples show what RADICAL needs and produces. The sample input may be modified to simulate other BWRs.

I. DRESDEN0.IN

DRESDEN0.IN is the input file for RADICAL which was used to simulate Dresden-2 BWR power plant water chemistry in this thesis.

The zero in the input file name implies that no hydrogen is injected at the feedwater line. Input files for hydrogen water chemistry simulation are the same, except that the hydrogen concentration at the inlet of the feedwater is specified for a specific hydrogen injection level; the levels for 0.3, 0.5, 0.8, and 2.1 ppm hydrogen injection are given in the feedwater section of the input file as comments.

This input file may be used as a template for creating input files for other power plants or experimental loops.

```
[JCHUN.RADICAL.DRESDEN]DRESDEN0.IN  IBE'S RX,DRESDEN-2,MULTI DNCMR 14 JUN 1990
HYDROGEN WATER CHEMISTRY - 0 PPM H2 ADDED AT FEEDWATER.
LAST MODIFIED: 18 JUNE 1990

$FILENAME
OUTFILE  = 'DRESDEN0.OUT',
PLOTFILE = 'DRESDEN0.PLOT',
SENSFILE = 'DRESDEN0.SENS',
$END

$SIZE
NSPECIES =          16,
NRX      =          47,
NSURFRX  =           1,
NCOMP    =          17,
NNODE    =           9,
NCYCLE   =           2,
$END

$CONTROL
NODESTART=     1,
TEMPREF  =   298.0,
LINLIN   = T,
SENS     = T,
PPBOUT   = T,
CYCLEOUT = 2*T,
$END

*123456789012345*1234123412341234
$COMPONENT
CORE BOILING        1   2   1
CORE BYPASS         1   2   1
UPPER PLENUM        2   3
FEEDWATER           9   3   1
MIXING PLENUM       3   4
UP DOWNCOMER1       4   5
UP DOWNCOMER2       4   5
UP DOWNCOMER3       4   5
UP DOWNCOMER4       4   5
LO DOWNCOMER1       5   6
LO DOWNCOMER2       5   6
LO DOWNCOMER3       5   6
LO DOWNCOMER4       5   6
SPACER              5   7
RECIRC              6   7
JET PUMP            7   8
LOWER PLENUM        8   1
$END

***************************************************************************
IBE.DAT                                                       21 MARCH 1990
LAST MODIFIED: 13 JUNE 1990

*FROM IBE, ET AL.;"BEHAVIOR OF NITROGEN COMPOUNDS IN RADIATION FIELD AND
NUCLEAR REACTOR SYSTEMS",
J. OF NUCLEAR SCIENCE AND TECHNOLOGY, 26[8], PP. 760-769 (AUG 1989)

*NSPECIES = 16,
```

```
*NRX       = 46,
*NSURFACE =  1,
*H20 EXPLICITLY DECLARED IN RX.

*GAMMA AND NEUTRON G-VALUES
 THESE ARE BURNS' HI-T G-VALUES (1980)

 $GVALUE
 e-        0.4000
           0.400D+00
           5.490D-04
 OH-          0.0000
           0.000D+00
           1.700D+01
 H2        2.000
           2.000D+00
           2.000D+00
 OH        0.7000
           0.700D+00
           1.700D+01
 HO2-         0.0000
           0.000D+00
           3.300D+01
 H2O2      0.00
           0.000D+00
           3.400D+01
 O2-          0.0000
           0.000D+00
           3.200D+01
 O2           0.0000
           0.000D+00
           3.200D+01
 H         0.3000
           0.300D+00
           1.000D+00
 H+        0.4000
           0.400D+00
           1.000D+00
 HO2          0.0000
           0.000D-00
           3.300D+01
 O2G          0.0000
           0.000D+00
           3.200D+01
 H2G          0.0000
           0.000D+00
           2.000D+00
 O            2.0000
           2.000D+00
           1.600D+01
 H2O          0.0000
           0.000D+00
           1.800D+01
 2H2O         0.0000
           0.000D+00
           3.600D+01
 $END OF GVALUE
```

```
 $NAME
 SPECIESNAME  = 'e- ',  'OH-',          'H2 ',      'OH ',   'HO2-',
                'H2O2 ','O2- ', 'O2 ',        'H ',        'H+ ',
                'HO2 ', 'O2G',       'H2G', 'O ','H2O ',
                '2H2O '
 $END

*REACTION NAME, REACTION, RATE CONSTANT AND ACTIVATION ENERGY
 WATER EXPLICITLY DECLARED

 $REACTION
 I 1     15 15  0 16  0  0  0   1.0D0          0.0
 I 2     16  0  0 15 15  0  0   1.0D0          0.0
 W 1      1 15  0  9  2  0  0   0.160000E+02   0.126000E+02
 W 2      1 10  0  9  0  0  0   0.240000E+11   0.126000E+02
 W 3      1  4  0  2  0  0  0   0.240000E+11   0.126000E+02
 W 4      1  6  0  4  2  0  0   0.130000E+11   0.126000E+02
 W 5      9  9  0  3  0  0  0   0.100000E+11   0.126000E+02
 W 6      1 11  0  5  0  0  0   0.200000E+11   0.126000E+02
 W 7      1  8  0  7  0  0  0   0.190000E+11   0.126000E+02
 W 8      1  1 16  2  2  3  0   1.640000E+06   0.126000E+02
 W 9      4  4  0  6  0  0  0   5.000000E+03   0.126000E+02
 W10     11  4  0  8 15  0  0   0.120000E+11   0.126000E+02
 W11      4  7  0  8  2  0  0   0.120000E+11   0.126000E+02
 W12      9  2  0  1 15  0  0   0.200000E+08   0.126000E+02
 W13      9  1 15  3  2  0  0   4.500000E+08   0.126000E+02
 W14      5  1 15  4  2  2  0   6.300000E+07   0.126000E+02
 W15     10  2  0 15  0  0  0   1.437800E+11   0.126000E+02
 W16      9  4  0 15  0  0  0   0.200000E+11   0.126000E+02
 W17      3  4  0  9 15  0  0   3.400000E+07   0.193000E+02
 W18      6  4  0 11 15  0  0   0.270000E+08   1.420000E+01
 W19      9  6  0  4 15  0  0   0.440000E+08   0.189000E+02
 W20      9  8  0 11  0  0  0   0.190000E+11   0.126000E+02
 W21     11  0  0 10  7  0  0   0.800000E+06   0.126000E+02
 W22     11  7  0  5  8  0  0   0.150000E+08   0.189000E+02
 W23     11 11  0  8  6  0  0   0.270000E+07   0.189000E+02
 W24      7  7 16  8  6  2  2   5.600000E+03   0.189000E+02
 W25      9 11  0  6  0  0  0   0.200000E+11   0.126000E+02
 W26      9  7  0  5  0  0  0   0.200000E+11   0.126000E+02
 W27      7  1 15  5  2  0  0   1.800000E+08   0.189000E+02
 W28      6  2  0  5 15  0  0   0.500000E+09   0.189000E+02
*W29     15  0  0 10  2  0  0   2.088400E-02   0.126D2
 W30      7 10  0 11  0  0  0   0.500000E+11   0.126000E+02
 W31      5 15  0  6  2  0  0   1.022000E+04   0.126000E+02
 W32      6  0  0  4  4  0  0   1.953000E-03   7.280000E+00
 W33     14 14  0  8  0  0  0   2.200000E+10   0.126000E+02
 W34     11 14  0  8  4  0  0   2.000000E+10   0.126000E+02
 W35      4 14  0  9  8  0  0   1.000000E-00   0.706000E+02
 W36     15 14  0  4  4  0  0   1.900000E+03   0.126000E+02
 W37      4 14  0 11  0  0  0   2.000000E+10   0.126000E+02
 W38      3 14  0  9  4  0  0   4.800000E+03   0.349000E+02
 W39      6 14  0 11  4  0  0   1.300000E+06   0.176000E+02
 W40      9 14  0  4  0  0  0   2.000000E+10   0.126000E+02
 H2G      3  0  0 13  0  0  0   30.D0          -1.D0
 H2L     13  0  0  3  0  0  0   10.D0          -1.D0
 O2G      8  0  0 12  0  0  0   23.D0          -1.D0
 O2L     12  0  0  8  0  0  0   12.D0          -1.D0
 SS       6  0  0 14 15  0  0   5.322D-7       66.9D0
```

```
 $END OF REACTION
***************************************************************************


*THESE PARAMETERS CLOSELY FOLLOW DRESDEN-2 REPORTED BY
 IBE, ET AL.,"RADIOLYTIC ENVIRONMENTS
 IN BOILING WATER REACTOR CORES", JOURNAL OF NUCLEAR SCIENCE AND
 TECHNOLOGY, 24[3], PP. 220-226 (MARCH 1987)
 AND
 RUIZ, ET AL.,"MODELING HYDROGEN WATER CHEMISTRY FOR BWR APPLICATIONS",
 EPRI NP-6386, JUNE 1989

 @CORE BOILING

 $POSITION
 XINITIAL =     0.0000000000000     ,
 XFINAL   =   370.0000000000000     ,
 XSTEP    =    50.0,
 XBOIL    =    66.0D0,
 $END

 $STATE
 TEMPIN   =   552.000000000000     ,
 TEMPOUT  =   558.0,
 GAMMARATE=     3.00E5 ,
 NEUTRATE =     4.17E5,
 VELINLET =   150.0,
 DENSLIQ  =     0.741,
 DENSGAS  =     3.62D-2,
 PRESSURE =    70.75,
 FLOWRATE =     0.8934,
 DIAMETER =     5.0,
 $END

 $DOSESHAPE
 MAXORDERD=    9,
 GAMMAC        =   0.0518421,0.0302066,-0.000636609,9.55961D-6,-9.27315D-8,
               5.61948D-10,-2.09953D-12,4.67807D-15,-5.68192D-18,2.88266D-21
 NEUTRONC =    1.D0,9*0.D0
 $END

 $VOIDFRACTION
 MAXORDERV=    5,
 VOIDC    =  -0.58134,1.1809D-2,-4.8206D-5,1.1537D-7,-1.7792D-10,1.3508D-13
 $END

 $INITIALCONC
 CONC     =    2*0.D0,2.5935D-6,2*0D0,
               5.44853D-7,0.D0,4.2839D-6,2*0.D0,
               4*0.D0,41.1666666667,
               1694.7
 $END

 $FLAG
 CALCSURF = F,
 VOIDFLAG = T,
 CALCSENS = T,
 WRITERX  = F,
```

```
 WRITEPARA= T,
 $END

 $SENSITIVITY
 NSENS     = 2,
 SENSSPECIES = 'H2O2','O2'
 $END

 @END OF CORE BOILING
******************************************************************
 @CORE BYPASS

 $POSITION
 XINITIAL =     0.0000000000000     ,
 XFINAL   =   370.0000000000000     ,
 XSTEP    =    50.0,
 XBOIL    =  9999.0D0,
 $END

 $STATE
 TEMPIN   =   552.000000000000     ,
 TEMPOUT  =   558.0,
 VELINLET =    19.220,
 FLOWRATE =     0.1066,
 $END

 $DOSESHAPE $

 $VOIDFRACTION
 VOIDC    =  6*0.D0
 $END

 $INITIALCONC
 CONC     =   2*0.D0,2.5935D-6,2*0D0,
              5.44853D-7,0.D0,4.2839D-6,2*0.D0,
              4*0.D0,41.1666666667,
              1694.7
 $END

 $FLAG $
 $SENSITIVITY $

 @END OF CORE BYPASS
******************************************************************
 @UPPER PLENUM

 $POSITION
 XLENGTH  =    40.0000000000000     ,
 XSTEP    =    10.0,
 XBOIL    =    66.0D0,
 $END

 $STATE
 TEMPIN   =   558.0,
 TEMPOUT  =   555.0,
 VELINLET =    20.0,
 FLOWRATE =     1.105,
 $END
```

```
 $DOSESHAPE
 MAXORDERD=     0,
 GAMMAC       =     1.D-3,
 NEUTRONC =     1.D-3,
 $END

 $VOIDFRACTION
 MAXORDERV=  1,
 VOIDC    =  0.63873,-1.4325D-4,5*0.D0,
 $END

 $INITIALCONC
 CONC     =   14*,41.1666666667,1694.7
 $END

 $FLAG
 CALCSENS = F,
 $END

 $SENSITIVITY $

 @END OF UPPER PLENUM
*******************************************************************
 @FEEDWATER

 $POSITION
 XLENGTH  =     1.0000000000000     ,
 XBOIL    =  9999.0,
 $END

 $STATE
 VELINLET =     1.0D6,
 FLOWRATE =     0.125,
 $END

 $DOSESHAPE $
 $VOIDFRACTION $

 $INITIALCONC
 CONC =   2*0.D0,0.0,2*0.D0,
          2*0.D0,8.1047D-7,2*0.D0,
          4*0.D0,41.1666666667,
          1694.7
 $END
 0.3 PPM H2 = 1.1115D-4
 0.5 PPM H2 = 1.8525D-4
 0.8 PPM H2 = 2.9640D-4
 2.1 PPM H2 = 7.7805D-4

 $FLAG $
 $SENSITIVITY $

 @END OF FEEDWATER
*******************************************************************
 @MIXING PLENUM

 $POSITION
```

```
XINITIAL =   410.0,
XLENGTH  =   130.0000000000000      ,
XSTEP    =    20.0,
XBOIL    =    66.0,
$END

$STATE
TEMPIN   =  555.0,
TEMPOUT  =  552.0,
VELINLET =   30.23,
FLOWRATE =    0.69,
$END

$DOSESHAPE
GAMMAC       =   1.D-4,
NEUTRONC =   1.D-4,
$END

$VOIDFRACTION
MAXORDERV=  1,
VOIDC     =  1.0353D-2,-1.9154D-5,5*0.D0,
$END

$INITIALCONC
CONC      =   14*,41.1666666667,1694.7
$END

$FLAG $
$SENSITIVITY $

@END OF MIXING PLENUM
*******************************************************************
@SPACER

$POSITION
XLENGTH  =      0.0000000000000      ,
$END

$STATE
FLOWRATE =    0.69,
$END

$DOSESHAPE $
$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF SPACER
*******************************************************************
@UP DOWNCOMER1

$POSITION
XINITIAL =   540.0,
XLENGTH  =    40.0000000000000      ,
XSTEP    =    20.0,
XBOIL    = 99999.0,
$END
```

```
$STATE
VELINLET =    40.0,
FLOWRATE =     0.31,
$END

$DOSESHAPE
GAMMAC        =     1.D-2,
NEUTRONC =     1.D-3,
$END

$VOIDFRACTION $

$INITIALCONC
CONC      =   12*,2*0.D0,41.1666666667,1694.7
$END

$FLAG $
$SENSITIVITY $

@END OF UP DOWNCOMER1
*******************************************************************
@UP DOWNCOMER2

$POSITION
XINITIAL =   540.0,
XLENGTH  =    40.0000000000000     ,
$END

$STATE
FLOWRATE =     0.33,
$END

$DOSESHAPE
GAMMAC        =     1.D-3,
NEUTRONC =     1.D-4,
$END

$VOIDFRACTION $

$INITIALCONC
CONC      =   12*,2*0.D0,41.1666666667,1694.7
$END

$FLAG $
$SENSITIVITY $

@END OF UP DOWNCOMER2
*******************************************************************
@UP DOWNCOMER3

$POSITION
XINITIAL =   540.0,
XLENGTH  =    40.0000000000000     ,
$END

$STATE
FLOWRATE =     0.30,
```

```
$END

$DOSESHAPE
GAMMAC      =     1.D-4,
NEUTRONC =     1.D-5,
$END

$VOIDFRACTION $

$INITIALCONC
CONC     =   12*,2*0.D0,41.1666666667,1694.7
$END

$FLAG $
$SENSITIVITY $

@END OF UP DOWNCOMER3
****************************************************************
@UP DOWNCOMER4

$POSITION
XINITIAL =   540.0,
XLENGTH  =    40.0000000000000     ,
$END

$STATE
FLOWRATE =     0.06,
$END

$DOSESHAPE
GAMMAC      =     1.D-4,
NEUTRONC =     1.D-6,
$END

$VOIDFRACTION $

$INITIALCONC
CONC     =   12*,2*0.D0,41.1666666667,1694.7
$END

$FLAG $
$SENSITIVITY $

@END OF UP DOWNCOMER4
****************************************************************
@LO DOWNCOMER1

$POSITION
XINITIAL =   540.0,
XLENGTH  =    80.0000000000000     ,
$END

$STATE
VELINLET =    24.242,
FLOWRATE =     0.31,
$END

$DOSESHAPE
```

```
GAMMAC       =      1.D-2,
NEUTRONC =     1.D-3,
$END

$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF LO DOWNCOMER1
*******************************************************************
@LO DOWNCOMER2

$POSITION
XINITIAL =   540.0,
XLENGTH  =    80.0000000000000      ,
$END

$STATE
FLOWRATE =     0.33,
$END

$DOSESHAPE
GAMMAC       =      1.D-3,
NEUTRONC =     1.D-4,
$END

$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF LO DOWNCOMER2
*******************************************************************
@LO DOWNCOMER3

$POSITION
XINITIAL =   540.0,
XLENGTH  =    80.0000000000000      ,
XSTEP    =    20.0,
$END

$STATE
FLOWRATE =     0.30,
$END

$DOSESHAPE
GAMMAC       =      1.D-4,
NEUTRONC =     1.D-5,
$END

$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF LO DOWNCOMER3
*******************************************************************
```

```
@LO DOWNCOMER4

$POSITION
XINITIAL =   540.0,
XLENGTH  =    80.0000000000000      ,
$END

$STATE
FLOWRATE =     0.06,
$END

$DOSESHAPE
GAMMAC       =      1.D-4,
NEUTRONC =     1.D-6,
$END

$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF LO DOWNCOMER4
******************************************************************
@RECIRC

$POSITION
XLENGTH  =   130.0000000000000,
XSTEP    =    20.0,
$END

$STATE
VELINLET =    30.230,
FLOWRATE =     0.310,
$END

$DOSESHAPE
GAMMAC       =   0.0,
NEUTRONC =   0.0,
$END

$VOIDFRACTION $
$INITIALCONC $

$FLAG
CALCSENS = T,
$END

$SENSITIVITY $

@END OF RECIRC
******************************************************************
@JET PUMP

$POSITION
XLENGTH  =   200.0000000000000,
XSTEP    =    50.0,
$END
```

```
$STATE
VELINLET =   100.0,
$END

$DOSESHAPE
GAMMAC        =     1.D-3,
NEUTRONC =     1.D-3,
$END

$VOIDFRACTION $
$INITIALCONC $

$FLAG
CALCSENS = F,
$END

$SENSITIVITY $

@END OF JET PUMP
*******************************************************************
@LOWER PLENUM

$POSITION
XLENGTH  =   140.0000000000000     ,
XSTEP    =    50.0,
$END

$STATE
VELINLET =    30.435,
$END

$DOSESHAPE
GAMMAC        =     1.D-3,
NEUTRONC =     1.D-3,
$END

$VOIDFRACTION $
$INITIALCONC $
$FLAG $
$SENSITIVITY $

@END OF LOWER PLENUM
```

II. DRESDEN0.OUT

This is the output listing of RADICAL for the input file DRESDEN0.IN. The complete output file consisted of two cycles, which was too extensive to list in this thesis. Only the first cycle is listed here. For each component, only the first and last positions are retained in this sample output.

For the final concentration calculation results, see section III, where a compact output form is listed as DRESDEN0.MAC.

```
          ________________________________________________________
          |                                                      |
          |              RADICAL CODE PACKAGE OUTPUT             |
          |                     VERSION: 1.0                     |
          |                                                      |
          |                18-JUN-90  17:03:26                   |
          ________________________________________________________

______________________________________________________________________________

                                    INPUT

______________________________________________________________________________

[JCHUN.RADICAL.DRESDEN]DRESDEN0.IN  IBE'S RX,DRESDEN-2,MULTI DNCMR 14 JUN 1990

      INPUT FILE NAME                   = DRESDEN0.IN
      OUTPUT FILE NAME                  = DRESDEN0.OUT
      PLOT FILE NAME                    = DRESDEN0.PLOT
      SENSITIVITY FILE NAME             = DRESDEN0.SENS

      NUMBER OF SPECIES EVALUATED       =       16
      NUMBER OF CHEMICAL REACTIONS      =       47
      NUMBER OF SURFACE REACTIONS       =        1
      NUMBER OF COMPONENTS              =       17
      NUMBER OF NODES                   =        9
      NUMBER OF CYCLES                  =        2

      STARTING NODE                     =        1
      REFERENCE TEMPERATURE             =      298.00000 Kelvin

      PlotOut                           =        T
      LinLin                            =        T
      SENS                              =        T
      NORMALIZE                         =        F
      PPBOUT                            =        T


                                FLOW-IN    FLOW-OUT    INITIAL
      COMPONENT NAME              NODE       NODE        CONC
      ----------------          --------   --------    --------
      CORE BOILING                 1          2           1
      CORE BYPASS                  1          2           1
      UPPER PLENUM                 2          3           0
      FEEDWATER                    9          3           1
      MIXING PLENUM                3          4           0
      UP DOWNCOMER1                4          5           0
      UP DOWNCOMER2                4          5           0
      UP DOWNCOMER3                4          5           0
      UP DOWNCOMER4                4          5           0
      LO DOWNCOMER1                5          6           0
      LO DOWNCOMER2                5          6           0
      LO DOWNCOMER3                5          6           0
      LO DOWNCOMER4                5          6           0
      SPACER                       5          7           0
      RECIRC                       6          7           0
      JET PUMP                     7          8           0
```

```
LOWER PLENUM            8            1            0

              GAMMA       NEUTRON      MOLECULAR
             G-VALUES     G-VALUES      WEIGHT
SPECIES     (#/100eV)    (#/100eV)     (g/mole)
--------    ---------    ---------    ---------
e-          0.40D+00     0.40D+00     0.55D-03
OH-         0.00D+00     0.00D+00     0.17D+02
H2          0.20D+01     0.20D+01     0.20D+01
OH          0.70D+00     0.70D+00     0.17D+02
HO2-        0.00D+00     0.00D+00     0.33D+02
H2O2        0.00D+00     0.00D+00     0.34D+02
O2-         0.00D+00     0.00D+00     0.32D+02
O2          0.00D+00     0.00D+00     0.32D+02
H           0.30D+00     0.30D+00     0.10D+01
H+          0.40D+00     0.40D+00     0.10D+01
HO2         0.00D+00     0.00D+00     0.33D+02
O2G         0.00D+00     0.00D+00     0.32D+02
H2G         0.00D+00     0.00D+00     0.20D+01
O           0.20D+01     0.20D+01     0.16D+02
H2O         0.00D+00     0.00D+00     0.18D+02
2H2O        0.00D+00     0.00D+00     0.36D+02
```

CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES

	REACTIONS								RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
I 1	H2O	H2O		>2H2O					0.10D+01	0.00D+00
I 2	2H2O			>H2O	H2O				0.10D+01	0.00D+00
W 1	e-	H2O		>H	OH-				0.16D+02	0.13D+02
W 2	e-	H+		>H					0.24D+11	0.13D+02
W 3	e-	OH		>OH-					0.24D+11	0.13D+02
W 4	e-	H2O2		>OH	OH-				0.13D+11	0.13D+02
W 5	H	H		>H2					0.10D+11	0.13D+02
W 6	e-	HO2		>HO2-					0.20D+11	0.13D+02
W 7	e-	O2		>O2-					0.19D+11	0.13D+02
W 8	e-	e-	2H2O	>OH-	OH-	H2			0.16D+07	0.13D+02
W 9	OH	OH		>H2O2					0.50D+04	0.13D+02
W10	HO2	OH		>O2	H2O				0.12D+11	0.13D+02
W11	OH	O2-		>O2	OH-				0.12D+11	0.13D+02
W12	H	OH-		>e-	H2O				0.20D+08	0.13D+02
W13	H	e-	H2O	>H2	OH-				0.45D+09	0.13D+02
W14	HO2-	e-	H2O	>OH	OH-	OH-			0.63D+08	0.13D+02
W15	H+	OH-		>H2O					0.14D+12	0.13D+02
W16	H	OH		>H2O					0.20D+11	0.13D+02
W17	H2	OH		>H	H2O				0.34D+08	0.19D+02
W18	H2O2	OH		>HO2	H2O				0.27D+08	0.14D+02
W19	H	H2O2		>OH	H2O				0.44D+08	0.19D+02
W20	H	O2		>HO2					0.19D+11	0.13D+02
W21	HO2			>H+	O2-				0.80D+06	0.13D+02
W22	HO2	O2-		>HO2-	O2				0.15D+08	0.19D+02
W23	HO2	HO2		>O2	H2O2				0.27D+07	0.19D+02
W24	O2-	O2-	2H2O	>O2	H2O2	OH-	OH-		0.56D+04	0.19D+02
W25	H	HO2		>H2O2					0.20D+11	0.13D+02
W26	H	O2-		>HO2-					0.20D+11	0.13D+02
W27	O2-	e-	H2O	>HO2-	OH-				0.18D+09	0.19D+02
W28	H2O2	OH-		>HO2-	H2O				0.50D+09	0.19D+02
W29	H2O			>H+	OH-				0.21D-01	0.13D+02
W30	O2-	H+		>HO2					0.50D+11	0.13D+02
W31	HO2-	H2O		>H2O2	OH-				0.10D+05	0.13D+02
W32	H2O2			>OH	OH				0.20D-02	0.73D+01
W33	O	O		>O2					0.22D+11	0.13D+02
W34	HO2	O		>O2	OH				0.20D+11	0.13D+02
W35	OH	O		>H	O2				0.10D+01	0.71D+02
W36	H2O	O		>OH	OH				0.19D+04	0.13D+02
W37	OH	O		>HO2					0.20D+11	0.13D+02
W38	H2	O		>H	OH				0.48D+04	0.35D+02
W39	H2O2	O		>HO2	OH				0.13D+07	0.18D+02
W40	H	O		>OH					0.20D+11	0.13D+02
H2G	H2			>H2G					0.30D+02	-0.10D+01
H2L	H2G			>H2					0.10D+02	-0.10D+01
O2G	O2			>O2G					0.23D+02	-0.10D+01
O2L	O2G			>O2					0.12D+02	-0.10D+01

```
SS  H2O2                          >O        H2O                      0.53D-06  0.67D+02
```

```
                OUTPUT FOR CYCLE    1 AT CORE BOILING


    INITIAL POSITION                    =        0.00000 cm
    FINAL POSITION                      =      370.00000 cm
    FLOW LENGTH                         =      370.00000 cm
    POSITION INCREMENT                  =       50.00000 cm
    POSITION OF ONSET OF BOILING        =       66.00000 cm

    INLET TEMPERATURE                   =      552.00000 Kelvin
    OUTLET TEMPERATURE                  =      558.00000 Kelvin
    INLET LIQUID VELOCITY               =      150.00000 cm/s
    PIPE INTERNAL DIAMETER              =        5.00000 cm
    WATER DENSITY                       =        0.74100 g/cc
    VAPOR DENSITY                       =        0.03620 g/cc
    PRESSURE                            =       70.75000 atm
    MASS FlowRate                       =    0.89340D+00 g/s

    SENSITIVITY SPECIES   1             = H2O2
    SENSITIVITY SPECIES   2             = O2

    SensStep                            =       135

    GAMMA DOSE RATE MULTIPLIER          =    0.30000D+06 Rad/s
    NEUTRON DOSE RATE MULTIPLIER        =    0.41700D+06 Rad/s
    GConvert                            =    0.76916D-09

    GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
    GAMMA COEFFICIENT  0                =    0.51842D-01
    GAMMA COEFFICIENT  1                =    0.30207D-01
    GAMMA COEFFICIENT  2                =   -0.63661D-03
    GAMMA COEFFICIENT  3                =    0.95596D-05
    GAMMA COEFFICIENT  4                =   -0.92731D-07
    GAMMA COEFFICIENT  5                =    0.56195D-09
    GAMMA COEFFICIENT  6                =   -0.20995D-11
    GAMMA COEFFICIENT  7                =    0.46781D-14
    GAMMA COEFFICIENT  8                =   -0.56819D-17
    GAMMA COEFFICIENT  9                =    0.28827D-20

    NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
    NEUTRON COEFFICIENT  0              =    0.10000D+01
    NEUTRON COEFFICIENT  1              =    0.00000D+00
    NEUTRON COEFFICIENT  2              =    0.00000D+00
    NEUTRON COEFFICIENT  3              =    0.00000D+00
    NEUTRON COEFFICIENT  4              =    0.00000D+00
    NEUTRON COEFFICIENT  5              =    0.00000D+00
    NEUTRON COEFFICIENT  6              =    0.00000D+00
    NEUTRON COEFFICIENT  7              =    0.00000D+00
    NEUTRON COEFFICIENT  8              =    0.00000D+00
    NEUTRON COEFFICIENT  9              =    0.00000D+00

    VOID FRACTION FUNCTION COEFFICIENTS
    VOID FRACTION  COEFFICIENT  0  =   -0.58134D+00
```

```
     VOID FRACTION  COEFFICIENT  1   =    0.11809D-01
     VOID FRACTION  COEFFICIENT  2   =   -0.48206D-04
     VOID FRACTION  COEFFICIENT  3   =    0.11537D-06
     VOID FRACTION  COEFFICIENT  4   =   -0.17782D-09
     VOID FRACTION  COEFFICIENT  5   =    0.13508D-12

     CalcSurf                        =        F
     VoidFlag                        =        T
     CalcSens                        =        T
     WriteRx                         =        F
     WritePara                       =        T

     RADIOLYSIS ABSOLUTE TOLERANCE   =    0.10000D-14
                RELATIVE TOLERANCE   =    0.10000D-04
     ADJOINT    ABSOLUTE TOLERANCE   =    0.10000D-09
                RELATIVE TOLERANCE   =    0.10000D-03
     RESPONSE   ABSOLUTE TOLERANCE   =    0.10000D-14
                RELATIVE TOLERANCE   =    0.10000D-04
```

```
   CYCLE     1        POSITION IN CORE BOILING     =      0.0000 cm
                    CONCENTRATIONS[ppb]  AT POSITION =      0.0000 cm

   e-      =     0.000000D+00 **     OH-      =     0.000000D+00 **
   H2      =     0.700000D+01 **     OH       =     0.000000D+00 **
   HO2-    =     0.000000D+00 **     H2O2     =     0.250000D+02 **
   O2-     =     0.000000D+00 **     O2       =     0.185000D+03 **
   H       =     0.000000D+00 **     H+       =     0.000000D+00 **
   HO2     =     0.000000D+00 **     O2G      =     0.000000D+00 **
   H2G     =     0.000000D+00 **     O        =     0.000000D+00 **
   H2O     =     0.100000D+10 **     2H2O     =     0.823336D+11 **

   NO. STEPS                    =      0
   TEMPERATURE (K)              =      0.00000
   LIQUID VELOCITY (CM/S)       =    150.00000
   GAS VELOCITY  (CM/S)         =      0.00000
   VOID FRACTION                =      0.00000
   GAMMA DOSE RATE (RAD/S)      =   0.00000D+00
   NEUTRON DOSE RATE (RAD/S)    =   0.00000D+00
```

```
   CYCLE     1        POSITION IN CORE BOILING     =    370.0000 cm
                    CONCENTRATIONS[ppb]  AT POSITION =    370.0000 cm

   e-      =     0.627058D-07 **     OH-      =     0.553092D+02 **
   H2      =     0.157086D+02 **     OH       =     0.213211D+01 **
   HO2-    =     0.148047D+00 **     H2O2     =     0.162650D+02 **
   O2-     =     0.285988D+01 **     O2       =     0.204904D+03 **
   H       =     0.115243D-02 **     H+       =     0.334745D+01 **
   HO2     =     0.460994D+00 **     O2G      =     0.364294D+03 **
   H2G     =     0.429573D+02 **     O        =     0.180306D-01 **
   H2O     =     0.100000D+10 **     2H2O     =     0.823336D+11 **

   O2G       =   0.297D-03 ATM
   H2G       =   0.560D-03 ATM
```

```
    NO. STEPS                     =       472
    TEMPERATURE (K)               =       558.00000
    LIQUID VELOCITY (CM/S)        =       350.29014
    GAS VELOCITY  (CM/S)          =       728.94583
    VOID FRACTION                 =         0.63649
    GAMMA DOSE RATE (RAD/S)       =     0.49351D+05
    NEUTRON DOSE RATE (RAD/S)     =     0.41700D+06
```

```
               RUN STATISTICS FOR CYCLE    1 AT CORE BOILING
```

```
REQUIRED RWORK SIZE   =       422
IWORK SIZE            =        36
NUMBER OF STEPS       =       472
# OF FUNC.- EVALS.    =       659
# OF JACOB.- EVALS    =       127
COMPONENT JOB TIME    =     21.79 seconds

CONCENTRATION PROFILE OF CORE BOILING     HAS BEEN EVALUATED SUCCESSFULLY!

LSODE--  AT CURRENT T (=R1), MXSTEP (=I1) STEPS
      TAKEN ON THIS CALL BEFORE REACHING TOUT     L
     IN ABOVE MESSAGE,  I1 =       500
     IN ABOVE MESSAGE,  R1 =  0.8250859426938E+02
LSODE--  AT CURRENT T (=R1), MXSTEP (=I1) STEPS
      TAKEN ON THIS CALL BEFORE REACHING TOUT     L
     IN ABOVE MESSAGE,  I1 =       500
     IN ABOVE MESSAGE,  R1 =  0.3608377528807E+03
```

```
         CORE BOILING     SENSITIVITY RESULTS FOR O2

          ============ ADJOINT RESULTS ============

e-       =   -0.169968D+01 **     OH-     =   -0.242486D+00 **
H2       =   -0.290595D+01 **     OH      =    0.145330D+01 **
HO2-     =    0.268444D+01 **     H2O2    =    0.292693D+01 **
O2-      =    0.414184D+01 **     O2      =    0.483807D+01 **
H        =   -0.145389D+01 **     H+      =    0.242486D+00 **
HO2      =    0.438432D+01 **     O2G     =    0.122240D+00 **
H2G      =   -0.539085D-01 **     O       =    0.290660D+01 **
H2O      =   -0.296610D-08 **     2H2O    =   -0.582393D-08 **


                                ABSOLUTE      RELATIVE
       PARAMETER               SENSITIVITY   SENSITIVITY
-------------------------     ------------  ------------

RATE CONST OF I  1             0.85517E-05   0.18887E+01
RATE CONST OF I  2            -0.85599E-05  -0.18905E+01
RATE CONST OF W  1             0.68435E-10   0.25860E-02
RATE CONST OF W  2             0.41482E-17   0.23512E+00
RATE CONST OF W  3             0.28215E-18   0.15993E-01
RATE CONST OF W  4            -0.22087E-16  -0.67811E+00
RATE CONST OF W  5             0.43841E-19   0.10354E-02
RATE CONST OF W  6            -0.31242E-18  -0.14757E-01
RATE CONST OF W  7             0.12135E-16   0.54453E+00
RATE CONST OF W  8             0.14261E-17   0.55235E-05
RATE CONST OF W  9             0.46302E-14   0.54676E-04
RATE CONST OF W10              0.85292E-17   0.24172E+00
RATE CONST OF W11              0.54228E-16   0.15368E+01
RATE CONST OF W12             -0.37790E-16  -0.17850E-02
RATE CONST OF W13              0.25938E-18   0.27567E-03
RATE CONST OF W14             -0.84689E-17  -0.12601E-02
RATE CONST OF W15             -0.37485E-18  -0.12729E+00
RATE CONST OF W16              0.10476E-17   0.49480E-01
RATE CONST OF W17             -0.23723E-13  -0.67160E+01
RATE CONST OF W18              0.12166E-13   0.10481E+01
RATE CONST OF W19             -0.24005E-15  -0.81572E-01
RATE CONST OF W20              0.22993E-16   0.10318E+01
RATE CONST OF W21             -0.29066E-14  -0.54917E-02
RATE CONST OF W22             -0.31309E-15  -0.36270E-01
RATE CONST OF W23             -0.49267E-16  -0.10273E-02
RATE CONST OF W24             -0.33643E-11  -0.14550E+00
RATE CONST OF W25             -0.31500E-17  -0.14879E+00
RATE CONST OF W26             -0.20048E-16  -0.94695E+00
RATE CONST OF W27             -0.80831E-16  -0.11237E+00
RATE CONST OF W28             -0.45789E-15  -0.17681E+01
RATE CONST OF W29              0.25804E-05   0.12727E+00
RATE CONST OF W30              0.46211E-19   0.54569E-02
RATE CONST OF W31              0.73326E-10   0.17698E+01
RATE CONST OF W32             -0.24589E-06  -0.41701E-03
```

```
RATE CONST OF W33              0.97093E-18   0.50447E-01
RATE CONST OF W34             -0.19059E-18  -0.90023E-02
RATE CONST OF W35              0.83464E-16   0.10764E-04
RATE CONST OF W36             -0.90400E-09  -0.40565E+01
RATE CONST OF W37              0.83953E-16   0.39655E+01
RATE CONST OF W38             -0.45949E-15  -0.34525E-03
RATE CONST OF W39              0.14587E-15   0.11469E-02
RATE CONST OF W40             -0.11358E-19  -0.53650E-03
RATE CONST OF H2G              0.53123E-04   0.20102E+03
RATE CONST OF H2L             -0.52583E-04  -0.66325E+02
RATE CONST OF O2G             -0.70184E-04  -0.20361E+03
RATE CONST OF O2L              0.55191E-04   0.83536E+02
GAMMA   G-VALUE OF e-         -0.24582E-03  -0.21716E+02
NEUTRON G-VALUE OF e-         -0.46311E-03  -0.40912E+02
GAMMA   G-VALUE OF H2         -0.39686E-03  -0.17530E+03
NEUTRON G-VALUE OF H2         -0.75340E-03  -0.33278E+03
GAMMA   G-VALUE OF OH          0.20051E-03   0.30998E+02
NEUTRON G-VALUE OF OH          0.37990E-03   0.58731E+02
GAMMA   G-VALUE OF H          -0.20260E-03  -0.13423E+02
NEUTRON G-VALUE OF H          -0.38302E-03  -0.25377E+02
GAMMA   G-VALUE OF H+          0.39786E-04   0.35148E+01
NEUTRON G-VALUE OF H+          0.74586E-04   0.65890E+01
GAMMA   G-VALUE OF O           0.40473E-03   0.17877E+03
NEUTRON G-VALUE OF O           0.76556E-03   0.33815E+03
CONCENTRATION OF   e-         -0.50560E+03  -0.97017E-02
CONCENTRATION OF   OH-        -0.35815E+01  -0.19068E+01
CONCENTRATION OF   H2         -0.28317E+01  -0.36026E+01
CONCENTRATION OF   OH          0.64331E+01   0.13341E+00
CONCENTRATION OF   HO2-        0.23790E+04   0.17678E+01
CONCENTRATION OF   H2O2       -0.20423E+02  -0.16176E+01
CONCENTRATION OF   O2-         0.94950E+01   0.13720E+00
CONCENTRATION OF   O2          0.46109E+01   0.46109E+01
CONCENTRATION OF   H          -0.48615E+03  -0.96069E-01
CONCENTRATION OF   H+          0.26628E+00   0.14582E+00
CONCENTRATION OF   HO2         0.99284E+01   0.22417E-01
CONCENTRATION OF   O2G         0.11790E+00   0.20890E+00
CONCENTRATION OF   H2G        -0.51337E-01  -0.17844E+00
CONCENTRATION OF   O           0.48204E+01   0.88921E-03
CONCENTRATION OF   H2O         0.19136E-06   0.17390E+01
CONCENTRATION OF   2H2O       -0.61672E-08  -0.23083E+01
```

CORE BOILING   SENSITIVITY RUN STATISTICS

```
                          ADJOINT                RESPONSE
                          -------                --------

REQUIRED RWORK SIZE   =     422                    9902
IWORK SIZE            =      36                     115
NUMBER OF STEPS       =     232                    1070
# OF FUNC.- EVALS.    =     334                    1593
# OF JACOB.- EVALS    =      63                     278
SENSITIVITY JOB TIME  =   26.99 seconds          321.39 seconds
```

```
SENSITIVITY OF O2         IN CORE BOILING      HAS BEEN EVALUATED SUCCESSFULLY!
```

```
            OUTPUT FOR CYCLE    1 AT CORE BYPASS

INITIAL POSITION                  =        0.00000 cm
FINAL POSITION                    =      370.00000 cm
FLOW LENGTH                       =      370.00000 cm
POSITION INCREMENT                =       50.00000 cm
POSITION OF ONSET OF BOILING      =     9999.00000 cm

INLET TEMPERATURE                 =      552.00000 Kelvin
OUTLET TEMPERATURE                =      558.00000 Kelvin
INLET LIQUID VELOCITY             =       19.22000 cm/s
PIPE INTERNAL DIAMETER            =        5.00000 cm
WATER DENSITY                     =        0.74100 g/cc
VAPOR DENSITY                     =        0.03620 g/cc
PRESSURE                          =       70.75000 atm
MASS FlowRate                     =    0.10660D+00 g/s

SENSITIVITY SPECIES   1           = H2O2
SENSITIVITY SPECIES   2           = O2

SensStep                          =      135

GAMMA DOSE RATE MULTIPLIER        =    0.30000D+06 Rad/s
NEUTRON DOSE RATE MULTIPLIER      =    0.41700D+06 Rad/s
GConvert                          =    0.76916D-09

GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
GAMMA COEFFICIENT  0              =    0.51842D-01
GAMMA COEFFICIENT  1              =    0.30207D-01
GAMMA COEFFICIENT  2              =   -0.63661D-03
GAMMA COEFFICIENT  3              =    0.95596D-05
GAMMA COEFFICIENT  4              =   -0.92731D-07
GAMMA COEFFICIENT  5              =    0.56195D-09
GAMMA COEFFICIENT  6              =   -0.20995D-11
GAMMA COEFFICIENT  7              =    0.46781D-14
GAMMA COEFFICIENT  8              =   -0.56819D-17
GAMMA COEFFICIENT  9              =    0.28827D-20

NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
NEUTRON COEFFICIENT  0            =    0.10000D+01
NEUTRON COEFFICIENT  1            =    0.00000D+00
NEUTRON COEFFICIENT  2            =    0.00000D+00
NEUTRON COEFFICIENT  3            =    0.00000D+00
NEUTRON COEFFICIENT  4            =    0.00000D+00
NEUTRON COEFFICIENT  5            =    0.00000D+00
NEUTRON COEFFICIENT  6            =    0.00000D+00
NEUTRON COEFFICIENT  7            =    0.00000D+00
NEUTRON COEFFICIENT  8            =    0.00000D+00
NEUTRON COEFFICIENT  9            =    0.00000D+00

CalcSurf                          =        F
VoidFlag                          =        T
```

```
  CalcSens                                   =        T
  WriteRx                                    =        F
  WritePara                                  =        T

  RADIOLYSIS ABSOLUTE TOLERANCE              =     0.10000D-14
             RELATIVE TOLERANCE              =     0.10000D-04
  ADJOINT    ABSOLUTE TOLERANCE              =     0.10000D-09
             RELATIVE TOLERANCE              =     0.10000D-03
  RESPONSE   ABSOLUTE TOLERANCE              =     0.10000D-14
             RELATIVE TOLERANCE              =     0.10000D-04
```

```
CYCLE     1        POSITION IN CORE BYPASS        =        0.0000 cm
              CONCENTRATIONS[ppb]  AT POSITION =        0.0000 cm

e-        =    0.000000D+00 **     OH-       =     0.000000D+00 **
H2        =    0.700000D+01 **     OH        =     0.000000D+00 **
HO2-      =    0.000000D+00 **     H2O2      =     0.250000D+02 **
O2-       =    0.000000D+00 **     O2        =     0.185000D+03 **
H         =    0.000000D+00 **     H+        =     0.000000D+00 **
HO2       =    0.000000D+00 **     O2G       =     0.000000D+00 **
H2G       =    0.000000D+00 **     O         =     0.000000D+00 **
H2O       =    0.100000D+10 **     2H2O      =     0.823336D+11 **

NO. STEPS                      =      0
TEMPERATURE (K)                =    558.00000
LIQUID VELOCITY (CM/S)         =     19.22000
GAS VELOCITY   (CM/S)          =      0.00000
VOID FRACTION                  =      0.00000
GAMMA DOSE RATE (RAD/S)        =   0.49351D+05
NEUTRON DOSE RATE (RAD/S)      =   0.41700D+06
```

```
CYCLE     1        POSITION IN CORE BYPASS        =     370.0000 cm
              CONCENTRATIONS[ppb]  AT POSITION =     370.0000 cm

e-        =    0.395577D-07 **     OH-       =     0.542862D+02 **
H2        =    0.348197D+02 **     OH        =     0.997196D+00 **
HO2-      =    0.443313D+00 **     H2O2      =     0.494938D+02 **
O2-       =    0.617936D+01 **     O2        =     0.389967D+03 **
H         =    0.617657D-03 **     H+        =     0.339992D+01 **
HO2       =    0.100721D+01 **     O2G       =     0.000000D+00 **
H2G       =    0.000000D+00 **     O         =     0.182557D-01 **
H2O       =    0.996883D+09 **     2H2O      =     0.823367D+11 **

NO. STEPS                      =    482
TEMPERATURE (K)                =    558.00000
LIQUID VELOCITY (CM/S)         =     19.22000
GAS VELOCITY   (CM/S)          =      0.00000
VOID FRACTION                  =      0.00000
GAMMA DOSE RATE (RAD/S)        =   0.49351D+05
NEUTRON DOSE RATE (RAD/S)      =   0.41700D+06
```

```
               RUN STATISTICS FOR CYCLE    1 AT CORE BYPASS
_______________________________________________________________________________

REQUIRED RWORK SIZE   =       422
IWORK SIZE            =        36
NUMBER OF STEPS       =       482
# OF FUNC.- EVALS.    =       700
# OF JACOB.- EVALS    =       118
COMPONENT JOB TIME    =     22.80 seconds

CONCENTRATION PROFILE OF CORE BYPASS      HAS BEEN EVALUATED SUCCESSFULLY!
```

```
           CORE BYPASS      SENSITIVITY RESULTS FOR O2


               ============ ADJOINT RESULTS ============

e-        =   -0.451586D+00 **     OH-       =   -0.926972D-01 **
H2        =   -0.717767D+00 **     OH        =    0.358884D+00 **
HO2-      =    0.625095D+00 **     H2O2      =    0.717792D+00 **
O2-       =    0.983995D+00 **     O2        =    0.435577D+00 **
H         =   -0.358885D+00 **     H+        =    0.926972D-01 **
HO2       =    0.107669D+01 **     O2G       =    0.000000D+00 **
H2G       =    0.000000D+00 **     O         =    0.717768D+00 **
H2O       =   -0.570880D-09 **     2H2O      =   -0.114217D-08 **


                                      ABSOLUTE      RELATIVE
          PARAMETER                 SENSITIVITY   SENSITIVITY
-------------------------           ------------  ------------

RATE CONST OF I 1                    0.12599D-05   0.17002D+00
RATE CONST OF I 2                   -0.12613D-05  -0.17020D+00
RATE CONST OF W 1                    0.24543D-10   0.56664D-03
RATE CONST OF W 2                    0.15025D-17   0.52036D-01
RATE CONST OF W 3                    0.47787D-19   0.16550D-02
RATE CONST OF W 4                   -0.94932D-17  -0.17808D+00
RATE CONST OF W 5                    0.56108D-20   0.80964D-04
RATE CONST OF W 6                   -0.12132D-18  -0.35012D-02
RATE CONST OF W 7                    0.12588D-17   0.34511D-01
RATE CONST OF W 8                    0.24603D-18   0.58223D-06
RATE CONST OF W 9                    0.37317D-15   0.26925D-05
RATE CONST OF W10                    0.13362D-16   0.23137D+00
RATE CONST OF W11                    0.84589D-16   0.14647D+01
RATE CONST OF W12                   -0.12820D-16  -0.36999D-03
RATE CONST OF W13                    0.39792D-19   0.25839D-04
RATE CONST OF W14                   -0.36043D-17  -0.32766D-03
RATE CONST OF W15                   -0.57349D-18  -0.11899D+00
RATE CONST OF W16                    0.12224D-17   0.35278D-01
RATE CONST OF W17                   -0.30779D-13  -0.53240D+01
RATE CONST OF W18                    0.17042D-13   0.89707D+00
RATE CONST OF W19                   -0.38581D-15  -0.80105D-01
RATE CONST OF W20                   -0.64838D-17  -0.17777D+00
RATE CONST OF W21                   -0.86789D-14  -0.10019D-01
RATE CONST OF W22                   -0.58420D-15  -0.41351D-01
RATE CONST OF W23                   -0.87975D-16  -0.11209D-02
RATE CONST OF W24                   -0.59869D-11  -0.15820D+00
RATE CONST OF W25                   -0.42808D-17  -0.12354D+00
RATE CONST OF W26                   -0.27909D-16  -0.80544D+00
RATE CONST OF W27                   -0.11146D-15  -0.94676D-01
RATE CONST OF W28                   -0.23420D-13  -0.55257D+02
RATE CONST OF W29                    0.39478D-05   0.11897D+00
RATE CONST OF W30                    0.13817D-18   0.99692D-02
RATE CONST OF W31                    0.37486D-08   0.55283D+02
RATE CONST OF W32                   -0.50346D-06  -0.52170D-03
```

```
    RATE CONST OF W33              0.12534D-17   0.39790D-01
    RATE CONST OF W34             -0.33066D-19  -0.95430D-03
    RATE CONST OF W35              0.98643D-16   0.77727D-05
    RATE CONST OF W36             -0.10671D-08  -0.29258D+01
    RATE CONST OF W37              0.98853D-16   0.28529D+01
    RATE CONST OF W38             -0.63929D-15  -0.29349D-03
    RATE CONST OF W39              0.23257D-15   0.11172D-02
    RATE CONST OF W40             -0.10423D-19  -0.30082D-03
    GAMMA   G-VALUE OF e-         -0.20747D-02  -0.11199D+03
    NEUTRON G-VALUE OF e-         -0.35738D-02  -0.19290D+03
    GAMMA   G-VALUE OF H2         -0.30746D-02  -0.82978D+03
    NEUTRON G-VALUE OF H2         -0.52994D-02  -0.14302D+04
    GAMMA   G-VALUE OF OH          0.15396D-02   0.14543D+03
    NEUTRON G-VALUE OF OH          0.26538D-02   0.25067D+03
    GAMMA   G-VALUE OF H          -0.15421D-02  -0.62426D+02
    NEUTRON G-VALUE OF H          -0.26589D-02  -0.10764D+03
    GAMMA   G-VALUE OF H+          0.52837D-03   0.28520D+02
    NEUTRON G-VALUE OF H+          0.90486D-03   0.48841D+02
    GAMMA   G-VALUE OF O           0.30831D-02   0.83208D+03
    NEUTRON G-VALUE OF O           0.53148D-02   0.14344D+04
    CONCENTRATION OF   e-         -0.16358D+05  -0.13510D+00
    CONCENTRATION OF   OH-        -0.17274D+03  -0.55367D+02
    CONCENTRATION OF   H2         -0.35647D+01  -0.57198D+01
    CONCENTRATION OF   OH          0.19146D+03   0.12183D+01
    CONCENTRATION OF   HO2-        0.45703D+05   0.57136D+02
    CONCENTRATION OF   H2O2       -0.42100D+03  -0.56957D+02
    CONCENTRATION OF   O2-         0.69637D+02   0.12360D+01
    CONCENTRATION OF   O2          0.38908D+01   0.38908D+01
    CONCENTRATION OF   H          -0.14974D+05  -0.11289D+01
    CONCENTRATION OF   H+          0.39731D+00   0.13490D+00
    CONCENTRATION OF   HO2         0.72047D+02   0.20194D+00
    CONCENTRATION OF   O           0.53496D+02   0.60850D-02
    CONCENTRATION OF   H2O         0.99540D-05   0.55265D+02
    CONCENTRATION OF   2H2O       -0.74168D-08  -0.16961D+01

________________________________________________________________________________

                 CORE BYPASS     SENSITIVITY RUN STATISTICS

________________________________________________________________________________

                                   ADJOINT                      RESPONSE
                                   -------                      --------

REQUIRED RWORK SIZE    =          422                          9902
IWORK SIZE             =           36                           115
NUMBER OF STEPS        =          213                           287
# OF FUNC.- EVALS.     =          261                           436
# OF JACOB.- EVALS     =           40                            86
SENSITIVITY JOB TIME   =        20.36 seconds                 89.52 seconds

SENSITIVITY OF O2      IN CORE BYPASS      HAS BEEN EVALUATED SUCCESSFULLY!
```

```
                    OUTPUT FOR CYCLE    1 AT UPPER PLENUM


      INITIAL POSITION                  =      370.00000 cm
      FINAL POSITION                    =      410.00000 cm
      FLOW LENGTH                       =       40.00000 cm
      POSITION INCREMENT                =       10.00000 cm
      POSITION OF ONSET OF BOILING      =       66.00000 cm

      INLET TEMPERATURE                 =      558.00000 Kelvin
      OUTLET TEMPERATURE                =      555.00000 Kelvin
      INLET LIQUID VELOCITY             =       20.00000 cm/s
      PIPE INTERNAL DIAMETER            =        5.00000 cm
      WATER DENSITY                     =        0.74100 g/cc
      VAPOR DENSITY                     =        0.03620 g/cc
      PRESSURE                          =       70.75000 atm
      MASS FlowRate                     =    0.11050D+01 g/s

      GAMMA DOSE RATE MULTIPLIER        =    0.30000D+06 Rad/s
      NEUTRON DOSE RATE MULTIPLIER      =    0.41700D+06 Rad/s
      GConvert                          =    0.76916D-09

      GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
      GAMMA COEFFICIENT  0              =    0.10000D-02

      NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
      NEUTRON COEFFICIENT  0            =    0.10000D-02

      VOID FRACTION FUNCTION COEFFICIENTS
      VOID FRACTION  COEFFICIENT  0     =    0.63873D+00
      VOID FRACTION  COEFFICIENT  1     =   -0.14325D-03

      CalcSurf                          =        F
      VoidFlag                          =        T
      CalcSens                          =        F
      WriteRx                           =        F
      WritePara                         =        T

      RADIOLYSIS ABSOLUTE TOLERANCE     =    0.10000D-14
                 RELATIVE TOLERANCE     =    0.10000D-04

    CYCLE     1         POSITION IN UPPER PLENUM      =       0.0000 cm
                    CONCENTRATIONS[ppb]  AT POSITION =     370.0000 cm

    e-      =     0.602382D-07 **     OH-      =     0.552001D+02 **
    H2      =     0.177459D+02 **     OH       =     0.201113D+01 **
    HO2-    =     0.179522D+00 **     H2O2     =     0.198072D+02 **
    O2-     =     0.321374D+01 **     O2       =     0.224632D+03 **
    H       =     0.109543D-02 **     H+       =     0.335305D+01 **
    HO2     =     0.519220D+00 **     O2G      =     0.364294D+03 **
    H2G     =     0.429573D+02 **     O        =     0.180546D-01 **
```

```
    H2O       =    0.100000D+10 **     2H2O      =    0.823336D+11 **

    O2G       =    0.297D-03 ATM
    H2G       =    0.560D-03 ATM

    NO. STEPS                    =       0
    TEMPERATURE (K)              =     558.00000
    LIQUID VELOCITY (CM/S)       =      42.83996
    GAS VELOCITY   (CM/S)        =      78.72172
    VOID FRACTION                =       0.58573
    GAMMA DOSE RATE (RAD/S)      =    0.49351D+05
    NEUTRON DOSE RATE (RAD/S)    =    0.41700D+06
```

```
    CYCLE     1         POSITION IN UPPER PLENUM     =     40.0000 cm
                   CONCENTRATIONS[ppb]  AT POSITION =    410.0000 cm

    e-        =    0.985198D-10 **     OH-       =    0.556405D+02 **
    H2        =    0.149466D+02 **     OH        =    0.499621D-02 **
    HO2-      =    0.331761D+00 **     H2O2      =    0.365326D+02 **
    O2-       =    0.141466D+01 **     O2        =    0.197798D+03 **
    H         =    0.256401D-05 **     H+        =    0.332723D+01 **
    HO2       =    0.224809D+00 **     O2G       =    0.380312D+03 **
    H2G       =    0.449454D+02 **     O         =    0.288543D-04 **
    H2O       =    0.100000D+10 **     2H2O      =    0.823336D+11 **

    O2G       =    0.310D-03 ATM
    H2G       =    0.586D-03 ATM

    NO. STEPS                    =     239
    TEMPERATURE (K)              =     555.00000
    LIQUID VELOCITY (CM/S)       =      42.41951
    GAS VELOCITY   (CM/S)        =      77.06845
    VOID FRACTION                =       0.58000
    GAMMA DOSE RATE (RAD/S)      =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)    =    0.41700D+03
```

```
               RUN STATISTICS FOR CYCLE    1 AT UPPER PLENUM
```

```
REQUIRED RWORK SIZE   =       422
IWORK SIZE            =        36
NUMBER OF STEPS       =       239
# OF FUNC.- EVALS.    =       293
# OF JACOB.- EVALS    =        39
COMPONENT JOB TIME    =      9.96 seconds

CONCENTRATION PROFILE OF UPPER PLENUM     HAS BEEN EVALUATED SUCCESSFULLY!
```

```
OUTPUT FOR CYCLE    1 AT FEEDWATER
```

```
INITIAL POSITION                  =      410.00000 cm
FINAL POSITION                    =      411.00000 cm
FLOW LENGTH                       =        1.00000 cm
POSITION INCREMENT                =       10.00000 cm
POSITION OF ONSET OF BOILING      =     9999.00000 cm

INLET TEMPERATURE                 =      555.00000 Kelvin
OUTLET TEMPERATURE                =      555.00000 Kelvin
INLET LIQUID VELOCITY             =  1000000.00000 cm/s
PIPE INTERNAL DIAMETER            =        5.00000 cm
WATER DENSITY                     =        0.74100 g/cc
VAPOR DENSITY                     =        0.03620 g/cc
PRESSURE                          =       70.75000 atm
MASS FlowRate                     =    0.12500D+00 g/s

GAMMA DOSE RATE MULTIPLIER        =    0.30000D+06 Rad/s
NEUTRON DOSE RATE MULTIPLIER      =    0.41700D+06 Rad/s
GConvert                          =    0.76916D-09

GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
GAMMA COEFFICIENT  0              =    0.10000D-02

NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
NEUTRON COEFFICIENT  0            =    0.10000D-02

CalcSurf                          =        F
VoidFlag                          =        T
CalcSens                          =        F
WriteRx                           =        F
WritePara                         =        T

RADIOLYSIS ABSOLUTE TOLERANCE     =    0.10000D-14
           RELATIVE TOLERANCE     =    0.10000D-04
```

```
CYCLE    1        POSITION IN FEEDWATER          =     0.0000 cm
               CONCENTRATIONS[ppb]  AT POSITION =   410.0000 cm

e-      =    0.000000D+00 **    OH-      =    0.000000D+00 **
H2      =    0.000000D+00 **    OH       =    0.000000D+00 **
HO2-    =    0.000000D+00 **    H2O2     =    0.000000D+00 **
O2-     =    0.000000D+00 **    O2       =    0.350001D+02 **
H       =    0.000000D+00 **    H+       =    0.000000D+00 **
HO2     =    0.000000D+00 **    O2G      =    0.000000D+00 **
H2G     =    0.000000D+00 **    O        =    0.000000D+00 **
H2O     =    0.100000D+10 **    2H2O     =    0.823336D+11 **

NO. STEPS                =        0
```

```
    TEMPERATURE (K)             =      555.00000
    LIQUID VELOCITY (CM/S)      =  1000000.00000
    GAS VELOCITY  (CM/S)        =        0.00000
    VOID FRACTION               =        0.00000
    GAMMA DOSE RATE (RAD/S)     =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)   =    0.41700D+03
```

```
    CYCLE     1         POSITION IN FEEDWATER          =      1.0000 cm
                     CONCENTRATIONS[ppb]  AT POSITION =    411.0000 cm

    e-     =    0.114723D-09 **    OH-     =    0.560316D+02 **
    H2     =    0.297698D-05 **    OH      =    0.249929D-04 **
    HO2-   =    0.122332D-13 **    H2O2    =    0.155902D-13 **
    O2-    =    0.101490D-05 **    O2      =    0.350001D+02 **
    H      =    0.271933D-06 **    H+      =    0.329598D+01 **
    HO2    =    0.275782D-06 **    O2G     =    0.000000D+00 **
    H2G    =    0.000000D+00 **    O       =    0.162223D-04 **
    H2O    =    0.100000D+10 **    2H2O    =    0.823336D+11 **

    NO. STEPS                   =        49
    TEMPERATURE (K)             =      555.00000
    LIQUID VELOCITY (CM/S)      =  1000000.00000
    GAS VELOCITY  (CM/S)        =        0.00000
    VOID FRACTION               =        0.00000
    GAMMA DOSE RATE (RAD/S)     =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)   =    0.41700D+03
```

```
              RUN STATISTICS FOR CYCLE     1 AT FEEDWATER
```

```
REQUIRED RWORK SIZE    =       422
IWORK SIZE             =        36
NUMBER OF STEPS        =        49
# OF FUNC.- EVALS.     =        60
# OF JACOB.- EVALS     =        11
COMPONENT JOB TIME     =      4.34  seconds

CONCENTRATION PROFILE OF FEEDWATER        HAS BEEN EVALUATED SUCCESSFULLY!
```

```
                   OUTPUT FOR CYCLE    1 AT MIXING PLENUM

      INITIAL POSITION                   =      410.00000 cm
      FINAL POSITION                     =      540.00000 cm
      FLOW LENGTH                        =      130.00000 cm
      POSITION INCREMENT                 =       20.00000 cm
      POSITION OF ONSET OF BOILING       =       66.00000 cm

      INLET TEMPERATURE                  =      555.00000 Kelvin
      OUTLET TEMPERATURE                 =      552.00000 Kelvin
      INLET LIQUID VELOCITY              =       30.23000 cm/s
      PIPE INTERNAL DIAMETER             =        5.00000 cm
      WATER DENSITY                      =        0.74100 g/cc
      VAPOR DENSITY                      =        0.03620 g/cc
      PRESSURE                           =       70.75000 atm
      MASS FlowRate                      =    0.69000D+00 g/s

      GAMMA DOSE RATE MULTIPLIER         =    0.30000D+06 Rad/s
      NEUTRON DOSE RATE MULTIPLIER       =    0.41700D+06 Rad/s
      GConvert                           =    0.76916D-09

      GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
      GAMMA COEFFICIENT  0               =    0.10000D-03

      NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
      NEUTRON COEFFICIENT  0             =    0.10000D-03

      VOID FRACTION FUNCTION COEFFICIENTS
      VOID FRACTION  COEFFICIENT  0      =    0.10353D-01
      VOID FRACTION  COEFFICIENT  1      =   -0.19154D-04

      CalcSurf                           =        F
      VoidFlag                           =        T
      CalcSens                           =        F
      WriteRx                            =        F
      WritePara                          =        T

      RADIOLYSIS ABSOLUTE TOLERANCE      =    0.10000D-14
                 RELATIVE TOLERANCE      =    0.10000D-04

    CYCLE      1        POSITION IN MIXING PLENUM     =       0.0000 cm
                      CONCENTRATIONS[ppb]  AT POSITION =     410.0000 cm

    e-       =     0.100166D-09 **    OH-      =     0.556802D+02 **
    H2       =     0.134276D+02 **    OH       =     0.449100D-02 **
    HO2-     =     0.298045D+00 **    H2O2     =     0.328200D+02 **
    O2-      =     0.127089D+01 **    O2       =     0.181254D+03 **
    H        =     0.233108D-05 **    H+       =     0.332405D+01 **
    HO2      =     0.201962D+00 **    O2G      =     0.380312D+03 **
    H2G      =     0.449454D+02 **    O        =     0.275705D-04 **
```

```
H2O        =    0.100000D+10 **      2H2O       =    0.823336D+11 **

O2G        =    0.310D-03 ATM
H2G        =    0.586D-03 ATM

NO. STEPS                      =       0
TEMPERATURE (K)                =     555.00000
LIQUID VELOCITY (CM/S)         =      30.30118
GAS VELOCITY   (CM/S)          =      37.37660
VOID FRACTION                  =       0.00250
GAMMA DOSE RATE (RAD/S)        =    0.30000D+03
NEUTRON DOSE RATE (RAD/S)      =    0.41700D+03
------------------------------------------------------------------------

CYCLE      1        POSITION IN MIXING PLENUM       =    130.0000 cm
                    CONCENTRATIONS[ppb]  AT POSITION =    540.0000 cm

e-         =    0.107478D-10 **      OH-        =    0.558284D+02 **
H2         =    0.125865D+02 **      OH         =    0.775042D-03 **
HO2-       =    0.418208D+00 **      H2O2       =    0.462441D+02 **
O2-        =    0.630371D+00 **      O2         =    0.168759D+03 **
H          =    0.379874D-06 **      H+         =    0.331640D+01 **
HO2        =    0.998457D-01 **      O2G        =    0.228867D+04 **
H2G        =    0.313170D+03 **      O          =    0.293047D-05 **
H2O        =    0.100011D+10 **      2H2O       =    0.823335D+11 **

O2G        =    0.186D-02 ATM
H2G        =    0.408D-02 ATM

NO. STEPS                      =     249
TEMPERATURE (K)                =     552.00000
LIQUID VELOCITY (CM/S)         =      30.23028
GAS VELOCITY   (CM/S)          =      37.26747
VOID FRACTION                  =       0.00001
GAMMA DOSE RATE (RAD/S)        =    0.30000D+02
NEUTRON DOSE RATE (RAD/S)      =    0.41700D+02
------------------------------------------------------------------------

               RUN STATISTICS FOR CYCLE    1 AT MIXING PLENUM

------------------------------------------------------------------------


REQUIRED RWORK SIZE    =       422
IWORK SIZE             =        36
NUMBER OF STEPS        =       249
# OF FUNC.- EVALS.     =       355
# OF JACOB.- EVALS     =        52
COMPONENT JOB TIME     =     11.61 seconds

CONCENTRATION PROFILE OF MIXING PLENUM    HAS BEEN EVALUATED SUCCESSFULLY!
```

```
OUTPUT FOR CYCLE    1 AT UP DOWNCOMER1

INITIAL POSITION                 =      540.00000 cm
FINAL POSITION                   =      580.00000 cm
FLOW LENGTH                      =       40.00000 cm
POSITION INCREMENT               =       20.00000 cm
POSITION OF ONSET OF BOILING     =    99999.00000 cm

INLET TEMPERATURE                =      552.00000 Kelvin
OUTLET TEMPERATURE               =      552.00000 Kelvin
INLET LIQUID VELOCITY            =       40.00000 cm/s
PIPE INTERNAL DIAMETER           =        5.00000 cm
WATER DENSITY                    =        0.74100 g/cc
VAPOR DENSITY                    =        0.03620 g/cc
PRESSURE                         =       70.75000 atm
MASS FlowRate                    =    0.31000D+00 g/s

GAMMA DOSE RATE MULTIPLIER       =    0.30000D+06 Rad/s
NEUTRON DOSE RATE MULTIPLIER     =    0.41700D+06 Rad/s
GConvert                         =    0.76916D-09

GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
GAMMA COEFFICIENT  0             =    0.10000D-01

NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
NEUTRON COEFFICIENT  0           =    0.10000D-02

CalcSurf                         =        F
VoidFlag                         =        T
CalcSens                         =        F
WriteRx                          =        F
WritePara                        =        T

RADIOLYSIS ABSOLUTE TOLERANCE    =    0.10000D-14
           RELATIVE TOLERANCE    =    0.10000D-04


CYCLE     1       POSITION IN UP DOWNCOMER1     =      0.0000 cm
              CONCENTRATIONS[ppb]  AT POSITION  =    540.0000 cm

e-      =   0.107478D-10 **     OH-     =   0.558284D+02 **
H2      =   0.125865D+02 **     OH      =   0.775042D-03 **
HO2-    =   0.418208D+00 **     H2O2    =   0.462441D+02 **
O2-     =   0.630371D+00 **     O2      =   0.168759D+03 **
H       =   0.379874D-06 **     H+      =   0.331640D+01 **
HO2     =   0.998457D-01 **     O2G     =   0.228867D+04 **
H2G     =   0.000000D+00 **     O       =   0.000000D+00 **
H2O     =   0.100000D+10 **     2H2O    =   0.823336D+11 **

NO. STEPS                   =        0
```

```
    TEMPERATURE (K)               =      552.00000
    LIQUID VELOCITY (CM/S)        =       40.00000
    GAS VELOCITY  (CM/S)          =        0.00000
    VOID FRACTION                 =        0.00000
    GAMMA DOSE RATE (RAD/S)       =    0.30000D+02
    NEUTRON DOSE RATE (RAD/S)     =    0.41700D+02
```

```
    CYCLE     1         POSITION IN UP DOWNCOMER1      =     40.0000 cm
                     CONCENTRATIONS[ppb]  AT POSITION =    580.0000 cm

    e-        =     0.522508D-09 **     OH-       =     0.555133D+02 **
    H2        =     0.113169D+02 **     OH        =     0.251769D-01 **
    HO2-      =     0.497462D+00 **     H2O2      =     0.553136D+02 **
    O2-       =     0.173743D+01 **     O2        =     0.153326D+03 **
    H         =     0.130023D-04 **     H+        =     0.333486D+01 **
    HO2       =     0.276757D+00 **     O2G       =     0.228867D+04 **
    H2G       =     0.000000D+00 **     O         =     0.139491D-03 **
    H2O       =     0.100000D+10 **     2H2O      =     0.823336D+11 **

    NO. STEPS                     =     148
    TEMPERATURE (K)               =      552.00000
    LIQUID VELOCITY (CM/S)        =       40.00000
    GAS VELOCITY  (CM/S)          =        0.00000
    VOID FRACTION                 =        0.00000
    GAMMA DOSE RATE (RAD/S)       =    0.30000D+04
    NEUTRON DOSE RATE (RAD/S)     =    0.41700D+03
```

```
                 RUN STATISTICS FOR CYCLE    1 AT UP DOWNCOMER1
```

```
REQUIRED RWORK SIZE   =       422
IWORK SIZE            =        36
NUMBER OF STEPS       =       148
# OF FUNC.- EVALS.    =       182
# OF JACOB.- EVALS    =        32
COMPONENT JOB TIME    =      7.25 seconds

CONCENTRATION PROFILE OF UP DOWNCOMER1    HAS BEEN EVALUATED SUCCESSFULLY!
```

```
                      OUTPUT FOR CYCLE     1 AT LO DOWNCOMER1


    INITIAL POSITION                    =      540.00000 cm
    FINAL POSITION                      =      620.00000 cm
    FLOW LENGTH                         =       80.00000 cm
    POSITION INCREMENT                  =       20.00000 cm
    POSITION OF ONSET OF BOILING        =    99999.00000 cm

    INLET TEMPERATURE                   =      552.00000 Kelvin
    OUTLET TEMPERATURE                  =      552.00000 Kelvin
    INLET LIQUID VELOCITY               =       24.24200 cm/s
    PIPE INTERNAL DIAMETER              =        5.00000 cm
    WATER DENSITY                       =        0.74100 g/cc
    VAPOR DENSITY                       =        0.03620 g/cc
    PRESSURE                            =       70.75000 atm
    MASS FlowRate                       =    0.31000D+00 g/s

    GAMMA DOSE RATE MULTIPLIER          =    0.30000D+06 Rad/s
    NEUTRON DOSE RATE MULTIPLIER        =    0.41700D+06 Rad/s
    GConvert                            =    0.76916D-09

    GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
    GAMMA COEFFICIENT  0                =    0.10000D-01

    NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
    NEUTRON COEFFICIENT  0              =    0.10000D-02

    CalcSurf                            =        F
    VoidFlag                            =        T
    CalcSens                            =        F
    WriteRx                             =        F
    WritePara                           =        T

    RADIOLYSIS ABSOLUTE TOLERANCE       =    0.10000D-14
               RELATIVE TOLERANCE       =    0.10000D-04


  CYCLE     1       POSITION IN LO DOWNCOMER1      =      0.0000 cm
                  CONCENTRATIONS[ppb]  AT POSITION =    540.0000 cm

  e-     =     0.180824D-09 **     OH-     =    0.556990D+02 **
  H2     =     0.119517D+02 **     OH      =    0.897234D-02 **
  HO2-   =     0.470654D+00 **     H2O2    =    0.521666D+02 **
  O2-    =     0.105903D+01 **     O2      =    0.160493D+03 **
  H      =     0.461789D-05 **     H+      =    0.332377D+01 **
  HO2    =     0.168334D+00 **     O2G     =    0.000000D+00 **
  H2G    =     0.000000D+00 **     O       =    0.483432D-04 **
  H2O    =     0.100001D+10 **     2H2O    =    0.823336D+11 **

  NO. STEPS                 =        0
```

```
TEMPERATURE (K)             =      552.00000
LIQUID VELOCITY (CM/S)      =       24.24200
GAS VELOCITY  (CM/S)        =        0.00000
VOID FRACTION               =        0.00000
GAMMA DOSE RATE (RAD/S)     =    0.30000D+02
NEUTRON DOSE RATE (RAD/S)   =    0.41700D+00
```

```
CYCLE     1        POSITION IN LO DOWNCOMER1     =     80.0000 cm
               CONCENTRATIONS[ppb]  AT POSITION =    620.0000 cm

e-        =     0.549851D-09 **     OH-       =     0.555753D+02 **
H2        =     0.939352D+01 **     OH        =     0.292640D-01 **
HO2-      =     0.468551D+00 **     H2O2      =     0.520411D+02 **
O2-       =     0.153018D+01 **     O2        =     0.139670D+03 **
H         =     0.139104D-04 **     H+        =     0.333115D+01 **
HO2       =     0.243477D+00 **     O2G       =     0.000000D+00 **
H2G       =     0.000000D+00 **     O         =     0.139512D-03 **
H2O       =     0.100001D+10 **     2H2O      =     0.823336D+11 **

NO. STEPS                   =      150
TEMPERATURE (K)             =      552.00000
LIQUID VELOCITY (CM/S)      =       24.24200
GAS VELOCITY  (CM/S)        =        0.00000
VOID FRACTION               =        0.00000
GAMMA DOSE RATE (RAD/S)     =    0.30000D+04
NEUTRON DOSE RATE (RAD/S)   =    0.41700D+03
```

```
           RUN STATISTICS FOR CYCLE    1 AT LO DOWNCOMER1
```

```
REQUIRED RWORK SIZE   =       422
IWORK SIZE            =        36
NUMBER OF STEPS       =       150
# OF FUNC.- EVALS.    =       180
# OF JACOB.- EVALS    =        31
COMPONENT JOB TIME    =      7.30 seconds

CONCENTRATION PROFILE OF LO DOWNCOMER1    HAS BEEN EVALUATED SUCCESSFULLY!
```

```
------------------------------------------------------------------------

                 OUTPUT FOR CYCLE    1 AT RECIRC

------------------------------------------------------------------------

    INITIAL POSITION                =      620.00000 cm
    FINAL POSITION                  =      750.00000 cm
    FLOW LENGTH                     =      130.00000 cm
    POSITION INCREMENT              =       20.00000 cm
    POSITION OF ONSET OF BOILING    =    99999.00000 cm

    INLET TEMPERATURE               =      552.00000 Kelvin
    OUTLET TEMPERATURE              =      552.00000 Kelvin
    INLET LIQUID VELOCITY           =       30.23000 cm/s
    PIPE INTERNAL DIAMETER          =        5.00000 cm
    WATER DENSITY                   =        0.74100 g/cc
    VAPOR DENSITY                   =        0.03620 g/cc
    PRESSURE                        =       70.75000 atm
    MASS FlowRate                   =    0.31000D+00 g/s

    SENSITIVITY SPECIES   1         = H2O2
    SENSITIVITY SPECIES   2         = O2

    SensStep                        =      153

    GAMMA DOSE RATE MULTIPLIER      =    0.30000D+06 Rad/s
    NEUTRON DOSE RATE MULTIPLIER    =    0.41700D+06 Rad/s
    GConvert                        =    0.76916D-09

    GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
    GAMMA COEFFICIENT  0            =    0.00000D+00

    NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
    NEUTRON COEFFICIENT  0          =    0.00000D+00

    CalcSurf                        =        F
    VoidFlag                        =        T
    CalcSens                        =        T
    WriteRx                         =        F
    WritePara                       =        T

    RADIOLYSIS ABSOLUTE  TOLERANCE  =    0.10000D-14
               RELATIVE  TOLERANCE  =    0.10000D-04
    ADJOINT    ABSOLUTE  TOLERANCE  =    0.10000D-09
               RELATIVE  TOLERANCE  =    0.10000D-03
    RESPONSE   ABSOLUTE  TOLERANCE  =    0.10000D-14
               RELATIVE  TOLERANCE  =    0.10000D-04

------------------------------------------------------------------------
 CYCLE     1        POSITION IN RECIRC              =       0.0000 cm
                 CONCENTRATIONS[ppb]  AT POSITION =     620.0000 cm

 e-        =     0.189901D-09 **     OH-      =     0.557074D+02 **
```

```
    H2       =    0.104514D+02 **    OH       =    0.103532D-01 **
    HO2-     =    0.545697D+00 **    H2O2     =    0.604790D+02 **
    O2-      =    0.977894D+00 **    O2       =    0.144612D+03 **
    H        =    0.495905D-05 **    H+       =    0.332400D+01 **
    HO2      =    0.155383D+00 **    O2G      =    0.000000D+00 **
    H2G      =    0.000000D+00 **    O        =    0.483493D-04 **
    H2O      =    0.100023D+10 **    2H2O     =    0.823334D+11 **

    NO. STEPS                    =        0
    TEMPERATURE (K)              =      552.00000
    LIQUID VELOCITY (CM/S)       =       30.23000
    GAS VELOCITY  (CM/S)         =        0.00000
    VOID FRACTION                =        0.00000
    GAMMA DOSE RATE (RAD/S)      =    0.30000D+02
    NEUTRON DOSE RATE (RAD/S)    =    0.41700D+00
________________________________________________________________________________

    CYCLE    1         POSITION IN RECIRC             =    130.0000 cm
                  CONCENTRATIONS[ppb]  AT POSITION =    750.0000 cm

    e-       =    0.622895D-14 **    OH-      =    0.558574D+02 **
    H2       =    0.102654D+02 **    OH       =    0.786641D-04 **
    HO2-     =    0.545447D+00 **    H2O2     =    0.601648D+02 **
    O2-      =    0.190379D+00 **    O2       =    0.143958D+03 **
    H        =    0.326262D-07 **    H+       =    0.330821D+01 **
    HO2      =    0.300797D-01 **    O2G      =    0.000000D+00 **
    H2G      =    0.000000D+00 **    O        =    0.494440D-16 **
    H2O      =    0.998159D+09 **    2H2O     =    0.823354D+11 **

    NO. STEPS                    =      240
    TEMPERATURE (K)              =      552.00000
    LIQUID VELOCITY (CM/S)       =       30.23000
    GAS VELOCITY  (CM/S)         =        0.00000
    VOID FRACTION                =        0.00000
    GAMMA DOSE RATE (RAD/S)      =    0.00000D+00
    NEUTRON DOSE RATE (RAD/S)    =    0.00000D+00

________________________________________________________________________________

              RUN STATISTICS FOR CYCLE    1 AT RECIRC

________________________________________________________________________________


REQUIRED RWORK SIZE    =       422
IWORK SIZE             =        36
NUMBER OF STEPS        =       240
# OF FUNC.- EVALS.     =       333
# OF JACOB.- EVALS     =        55
COMPONENT JOB TIME     =     11.62 seconds

CONCENTRATION PROFILE OF RECIRC          HAS BEEN EVALUATED SUCCESSFULLY!
```

```
          RECIRC              SENSITIVITY RESULTS FOR O2


            ============= ADJOINT RESULTS =============

e-       =   -0.384494D+00 **     OH-      =     0.397681D-05 **
H2       =   -0.394347D-02 **     OH       =    -0.400419D-01 **
HO2-     =   -0.128414D-01 **     H2O2     =    -0.128454D-01 **
O2-      =    0.565971D+00 **     O2       =    -0.185274D-04 **
H        =   -0.433945D+00 **     H+       =    -0.397719D-05 **
HO2      =    0.565967D+00 **     O2G      =     0.000000D+00 **
H2G      =    0.000000D+00 **     O        =    -0.795751D-01 **
H2O      =   -0.717518D-12 **     2H2O     =    -0.119067D-11 **


                                      ABSOLUTE       RELATIVE
         PARAMETER                   SENSITIVITY    SENSITIVITY
---------------------------         ------------   ------------


RATE CONST OF I 1                   -0.28840D-10   -0.92307D-05
RATE CONST OF I 2                    0.28850D-10    0.92337D-05
RATE CONST OF W 1                   -0.12358D-14   -0.65708D-07
RATE CONST OF W 2                   -0.73902D-22   -0.58940D-05
RATE CONST OF W 3                    0.76803D-25    0.61253D-08
RATE CONST OF W 4                    0.28045D-21    0.12115D-04
RATE CONST OF W 5                    0.22224D-25    0.73854D-09
RATE CONST OF W 6                   -0.30461D-24   -0.20245D-07
RATE CONST OF W 7                   -0.95110D-22   -0.60051D-05
RATE CONST OF W 8                    0.13361D-24    0.72813D-12
RATE CONST OF W 9                    0.50919D-22    0.84605D-12
RATE CONST OF W10                    0.94411D-20    0.37648D-03
RATE CONST OF W11                    0.61556D-19    0.24546D-02
RATE CONST OF W12                    0.75864D-20    0.50420D-06
RATE CONST OF W13                    0.51381D-25    0.76835D-10
RATE CONST OF W14                    0.10739D-21    0.22482D-07
RATE CONST OF W15                   -0.57360D-18   -0.27406D+00
RATE CONST OF W16                    0.12224D-17    0.81242D-01
RATE CONST OF W17                   -0.30780D-13   -0.12070D+02
RATE CONST OF W18                    0.17042D-13    0.20582D+01
RATE CONST OF W19                   -0.38596D-15   -0.18184D+00
RATE CONST OF W20                   -0.64828D-17   -0.40931D+00
RATE CONST OF W21                   -0.86638D-14   -0.23033D-01
RATE CONST OF W22                   -0.58340D-15   -0.93703D-01
RATE CONST OF W23                   -0.87853D-16   -0.25399D-02
RATE CONST OF W24                   -0.59780D-11   -0.35846D+00
RATE CONST OF W25                   -0.42808D-17   -0.28451D+00
RATE CONST OF W26                   -0.27908D-16   -0.18548D+01
RATE CONST OF W27                   -0.11146D-15   -0.21483D+00
RATE CONST OF W28                   -0.26810D-13   -0.14354D+03
RATE CONST OF W29                    0.39486D-05    0.27403D+00
RATE CONST OF W30                    0.13793D-18    0.22918D-01
RATE CONST OF W31                    0.42831D-08    0.14546D+03
RATE CONST OF W32                   -0.63169D-05   -0.15263D-01
```

```
RATE CONST OF W33               0.12534D-17   0.91631D-01
RATE CONST OF W34              -0.33066D-19  -0.21976D-02
RATE CONST OF W35               0.98643D-16   0.15625D-04
RATE CONST OF W36              -0.10671D-08  -0.67377D+01
RATE CONST OF W37               0.98853D-16   0.65699D+01
RATE CONST OF W38              -0.63929D-15  -0.64147D-03
RATE CONST OF W39               0.23257D-15   0.25429D-02
RATE CONST OF W40              -0.10423D-19  -0.69275D-03
GAMMA   G-VALUE OF e-          -0.20747D-02  -0.26562D+03
NEUTRON G-VALUE OF e-          -0.35738D-02  -0.45754D+03
GAMMA   G-VALUE OF H2          -0.30746D-02  -0.19682D+04
NEUTRON G-VALUE OF H2          -0.52994D-02  -0.33923D+04
GAMMA   G-VALUE OF OH           0.15396D-02   0.34493D+03
NEUTRON G-VALUE OF OH           0.26538D-02   0.59457D+03
GAMMA   G-VALUE OF H           -0.15421D-02  -0.14807D+03
NEUTRON G-VALUE OF H           -0.26589D-02  -0.25531D+03
GAMMA   G-VALUE OF H+           0.52837D-03   0.67645D+02
NEUTRON G-VALUE OF H+           0.90486D-03   0.11585D+03
GAMMA   G-VALUE OF O            0.30831D-02   0.19736D+04
NEUTRON G-VALUE OF O            0.53148D-02   0.34021D+04
CONCENTRATION OF   e-          -0.17227D+05  -0.50078D-07
CONCENTRATION OF   OH-         -0.19605D+03  -0.15268D+03
CONCENTRATION OF   H2          -0.35650D+01  -0.42786D+01
CONCENTRATION OF   OH           0.19243D+03   0.21035D-03
CONCENTRATION OF   HO2-         0.50415D+05   0.19423D+03
CONCENTRATION OF   H2O2        -0.46507D+03  -0.19169D+03
CONCENTRATION OF   O2-          0.70620D+02   0.98686D-01
CONCENTRATION OF   O2           0.38909D+01   0.38909D+01
CONCENTRATION OF   H           -0.15642D+05  -0.12680D-03
CONCENTRATION OF   H+           0.39721D+00   0.31143D+00
CONCENTRATION OF   HO2          0.73026D+02   0.15624D-01
CONCENTRATION OF   O            0.55104D+02   0.36396D-16
CONCENTRATION OF   H2O          0.11336D-04   0.14889D+03
CONCENTRATION OF   2H2O        -0.74143D-08  -0.40218D+01

---------------------------------------------------------------------------------

            RECIRC          SENSITIVITY RUN STATISTICS

---------------------------------------------------------------------------------

                             ADJOINT                       RESPONSE
                             -------                       --------

REQUIRED RWORK SIZE   =        422                          9902
IWORK SIZE            =         36                           115
NUMBER OF STEPS       =        284                           314
# OF FUNC.- EVALS.    =        422                           501
# OF JACOB.- EVALS    =         85                            95
SENSITIVITY JOB TIME  =      35.54 seconds                 97.84 seconds

SENSITIVITY OF O2       IN RECIRC          HAS BEEN EVALUATED SUCCESSFULLY!
```

```
------------------------------------------------------------------------

                OUTPUT FOR CYCLE    1 AT JET PUMP

------------------------------------------------------------------------

    INITIAL POSITION                   =      750.00000 cm
    FINAL POSITION                     =      950.00000 cm
    FLOW LENGTH                        =      200.00000 cm
    POSITION INCREMENT                 =       50.00000 cm
    POSITION OF ONSET OF BOILING       =    99999.00000 cm

    INLET TEMPERATURE                  =      552.00000 Kelvin
    OUTLET TEMPERATURE                 =      552.00000 Kelvin
    INLET LIQUID VELOCITY              =      100.00000 cm/s
    PIPE INTERNAL DIAMETER             =        5.00000 cm
    WATER DENSITY                      =        0.74100 g/cc
    VAPOR DENSITY                      =        0.03620 g/cc
    PRESSURE                           =       70.75000 atm
    MASS FlowRate                      =    0.31000D+00 g/s

    GAMMA DOSE RATE MULTIPLIER         =    0.30000D+06 Rad/s
    NEUTRON DOSE RATE MULTIPLIER       =    0.41700D+06 Rad/s
    GConvert                           =    0.76916D-09

    GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
    GAMMA COEFFICIENT  0               =    0.10000D-02

    NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
    NEUTRON COEFFICIENT  0             =    0.10000D-02

    CalcSurf                           =        F
    VoidFlag                           =        T
    CalcSens                           =        F
    WriteRx                            =        F
    WritePara                          =        T

    RADIOLYSIS ABSOLUTE TOLERANCE      =    0.10000D-14
               RELATIVE TOLERANCE      =    0.10000D-04


------------------------------------------------------------------------
 CYCLE     1        POSITION IN JET PUMP          =       0.0000 cm
                  CONCENTRATIONS[ppb]  AT POSITION =     750.0000 cm

 e-      =    0.124771D-09 **    OH-       =    0.557481D+02 **
 H2      =    0.114290D+02 **    OH        =    0.621530D-02 **
 HO2-    =    0.493840D+00 **    H2O2      =    0.546460D+02 **
 O2-     =    0.789747D+00 **    O2        =    0.155367D+03 **
 H       =    0.319646D-05 **    H+        =    0.331895D+01 **
 HO2     =    0.125475D+00 **    O2G       =    0.000000D+00 **
 H2G     =    0.000000D+00 **    O         =    0.333568D-04 **
 H2O     =    0.999433D+09 **    2H2O      =    0.823342D+11 **

 NO. STEPS                     =        0
```

```
    TEMPERATURE (K)              =      552.00000
    LIQUID VELOCITY (CM/S)       =      100.00000
    GAS VELOCITY  (CM/S)         =        0.00000
    VOID FRACTION                =        0.00000
    GAMMA DOSE RATE (RAD/S)      =    0.00000D+00
    NEUTRON DOSE RATE (RAD/S)    =    0.00000D+00
```

```
    CYCLE     1        POSITION IN JET PUMP           =    200.0000 cm
                     CONCENTRATIONS[ppb]  AT POSITION =    950.0000 cm

    e-        =    0.112529D-09 **     OH-       =     0.556043D+02 **
    H2        =    0.100869D+02 **     OH        =     0.660891D-02 **
    HO2-      =    0.624009D+00 **     H2O2      =     0.692371D+02 **
    O2-       =    0.121617D+01 **     O2        =     0.137332D+03 **
    H         =    0.334553D-05 **     H+        =     0.332776D+01 **
    HO2       =    0.193297D+00 **     O2G       =     0.000000D+00 **
    H2G       =    0.000000D+00 **     O         =     0.293042D-04 **
    H2O       =    0.999509D+09 **     2H2O      =     0.823341D+11 **

    NO. STEPS                    =      148
    TEMPERATURE (K)              =      552.00000
    LIQUID VELOCITY (CM/S)       =      100.00000
    GAS VELOCITY  (CM/S)         =        0.00000
    VOID FRACTION                =        0.00000
    GAMMA DOSE RATE (RAD/S)      =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)    =    0.41700D+03
```

```
                 RUN STATISTICS FOR CYCLE    1 AT JET PUMP
```

```
REQUIRED RWORK SIZE    =      422
IWORK SIZE             =       36
NUMBER OF STEPS        =      148
# OF FUNC.- EVALS.     =      205
# OF JACOB.- EVALS     =       40
COMPONENT JOB TIME     =     8.25 seconds

CONCENTRATION PROFILE OF JET PUMP         HAS BEEN EVALUATED SUCCESSFULLY!
```

```
                    OUTPUT FOR CYCLE     1 AT LOWER PLENUM


     INITIAL POSITION                 =      950.00000 cm
     FINAL POSITION                   =     1090.00000 cm
     FLOW LENGTH                      =      140.00000 cm
     POSITION INCREMENT               =       50.00000 cm
     POSITION OF ONSET OF BOILING     =    99999.00000 cm

     INLET TEMPERATURE                =      552.00000 Kelvin
     OUTLET TEMPERATURE               =      552.00000 Kelvin
     INLET LIQUID VELOCITY            =       30.43500 cm/s
     PIPE INTERNAL DIAMETER           =        5.00000 cm
     WATER DENSITY                    =        0.74100 g/cc
     VAPOR DENSITY                    =        0.03620 g/cc
     PRESSURE                         =       70.75000 atm
     MASS FlowRate                    =    0.31000D+00 g/s

     GAMMA DOSE RATE MULTIPLIER       =    0.30000D+06 Rad/s
     NEUTRON DOSE RATE MULTIPLIER     =    0.41700D+06 Rad/s
     GConvert                         =    0.76916D-09

     GAMMA DOSE SHAPE FUNCTION COEFFICIENTS
     GAMMA COEFFICIENT  0             =    0.10000D-02

     NEUTRON DOSE SHAPE FUNCTION COEFFICIENTS
     NEUTRON COEFFICIENT  0           =    0.10000D-02

     CalcSurf                         =        F
     VoidFlag                         =        T
     CalcSens                         =        F
     WriteRx                          =        F
     WritePara                        =        T

     RADIOLYSIS ABSOLUTE TOLERANCE    =    0.10000D-14
                RELATIVE TOLERANCE    =    0.10000D-04


   CYCLE     1        POSITION IN LOWER PLENUM      =       0.0000 cm
                   CONCENTRATIONS[ppb]  AT POSITION =     950.0000 cm

   e-       =    0.112529D-09 **   OH-      =    0.556043D+02 **
   H2       =    0.100869D+02 **   OH       =    0.660891D-02 **
   HO2-     =    0.624009D+00 **   H2O2     =    0.692371D+02 **
   O2-      =    0.121617D+01 **   O2       =    0.137332D+03 **
   H        =    0.334553D-05 **   H+       =    0.332776D+01 **
   HO2      =    0.193297D+00 **   O2G      =    0.000000D+00 **
   H2G      =    0.000000D+00 **   O        =    0.293042D-04 **
   H2O      =    0.999509D+09 **   2H2O     =    0.823341D+11 **

   NO. STEPS               =       0
```

```
    TEMPERATURE (K)               =      552.00000
    LIQUID VELOCITY (CM/S)        =       30.43500
    GAS VELOCITY  (CM/S)          =        0.00000
    VOID FRACTION                 =        0.00000
    GAMMA DOSE RATE (RAD/S)       =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)     =    0.41700D+03
____________________________________________________________________________

    CYCLE     1        POSITION IN LOWER PLENUM       =    140.0000 cm
                    CONCENTRATIONS[ppb]  AT POSITION =   1090.0000 cm

    e-       =    0.117822D-09 **     OH-       =    0.556086D+02 **
    H2       =    0.808841D+01 **     OH        =    0.761945D-02 **
    HO2-     =    0.723335D+00 **     H2O2      =    0.902534D+02 **
    O2-      =    0.110577D+01 **     O2        =    0.116207D+03 **
    H        =    0.370703D-05 **     H+        =    0.332757D+01 **
    HO2      =    0.175740D+00 **     O2G       =    0.000000D+00 **
    H2G      =    0.000000D+00 **     O         =    0.293060D-04 **
    H2O      =    0.999529D+09 **     2H2O      =    0.823341D+11 **

    NO. STEPS                     =       17
    TEMPERATURE (K)               =      552.00000
    LIQUID VELOCITY (CM/S)        =       30.43500
    GAS VELOCITY  (CM/S)          =        0.00000
    VOID FRACTION                 =        0.00000
    GAMMA DOSE RATE (RAD/S)       =    0.30000D+03
    NEUTRON DOSE RATE (RAD/S)     =    0.41700D+03

____________________________________________________________________________

             RUN STATISTICS FOR CYCLE    1 AT LOWER PLENUM

____________________________________________________________________________


REQUIRED RWORK SIZE     =       422
IWORK SIZE              =        36
NUMBER OF STEPS         =        17
# OF FUNC.- EVALS.      =        24
# OF JACOB.- EVALS      =         5
COMPONENT JOB TIME      =      3.59 seconds

CONCENTRATION PROFILE OF LOWER PLENUM     HAS BEEN EVALUATED SUCCESSFULLY!

TOTAL JOB TIME          =   1822.21 seconds
```

III. DRESDEN0.MAC

DRESDEN0.MAC lists the final calculation results in a compact columnar form which can be read by plotting software on the Apple Macintosh computer system. The plots in this thesis have been produced this way using Kaleida Graph 2.0 on the Macintosh II computer.

```
[JCHUN.RADICAL.DRESDEN]DRESDEN0.IN  IBE'S RX DRESDEN-2 MULTI DNCMR 14 JUN 1990

  -1
  16
 DISTANCE     OH-        H2         H2O2       O2          H+        O2G        H2G
CORE BOILING          9
   0.0000   55.6086    8.0884    80.2534   116.2071     3.3276     0.0000     0.0000
  50.0000   54.6147   29.8070    36.5589   306.2994     3.3885     0.0000     0.0000
 100.0000   54.7570   26.5267    33.3413   291.0058     3.3798   310.9055    41.4764
 150.0000   55.0507   20.5696    22.8632   246.5549     3.3617   336.2883    42.2959
 200.0000   55.1977   17.6263    18.7813   216.3710     3.3528   315.5397    38.7574
 250.0000   55.2709   16.1785    16.9004   199.8160     3.3483   305.8553    37.3214
 300.0000   55.2920   15.7738    16.3587   195.4751     3.3470   317.4440    38.7752
 350.0000   55.2926   15.7791    16.4866   197.0545     3.3469   340.6656    41.7463
 370.0000   55.3045   15.5482    16.4555   195.5373     3.3462   346.4663    42.4800
CORE BYPASS           9
   0.0000   55.6086    8.0884    80.2534   116.2071     3.3276     0.0000     0.0000
  50.0000   54.2106   38.6111    54.3743   367.1799     3.4138     0.0000     0.0000
 100.0000   54.0937   41.0121    58.6815   383.9596     3.4212     0.0000     0.0000
 150.0000   54.0638   41.5483    59.8294   387.6090     3.4231     0.0000     0.0000
 200.0000   54.0609   41.4931    59.9293   387.1144     3.4231     0.0000     0.0000
 250.0000   54.0780   41.0390    59.4160   383.7843     3.4220     0.0000     0.0000
 300.0000   54.1584   39.2530    56.7696   371.0269     3.4169     0.0000     0.0000
 350.0000   54.3482   35.1866    50.5731   342.0874     3.4049     0.0000     0.0000
 370.0000   54.4943   32.0940    46.0024   320.0280     3.3956     0.0000     0.0000
UPPER PLENUM          5
 370.0000   55.2182   17.3120    19.6052   208.8081     3.3514   346.4663    42.4800
 380.0000   55.6754   14.5454    24.3350   185.6694     3.3251   357.0546    43.7410
 390.0000   55.6647   14.6143    28.3343   186.1672     3.3258   358.0058    43.9476
 400.0000   55.6544   14.6833    32.2527   186.6697     3.3264   358.9610    44.1545
 410.0000   55.6446   14.7523    36.0925   187.1731     3.3271   359.9177    44.3613
FEEDWATER             2
 410.0000    0.0000    0.0000     0.0000    35.0001     0.0000     0.0000     0.0000
 411.0000   56.0316    0.0000     0.0000    35.0001     3.2960     0.0000     0.0000
MIXING PLENUM         8
 410.0000   55.6839   13.2530    32.4246   171.7084     3.3239   359.9177    44.3613
 430.0000   55.8516   13.1350    34.8556   170.1497     3.3146   336.0141    40.8373
 450.0000   55.8544   13.0035    36.9260   168.1187     3.3154   333.9760    40.7033
 470.0000   55.8494   12.8723    38.9559   166.1094     3.3156   333.1038    40.7472
 490.0000   55.8461   12.7415    40.9459   164.1218     3.3160   334.6203    41.1362
 510.0000   55.8539   12.6113    42.8957   162.1565     3.3169   343.1899    42.5536
 530.0000   55.8446   12.4815    44.8052   160.2137     3.3169   398.7878    50.8554
 540.0000   55.8439   12.4168    45.7450   159.2507     3.3171  2160.1959   308.9722
UP DOWNCOMER1         3
 540.0000   55.8439   12.4168    45.7450   159.2507     3.3171  2160.1959     0.0000
 560.0000   55.5143   11.7206    51.1677   150.1067     3.3348  2160.1959     0.0000
 580.0000   55.5206   11.1650    54.3230   144.2079     3.3344  2160.1959     0.0000
UP DOWNCOMER2         3
 540.0000   55.8439   12.4168    45.7450   159.2507     3.3171  2160.1959     0.0000
 560.0000   55.7050   12.1211    49.5746   154.6934     3.3234  2160.1959     0.0000
 580.0000   55.6982   11.8402    53.3401   150.6643     3.3230  2160.1959     0.0000
UP DOWNCOMER3         3
 540.0000   55.8439   12.4168    45.7450   159.2507     3.3171  2160.1959     0.0000
 560.0000   55.8645   12.3488    46.5792   158.4401     3.3139  2160.1959     0.0000
 580.0000   55.8628   12.2800    47.3307   157.5331     3.3140  2160.1959     0.0000
UP DOWNCOMER4         3
 540.0000   55.8439   12.4168    45.7450   159.2507     3.3171  2160.1959     0.0000
 560.0000   55.8699   12.3537    46.5158   158.5261     3.3136  2160.1959     0.0000
```

```
  580.0000    55.8684    12.2896    47.1941   157.6918     3.3137 2160.1959    0.0000
 LO DOWNCOMER1           5
  540.0000    55.7027    11.7898    51.4732   151.1451     3.3235    0.0000    0.0000
  560.0000    55.5243    10.8958    55.6427   141.4494     3.3342    0.0000    0.0000
  580.0000    55.5421    10.2268    55.8205   136.0722     3.3331    0.0000    0.0000
  600.0000    55.5626     9.6952    53.7238   132.8664     3.3319    0.0000    0.0000
  620.0000    55.5844     9.2542    50.5130   130.9092     3.3306    0.0000    0.0000
 LO DOWNCOMER2           5
  540.0000    55.7027    11.7898    51.4732   151.1451     3.3235    0.0000    0.0000
  560.0000    55.6929    11.3452    57.2626   144.8536     3.3241    0.0000    0.0000
  580.0000    55.6840    10.9242    62.4752   139.0197     3.3246    0.0000    0.0000
  600.0000    55.6763    10.5259    67.1350   133.6300     3.3251    0.0000    0.0000
  620.0000    55.6698    10.1497    71.2684   128.6669     3.3255    0.0000    0.0000
 LO DOWNCOMER3           5
  540.0000    55.7027    11.7898    51.4732   151.1451     3.3235    0.0000    0.0000
  560.0000    55.8508    11.6796    52.9183   150.0771     3.3148    0.0000    0.0000
  580.0000    55.8550    11.5673    54.0422   148.6454     3.3153    0.0000    0.0000
  600.0000    55.8650    11.4553    55.1460   147.2251     3.3162    0.0000    0.0000
  620.0000    55.8803    11.3435    56.2296   145.8165     3.3173    0.0000    0.0000
 LO DOWNCOMER4           5
  540.0000    55.7027    11.7898    51.4732   151.1451     3.3235    0.0000    0.0000
  560.0000    55.8559    11.6870    52.8174   150.2009     3.3144    0.0000    0.0000
  580.0000    55.8278    11.5821    53.8306   148.8804     3.3130    0.0000    0.0000
  600.0000    55.8156    11.4773    54.8268   147.5693     3.3126    0.0000    0.0000
  620.0000    55.8227    11.3727    55.8063   146.2676     3.3133    0.0000    0.0000
 RECIRC                  8
  620.0000    55.7156    10.3036    59.3949   135.5629     3.3239    0.0000    0.0000
  640.0000    55.9192    10.2759    59.7261   135.8596     3.3118    0.0000    0.0000
  660.0000    55.8524    10.2476    59.6108   135.6904     3.3077    0.0000    0.0000
  680.0000    55.8390    10.2193    59.4946   135.5196     3.3069    0.0000    0.0000
  700.0000    55.8552    10.1911    59.3787   135.3493     3.3078    0.0000    0.0000
  720.0000    55.8476    10.1630    59.2626   135.1794     3.3073    0.0000    0.0000
  740.0000    55.8299    10.1349    59.1467   135.0100     3.3063    0.0000    0.0000
  750.0000    55.8228    10.1209    59.0887   134.9254     3.3058    0.0000    0.0000
 JET PUMP                5
  750.0000    55.7400    11.2724    53.8340   146.1170     3.3180    0.0000    0.0000
  800.0000    55.6070    10.9020    58.0270   140.7585     3.3259    0.0000    0.0000
  850.0000    55.5969    10.5627    61.8483   136.2415     3.3259    0.0000    0.0000
  900.0000    55.5843    10.2447    65.1816   132.1273     3.3256    0.0000    0.0000
  950.0000    55.5706     9.9471    68.0573   128.3931     3.3252    0.0000    0.0000
 LOWER PLENUM            4
  950.0000    55.5706     9.9471    68.0573   128.3931     3.3252    0.0000    0.0000
 1000.0000    55.5669     9.0988    74.6890   118.4949     3.3254    0.0000    0.0000
 1050.0000    55.5699     8.4196    77.8158   111.6098     3.3252    0.0000    0.0000
 1090.0000    55.5762     7.9742    78.4263   107.7809     3.3248    0.0000    0.0000
```

APPENDIX • E

Reaction Sets

The reaction sets listed in this appendix have been compiled from various sources to provide readily available reaction sets which can be experimented with in simulations using RADICAL. Water reaction sets comprise the main reaction sets used in RADICAL for BWR water chemistry studies. Metal impurity reaction sets may be useful for studying the impurity effects on water chemistry. Nitrogen reaction sets may be useful in nitrogen-16 carryover simulations.

Besides the reaction sets compiled here, there are numerous others reported elsewhere. A reaction set should be used with a compatible set of g-values so that the combination describes a system under simulation in a manner consistent with measurements.. This is not a straight-forward process and a number of sets may have to be tried until a suitable combination is found. It should be kept in mind that different combinations of reaction sets and g-values can give wildly different simulation results, and careful review of these sets is recommended before attempting a simulation (for instance, see Mason [1990] for review of reaction sets and g-values).

I. Ibe's Water Reaction Set

This reaction set was used in simulating Dresden-2 water chemistry in this thesis. This set was also used by Ibe, et al. to study the water chemistry of Dresden-2 and

Oskarshamn-2 [Ibe 1986, 1987, 1989]. The first two reactions which are pseudo-reactions for water and the last five reactions which are mass transfer and surface decomposition reactions have been added for the present study.

The activation energies for mass transfer reactions are set to a negative value to flag RADICAL that these are not ordinary chemical reactions. The rate constant for ss, the hydrogen peroxide surface decomposition reaction, is input for 1 cm diameter pipe; it is scaled according to the pipe diameter of each component as the code runs (see Ch. 4.Sec. VII and Lin [1989] for more detail on diameter -dependent surface decomposition rates).

Ibe's Water
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K)

	REACTIONS							RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
I 1	H2O	H2O		>2H2O				0.10D+01	0.00D+00
I 2	2H2O			>H2O	H2O			0.10D+01	0.00D+00
W 1	e-	H2O		>H	OH-			0.16D+02	0.13D+02
W 2	e-	H+		>H				0.24D+11	0.13D+02
W 3	e-	OH		>OH-				0.24D+11	0.13D+02
W 4	e-	H2O2		>OH	OH-			0.13D+11	0.13D+02
W 5	H	H		>H2				0.10D+11	0.13D+02
W 6	e-	HO2		>HO2-				0.20D+11	0.13D+02
W 7	e-	O2		>O2-				0.19D+11	0.13D+02
W 8	e-	e-	2H2O	>OH-	OH-	H2		0.16D+07	0.13D+02
W 9	OH	OH		>H2O2				0.50D+04	0.13D+02
W10	HO2	OH		>O2	H2O			0.12D+11	0.13D+02
W11	OH	O2-		>O2	OH-			0.12D+11	0.13D+02
W12	H	OH-		>e-	H2O			0.20D+08	0.13D+02
W13	H	e-	H2O	>H2	OH-			0.45D+09	0.13D+02
W14	HO2-	e-	H2O	>OH	OH-	OH-		0.63D+08	0.13D+02
W15	H+	OH-		>H2O				0.14D+12	0.13D+02
W16	H	OH		>H2O				0.20D+11	0.13D+02
W17	H2	OH		>H	H2O			0.34D+08	0.19D+02
W18	H2O2	OH		>HO2	H2O			0.27D+08	0.14D+02
W19	H	H2O2		>OH	H2O			0.44D+08	0.19D+02
W20	H	O2		>HO2				0.19D+11	0.13D+02
W21	HO2			>H+	O2-			0.80D+06	0.13D+02
W22	HO2	O2-		>HO2-	O2			0.15D+08	0.19D+02
W23	HO2	HO2		>O2	H2O2			0.27D+07	0.19D+02
W24	O2-	O2-	2H2O	>O2	H2O2	OH-	OH-	0.56D+04	0.19D+02
W25	H	HO2		>H2O2				0.20D+11	0.13D+02
W26	H	O2-		>HO2-				0.20D+11	0.13D+02
W27	O2-	e-	H2O	>HO2-	OH-			0.18D+09	0.19D+02
W28	H2O2	OH-		>HO2-	H2O			0.50D+09	0.19D+02
W29	H2O			>H+	OH-			0.21D-01	0.13D+02
W30	O2-	H+		>HO2				0.50D+11	0.13D+02
W31	HO2-	H2O		>H2O2	OH-			0.10D+05	0.13D+02
W32	H2O2			>OH	OH			0.20D-02	0.73D+01
W33	O	O		>O2				0.22D+11	0.13D+02
W34	HO2	O		>O2	OH			0.20D+11	0.13D+02
W35	OH	O		>H	O2			0.10D+01	0.71D+02
W36	H2O	O		>OH	OH			0.19D+04	0.13D+02
W37	OH	O		>HO2				0.20D+11	0.13D+02
W38	H2	O		>H	OH			0.48D+04	0.35D+02
W39	H2O2	O		>HO2	OH			0.13D+07	0.18D+02
W40	H	O		>OH				0.20D+11	0.13D+02
H2G	H2			>H2G				0.30D+02	-0.10D+01
H2L	H2G			>H2				0.10D+02	-0.10D+01
O2G	O2			>O2G				0.23D+02	-0.10D+01
O2L	O2G			>O2				0.12D+02	-0.10D+01
SS	H2O2			>O	H2O			0.53D-06	0.67D+02

II. Ruiz's Water Reaction Set

This reaction set is used by Ruiz, et al. in simulation of nine BWRs using FACSIMILE [Ruiz 1989].

To implement this reaction set in RADICAL, the pseudo-reactions for water, `I1` and `I2`, in Ibe's water reaction set should be added along with the mass transfer reactions (`H2G`, `H2L`, `O2G`, and `O2L`). Reaction `W30` is the hydrogen peroxide decomposition reaction and has a rate constant which is divided by the hydrogen peroxide concentration. Since RADICAL does not allow a dynamic change of rate constants, the rate constant for `W30` should be appropriately set in the beginning of simulation, or one should use the reaction `SS` in Ibe's water reaction set.

Ruiz's Water
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

	REACTIONS						RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
W 1	e-	H2O		>H	OH-		1.60D+01	1.26D+01
W 2	e-	H+		>H			2.40D+10	1.26D+01
W 3	e-	OH		>OH-			2.00D+10	1.26D+01
W 4	e-	H2O2		>OH	OH-		1.30D+10	1.26D+01
W 5	H	H		>H2			1.00D+10	1.26D+01
W 6	e-	HO2		>HO2-			2.00D+10	1.26D+01
W 7	e-	O2		>O2-			1.90D+10	1.26D+01
W 8	e-	e-		>OH-	OH-	H2	5.00D+09	1.26D+01
W 9	OH	OH		>H2O2			4.50D+09	1.26D+01
W10	OH	HO2		>H2O	O2		1.20D+10	1.26D+01
W11	OH	O2-		>OH-	O2		1.20D+10	1.26D+01
W12	OH-	H		>e-	H2O		2.00D+07	1.88D+01
W13	e-	H	H2O	>OH-	H2		2.50D+10	1.26D+01
W14	e-	HO2-	H2O	>OH	OH-	OH-	3.50D+09	1.26D+01
W15	H+	OH-		>H2O			1.44D+11	1.26D+01
W16	H2O			>H+	OH-		2.60D-05	1.26D+01
W17	H	OH		>H2O			2.00D+10	1.26D+01
W18	OH	H2		>H	H2O		4.00D+07	1.92D+01
W19	OH	H2O2		>H2O	HO2		2.25D+07	1.44D+01
W20	H	H2O2		>OH	H2O		9.00D+07	1.88D+01
W21	H	O2		>HO2			1.90D+10	1.26D+01
W22	HO2			>O2-	H+		8.00D+05	1.26D+01
W23	O2-	H+		>HO2			5.00D+10	1.26D+01
W24	HO2	HO2		>H2O2	O2		2.70D+06	1.88D+01
W25	O2-	O2-	2H2O	>H2O2	O2	2OH-	1.70D+07	1.88D+01
W26	H	HO2		>H2O2			2.00D+10	1.26D+01
W27	H	O2-		>HO2-			2.00D+10	1.26D+01
W28	e-	O2-		>HO2-	OH-		1.30D+08	1.88D+01
W29	OH-	H2O2		>HO2-	H2O		1.80D+08	1.88D+01
W30	H2O2	H2O2		>H2O	H2O	O2	0.3/H2O2	

III. Notre Dame Water Reaction Set

This reaction set is compiled by the Radiation Chemistry Data Center at the University of Notre Dame and was used by Scott Simonson in his radioactive waste package simulations [Simonson 1988]. The reaction set here is duplicated from Simonson's thesis; it is included here as an alternate choice to the two sets listed previously. Unlike the previous reaction sets, water is implicitly declared in this reaction set.

All Notre Dame reaction sets listed in this appendix are compiled by the Radiation Chemistry Data Center at the University of Notre Dame and listed in Simonson's thesis. The Radiation Chemistry Data Center keeps an extensive database of data related to radiation chemistry and photochemistry and may prove to be a valuable source of parameters needed in water chemistry studies. The center may be reached through Dr. Alberta B. Ross, Radiation Chemistry Data Center, Radiation Laboratory, University of Notre Dame, Notre Dame, Indiana, 46556-0768, (219) 239-6527, BITNET: RCDC@NDRADLAB.

Notre Dame Water
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES at 25 °C (298 K).

			REACTIONS				RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
W 1	e-		>H	OH-			0.40D+02	0.13D+02
W 2	e-	H+	>H				0.60D+11	0.13D+02
W 3	e-	OH	>OH-				0.75D+11	0.13D+02
W 4	e-	H2O2	>OH	OH-			0.32D+11	0.13D+02
W 5	H	H	>H2				0.25D+11	0.13D+02
W 6	e-	HO2	>HO2-				0.50D+11	0.13D+02
W 7	e-	O2	>O2-				0.47D+11	0.13D+02
W 8	e-	e-	>OH-	OH-	H2		0.12D+11	0.13D+02
W 9	OH	OH	>H2O2				0.11D+11	0.13D+02
W10	OH-	H	>e-				0.78D+08	0.19D+02
W11	e-	H	>H2	OH-			0.62D+11	0.13D+02
W12	e-	HO2-	>OH	OH-	OH-		0.87D+10	0.13D+02
W13	H	OH	>				0.50D+11	0.13D+02
W14	OH	H2	>H				0.11D+09	0.13D+02
W14	H		>H2	OH			0.49D-01	0.85D+02
W15	H	O2	>HO2				0.47D+11	0.13D+02
W16	H	HO2	>H2O2				0.50D+11	0.13D+02
W17	H	O2-	>HO2-				0.50D+11	0.13D+02
W18	e-	O2-	>HO2-	OH-			0.51D+11	0.19D+02
W19	H	H2O2	>OH				0.24D+09	0.14D+02
W20	OH	H2O2	>HO2				0.41D+08	0.82D+01
W21	OH	HO2	>O2				0.30D+11	0.13D+02
W22	OH-	H2O2	>HO2-				0.70D+09	0.19D+02
W22	HO2-		>OH-	H2O2			0.22D+07	0.19D+02
W24	H+	O2-	>HO2				0.12D+12	0.13D+02
W24	HO2		>H+	O2-			0.20D+07	0.13D+02
W25	HO2	O2-	>HO2-	O2			0.58D+08	0.19D+02
W26	O2-	O2-	>H2O2	O2	OH-	OH-	0.66D+08	0.19D+02
W27	HO2	HO2	>H2O2	O2			0.11D+08	0.19D+02
W28	H+	OH-	>				0.14D+12	0.00D+00
W28			>H+	OH-			0.78D-01	0.00D+00
W29	OH	O2-	>O2	OH-			0.30D+11	0.13D+02
AE1	O2		>O2G				0.10D+07	0.00D+00
AE1	O2G		>O2				0.42D+03	0.00D+00

IV. Ibe's Nitrogen Reaction Set

A nitrogen reaction set may be added to a water reaction set to study nitrite, nitrate, ammonia formation, and N-16 carryover. This reaction set has been used by Ibe to investigate formation of nitrogen compounds in N_2-H_2O systems under radiation [Ibe 1989]. This becomes particularly important in hydrogen water chemistry since the release of radioactive ammonia gas through the secondary system in BWRs has been one of the major side effects of hydrogen addition.

Use this reaction set along with a water reaction set to simulate nitrogen behavior in BWRs. Water is explicitly declared in this reaction set.

Ibe's Nitrogen
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

	REACTIONS							RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
N41	N	O2		>NO	O			2.27D+04	1.26D+01
N42	NO	H		>NH	O			1.00D+04	1.26D+01
N43	N	H		>NH				2.00D+07	1.26D+01
N44	N	OH		>H	NO			3.20D+10	1.26D+01
N45	N	N		>N2				1.00D+09	1.26D+01
N46	NO	O		>NO2				1.66D+09	1.26D+01
N47	NO	O2		>NO2	O			1.00D+03	1.26D+01
N48	N	H2		>NH2				0.10D+00	1.26D+01
N49	NO	OH		>H+	NO2-			8.90D+09	1.26D+01
N50	NO2	H		>NO	OH			7.55D+10	1.26D+01
N51	NO2	NO2	H2O	>H+	H+	NO2-	NO3-	1.00D+07	1.26D+01
N52	NH	OH		>N	H2O			1.00D+04	1.26D+01
N53	NH	H2		>NH3				5.00D+00	1.26D+01
N54	NH	O2		>NO	OH			1.00D+07	1.26D+01
N55	NH2	OH		>NH	H2O			7.50D+09	1.26D+01
N56	NH2	O2		>NH	HO2			1.00D+04	1.26D+01
N57	NH2	H2		>NH3	H			3.00D+05	3.57D+01
N58	NH3	OH		>NH2	H2O			1.00D+09	1.26D+01
N59	NH3	O		>NH2	OH			1.00D+09	1.26D+01
N60	NH3	H2O		>NH4	OH			8.00D+05	1.26D+01
N61	NO2-	H2O2		>NO3-	H2O			1.00D+10	1.26D+01
N62	NO2-	H		>NO	OH-			1.60D+10	1.26D+01
N63	NO3-	H		>NO2	OH-			4.70D+06	1.26D+01
N64	NH4+	OH-		>NH3	H2O			8.00D+09	2.52D+01
N65	NO	NO	O2	>NO2	NO2			1.40D+07	1.26D+01
N66	N2	H2O		>NH2	NO			3.00D+09	3.44D+01
N67	H2O	H2O		>2H2O				1.00D+08	2.60D+01
N68	e-	H2O	NO3-	>NO2	OH-	OH-		1.10D+10	1.26D+01
N69	H+	NO2-	e-	>NO	OH-			1.00D+09	1.26D+01
N70	H	NH3		>NH2	H2			2.65D+09	2.60D+01
N71	NH3			>NH2	H			1.00D+02	1.26D+01
N72	NH2	NH2		>N2H4				1.00D+03	1.26D+01
N73	H	H	N2H4	>N2	H2	H2	H2	1.00D+05	1.26D+01

V. Notre Dame Nitrogen Reaction Set

Notre Dame Nitrogen
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

				REACTIONS					RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
A01	O	O		>O2					0.55D+11	0.13D+02
A02	O	HO2		>O2	OH				0.50D+11	0.13D+02
A03	O	OH		>O2	H				0.16D+03	0.70D+02
A04	O			>OH	OH				0.37D+05	0.41D+02
A05	O	OH		>HO2					0.50D+11	0.13D+02
A06	O	H2		>H	OH				0.59D+05	0.35D+02
A07	O	H2O2		>HO2	OH				0.46D+07	0.18D+02
A08	O	H		>OH					0.50D+11	0.13D+02
A09	N	O2		>O	NO				0.56D+05	0.13D+02
A10	NO	H		>NH	O				0.25D+05	0.13D+02
A11	N	H		>NH					0.50D+08	0.13D+02
A12	N	OH		>H	NO				0.80D+11	0.13D+02
A13	N	N		>N2					0.25D+10	0.13D+02
A14	NO	O		>NO2					0.41D+10	0.13D+02
A15	NO	O2		>NO2	O				0.25D+04	0.13D+02
A16	N	H2		>NH2					0.25D+00	0.13D+02
A17	NO	OH		>NO2-	H+				0.22D+11	0.13D+02
A18	NO2	H		>NO	OH				0.19D+12	0.13D+02
A19	NO2	NO2		>H+	H+	NO2-	NO3-		0.25D+08	0.13D+02
A20	NH	OH		>N					0.25D+05	0.13D+02
A21	NH	H2		>NH3					0.12D+02	0.13D+02
A22	NH	O2		>NO	OH				0.25D+08	0.13D+02
A23	NH2	OH		>NH					0.19D+11	0.13D+02
A24	NH2	O2		>NH	HO2				0.25D+05	0.13D+02
A25	NH2	H2		>NH3	H				0.39D+07	0.36D+02
A26	NH3	O		>NH2	OH				0.25D+10	0.13D+02
A27	NH3	OH		>NH2					0.25D+10	0.13D+02
A28	NO2-	H2O2		>NO3-					0.25D+11	0.13D+02
A29	NO2-	H		>NO	OH-				0.40D+11	0.13D+02
A30	NO3-	H		>NO2	OH-				0.12D+08	0.13D+02
A31	NO	NO	O2	>NO2	NO2				0.35D+08	0.13D+02
A32	NH3	H		>NH2	H2				0.17D+11	0.26D+02
A33	NH3			>NH2	H				0.25D+03	0.13D+02
A34	NH2	NH2		>N2H4					0.25D+04	0.13D+02
A35	H	H	N2H4	>N2	N2	H2	H2		0.25D+06	0.13D+02
A36	e-	NO3-		>NO2	OH-	OH-			0.27D+11	0.13D+02
A37	H+	NO2-	e-	>NO	OH-				0.25D+10	0.13D+02

VI. Ruiz's Metallic Impurity Reaction Set

Metallic impurity ions such as copper, iron, and nickel may cause significant effects on water chemistry in certain regions of the BWR. For instance, these ions act as catalysts, and the effect may range from reducing the primary chemical yields (g-values) of some species to changing the normal chemical reaction path in some cases [Ruiz 1989].

The presence of copper impurities in the recirculation line has been identified to cause disagreement between experimental and simulated results; in this case a copper reaction set may be added to a water reaction set in an input file to include the effect of copper impurities.

Ruiz's Metal Impurity
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

	REACTIONS						RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
M 1	CU2+	H		>CU+	H+		9.8D+08	
M 2	CU2+	e-		>CU+	H2O		4.0D+10	
M 3	CU+	H2O2		>CU2+	OH	OH-	2.3D+09	
M 4	CU+	HO2	H2O	>CU2+	H2O2	OH-	6.0D+08	
M 5	CU2+	HO2		>CU+	H+	O2	2.1D+08	
M 6	FE2+	OH		>FE3+	OH-		3.4D+08	
M 7	FE3+	H		>FE2+	H+		5.0D+08	
M 8	FE3+	e-		>FE2+	H2O		5.0D+10	
M 9	FE2+	HO2		>FE3+	HO2-		2.1D+06	
M10	CL-	OH		>CL	OH-		1.0D+06	
M11	BR-	OH		>BR	OH-		1.0D+04	
M12	I-	OH		>I	OH-		1.5D+10	

VII. Notre Dame Iron Reaction Set

Notre Dame Iron
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

	REACTIONS						RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
F 1	FE2+	OH	>FE3+	OH-			0.57D++09	0.13D+02
F 2	FE2+	e-	>FE+				0.55D+11	0.13D+02
F 3	FE+	OH	>FEOH+				0.70D+09	0.13D+02
F 4	FE+	H2O2	>FE2+	OH-	OH		0.13D+03	0.13D+02
F 5	FE+	O2-	>FE2+	OH-	OH-	H2O2	0.88D+09	0.13D+02
F 6	H	FE2+	>FEH2+				0.34D+07	0.13D+02
F 7	FEH2+	H+	>FE3+	H2			0.26D+05	0.13D+02
F 8	FE+	H	>FEH+				0.30D+07	0.13D+02
F 9	FEH+	H+	>FE2+	H2			0.23D+05	0.13D+02
F10	FE2+	H2O2	>FE3+	OH-	OH		0.15D+03	0.13D+02
F11	FE2+	O2-	>FE3+	OH-	OH-	H2O2	0.99D+09	0.13D+02
F12	FE3+	e-	>FE2+				0.50D+11	0.13D+02
F13	FE3+	O2-	>FE2+	O2			0.99D+09	0.13D+02
F14	FE3+	H	>FE2+	H+			0.65D+07	0.13D+02
F15	FE3+		>FEOH2+	H+			0.75D+08	0.13D+02
F16	FEOH2+	H+	>FE3+				0.12D+11	0.13D+02
F17	FEOH2+		>FE(OH)2+H+				0.15D+06	0.13D+02
F18	FE(OH)2+H+		>FEOH2+				0.20D+11	0.13D+02
F19	FE(OH)2+FE(OH)2+		>FEOOH	FEOH2+			0.12D+04	0.13D+02
FQ1	H+	FEOH+	>FE2+				0.10D+11	0.00D+00
FQ1	FE2+		>H+	FEOH+			0.40D+03	0.00D+00
FQ3	FEOH2+	H+	>FE3+				0.10D+11	0.00D+00
FQ3	FE3+		>FEOH2+	H+			0.13D+10	0.00D+00

VIII. Notre Dame Nickel Reaction Set

Notre Dame Nickel
CHEMICAL REACTIONS, RATE CONSTANTS, AND ACTIVATION ENERGIES
at 25 °C (298 K).

	REACTIONS						RATE CONSTANT	ACTIVATION ENERGIES (KJ/MOL-K)
NI1	NI2+	e-		>NI+			0.55D+11	0.13D+02
NI2	NI2+	H		>NI+	H+		0.50D+06	0.13D+02
NI3	NI+	H2O2		>NI2+	OH-	OH	0.99D+08	0.13D+02
NI4	NI+	OH		>NI2+	OH-		0.50D+11	0.13D+02
NI5	NI+	O2		>NI2+	O2-		0.55D+11	0.13D+02
NE1	H+	NIOH+		>NI2+			0.10D+11	0.00D+00
NE1	NI2+			>H+	NIOH+		0.14D+03	0.00D+00
NE2	NI2+	OH-	OH-	>NI(OH)2			0.10D+11	0.00D+00
NE2	NI(OH)2			>OH-	OH-	NI2+	0.10D-06	0.00D+00

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