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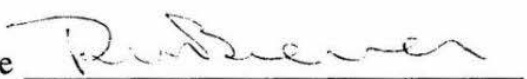
Signature 

Date 20 April 1993

ANALYSIS OF A HYPOTHETICAL ARRAY CRITICALITY ACCIDENT INVOLVING UNITS OF AQUEOUS URANYL FLUORIDE

A Thesis Presented for the Master of Science Degree

The University of Tennessee, Knoxville

Roger W. Brewer

August 1993

DEDICATION

This thesis is dedicated to my mother and father, Sara F. Brewer and Clifford N. Brewer. They have always supported me in everything I have done, and allowed me the freedom to succeed and fail.

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I would like to thank my major professor, Dr. H. L. Dodds, for his patience and guidance. I would also like to thank the other committee members, Dr. P. N. Stevens and Dr. A. Ruggles. I wish to thank J. C. Ingram and all other Martin Marietta employees for their help as well as Dr. D. J. Mather from the United Kingdom Atomic Energy Authority for his assistance. I would like to thank my wife, Sarah, for her support and understanding. Finally, I wish to express my thanks to the members of my family, Clifford N. Brewer, Sara F. Brewer, Patricia J. Kile, Donovan Picarella, and Clint Kile.

Abstract

In this study a model is developed to predict the results of a hypothetical nuclear excursion involving an array of six polyethylene bottles containing an aqueous solution of low-enriched UO_2F_2. The computer model calculates the power history, the total energy release, and various thermal-hydraulic parameters. The model employs point neutronics coupled with simple lumped parameter feedback.

The model has been used to predict the results of various nuclear excursion experiments. Good agreement with the experiments for the initial peak fission rate, the total number of fissions, and for some of the subsequent fission pulses is demonstrated. For the six bottle array, ramp insertion rates of 0.5 \$/sec to 35.0 \$/sec and a step of 35.0 \$ are postulated. The peak fission rates range from 3.1×10^{16} fissions/sec to 1.9×10^{22} fissions/sec. The total number of fissions range from 3.3×10^{16} fissions to 7.7×10^{18} fissions. Most of the array results appear to be quite reasonable.

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CHAPTER I

Introduction

Background

The work presented herein shows the analysis of a hypothetical nuclear excursion of an array of six polyethylene bottles containing aqueous uranyl fluoride. Knowledge concerning the excursion of an array of units which contain a fissile solution has been limited. It has long been thought that arrays have the capacity for a large total energy release with possibly explosive results[1] and, currently no excursion analysis codes which treat arrays of fissile solutions are known to exist. Also considering the fact that fissile solution units are normally stored in close proximity to each other, there exists a need to investigate a hypothetical excursion accident of such an array of units. Such information is required for accident dose assessments and emergency planning.

Problem Description

The problem which is the subject of this study involves the storage of over 100 polyethylene bottles, each bottle containing roughly 24 liters of aqueous low-enriched uranyl fluoride. Previous critical experiment results have indicated that five of these bottles in direct contact and unreflected are critical.[2] The compilation of all the pertinent critical experiment results are shown in Figure 1. The bottles are currently stored with no restraining devices.[3] Thus, an earthquake or some kind of operator error could result in a criticality accident.

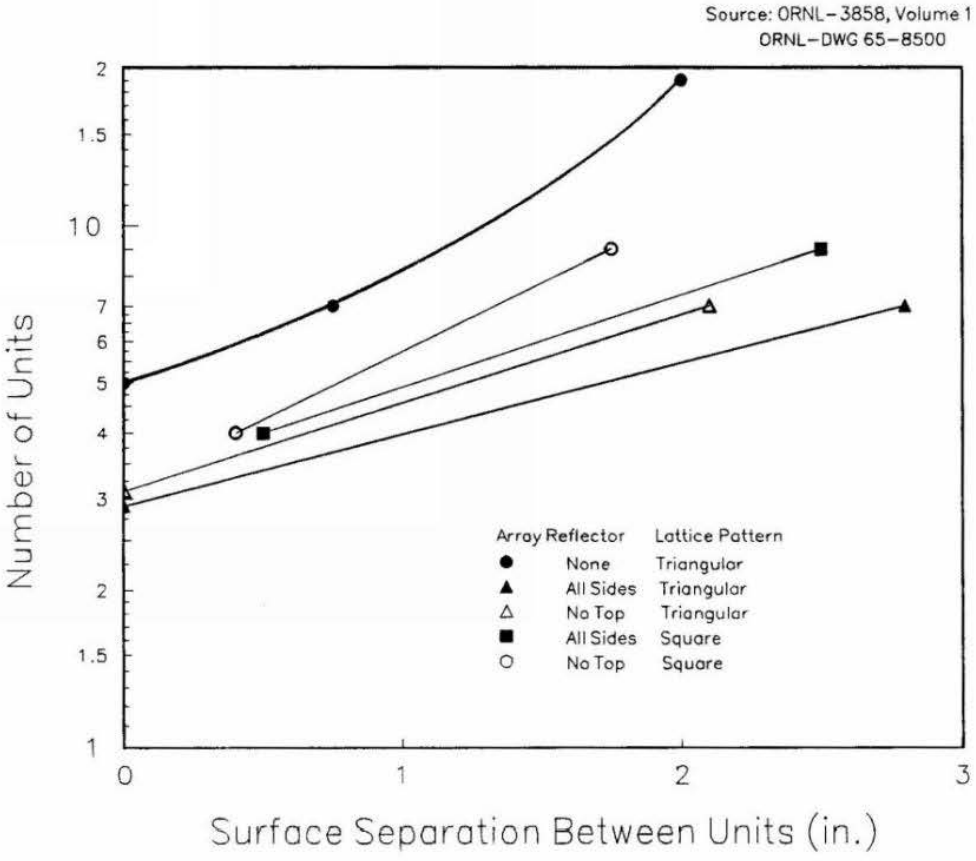

Figure 1: Critical Planar Arrays of Aqueous $U(4.98)O_2F_2$ Solution at a Concentration of 901 g of Uranium per Liter.

The UO_2F_2 solution in the bottles has a maximum enrichment of 4.98 weight percent U^{235}. This means that each bottle contains a maximum of 1.1 Kg of U^{235} ($H/U^{235}=496$). The solution has a specific gravity of 1.9875 and the uranium concentration is approximately 901 grams of uranium per liter of solution. The bottles themselves are molded polyethylene with a diameter of 10.75 inches and wall thicknesses of 0.10 inch on the side and 0.25 inch on the bottom. They are concave up on the bottom with a screw cap on the top. The bottles are normally stored in a square lattice pattern

with a surface separation distance of 2 feet.[3] The hypothetical accident involves the accidental moving together of six bottles simultaneously as shown in Figure 2.

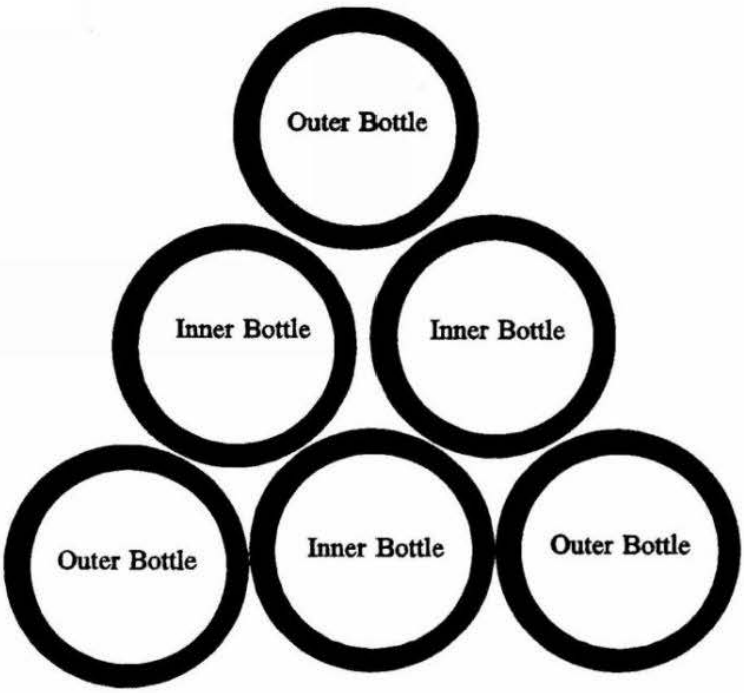

Figure 2: Postulated Accident Bottle Arrangement

Objectives

The primary objective of this study is to predict the time-dependent neutronic and thermal-hydraulic behavior of the system in question. The computer model developed in this work calculates the power as a function of time and the total energy release as well as other parameters of interest. A computer code called SKINATH[4] was formulated a number of years ago to solve point kinetics with simple thermal-hydraulic feedback. For the purposes of this study, SKINATH has been modified to reflect the aspects of the six

bottle array system involved. This modification is henceforth referred to as SKINATH-AR. SKINATH uses the Livermore Solver of Ordinary Differential Equations to solve the differential equations associated with the neutronics and thermal-hydraulics.[5]

Previous Work

A significant amount of work has been performed in excursion studies over the years much of which involved excursions of fissile solutions. One important study was the CRAC experiments. The CRAC experiments were conducted using a highly enriched uranyl nitrate solution in 300 mm and 800 mm diameter cylinders.[6] Another set of experiments which proved useful are the SHEBA experiments. These experiments were performed using UO_2F_2 at an enrichment of 4.8% and a concentration of 1000 g U per liter.[7] The SHEBA specifications closely reflect the composition of the solution in the bottles which are the subject of this study.

Numerous other studies of nuclear excursions have been published by many people and organizations. One such study concerns the effect of a weak neutron source on the initiation of a chain reaction.[8] Another study whose purpose was to model excursions of solutions employs an empirical quenching coefficient to approximate the thermal-hydraulic feedback associated with a fissile solution.[9] Additional studies include those performed by Lutz and Hetrick.[10,11] Hetrick has done a significant amount of work on modeling fissile solution excursions with particular attention being paid to the subsequent power pulses. Lutz studied excursions in general and made recommendations on modeling such excursions with point neutronics.

Many computer models have been developed to model nuclear excursions using point neutronics as well as space-time neutronics. Examples include CRITEX,[12] CREST,[13] PAD,[14] and SKINATH.[4] All previous work using SKINATH involved single fissile units. More recently, studies using SKINATH centered around powder systems, but it has also been used for fissile solutions.[15,16] Hypothetical excursion accidents involving arrays of fissile solution units have not been modeled prior to this study.

Scope

This chapter provides much of the background material for this problem. The following chapter discusses the theory and the procedure used in solving the problem. The third chapter provides results obtained with SKINATH-AR. The fourth chapter presents the validation efforts and the fifth chapter states the conclusions of this research. Finally, the last chapter describes the recommendations for future work. Several appendices are included which provide more detailed information on the material contained herein.

CHAPTER II

Accident Model

Neutronics

Assumptions

The neutronic model utilized in this study employs point neutronics which inherently assumes that the system is a point (no spatial effects occur).[17] Six delayed neutron precursor groups for thermal fission of U^{235} are used.[18] The change in liquid level in a bottle due to evaporation is assumed to have no effect (reactivity feedback associated with leakage due to the changing level in a bottle is not considered). Since a bulk averaged thermal-hydraulic model is used, no attention is given to the axial or radial distribution of vapor, steam voids, or radiolytic gas.

Point Neutronics

The excursion model developed in this work employs point neutronics coupled with simple lumped parameter feedback.[4] The fission rate (referred to as the power in the rest of this report) of the array as a function of time is calculated using point kinetics equations as shown below:[17,18]

$$\frac{dn}{dt} = \frac{(\rho_{tot} - \beta)}{\Lambda} n(t) + \sum_{i=1}^{6} \lambda_i C_i(t) \qquad (1)$$

$$\frac{dC_i}{dt} = \frac{\beta_i}{\Lambda} n(t) - \lambda_i C_i(t) \ , \ i=1,2,\cdots,6 \qquad (2)$$

where

n = power of the entire array as a function of time (fissions/sec)
t = time (sec)
ρ_{tot} = total reactivity ($\Delta k/k$)
β = total delayed neutron fraction
Λ = mean generation time (sec)
C_i = delayed neutron precursor concentration for group i (# of nuclei/sec)
λ_i = decay constant for precursor group i (sec^{-1})
β_i = delayed neutron fraction for precursor group i.

The total reactivity is represented as shown below:

$$\rho_{tot} = \rho_{ext} + \sum_{\ell=1}^{N} [\frac{\partial \rho}{\partial T}(T-T_0) + \frac{\partial \rho}{\partial V}(V_{gas}-V_0) + \frac{\partial \rho}{\partial V} V_{steam}]_\ell \ , \qquad (3)$$

where

N = total number of bottles
ℓ = subscript which refers to bottle "ℓ" in the array
ρ_{ext} = external reactivity ($\Delta k/k$)
T = bulk fluid temperature (°C)
T_o = initial temperature (°C)
V_{gas} = volume of gas produced (m^3)
V_o = initial volume of dissolved gas (m^3)
V_{steam} = volume of steam produced (m^3).

The feedback due to temperature is attributed to thermal expansion, spectral changes, and the doppler effect. The reactivity feedback from gas production is a function of the volume of gas produced[12] (H_2 and O_2 from radiolysis of H_2O as well as O_2 and F_2 from the break up of UO_2F_2). The feedback from steam is a function of the volume of steam produced.

The total number of fissions (referred to as the total energy release from here on) is calculated using the following equation:

$$P_{fiss}(t') = \int_0^t n(t')\, dt' , \qquad (4)$$

where

P_{fiss} = total energy release from t′=0 to t′=t.

Delayed Neutron Precursors

Delayed neutrons in excursion analyses can be an important factor in determining the speed and magnitude of the power transient. The values for delayed neutron decay constants and delayed neutron fractions were selected from reference 18 and are shown in Table 1.

Table 1: Delayed Neutron Parameters

i	λ_i (sec^{-1})	β_i
1	0.0127	0.000247
2	0.0317	0.0013845
3	0.115	0.001222
4	0.311	0.0026455
5	1.4	0.000832
6	3.87	0.000169

Generation Time

The generation time used is calculated by KENO, a module of SCALE, and this parameter compares favorably with the generation time of other sources as shown in the results.[19,20] The generation time yielded by KENO represents the average time between successive generations of neutrons omitting the first three generations.[20] The generation time for the six bottle array is 3.33×10^{-5} sec.

Initial Source Strength

The initial growth of power in a supercritical system is stochastic, particularly in the presence of a "weak" neutron source. This means that the development of the first persistent fission chain is statistical in nature and the time at which the chain develops must reflect the statistical nature of this phenomena. The neutron source studied here meets the criteria set forth by Hansen in defining a "weak" neutron source as shown below:[8]

$$\frac{2\,S\,\tau}{\bar{\nu}\,\Gamma_2} = 0.095 \ll 1\ , \tag{5}$$

where

S = neutron source strength (neutrons/sec)
τ = mean neutron lifetime (sec)
ν = average number of neutrons per fission (neutrons/fission)

$$\Gamma_2 = \frac{\overline{\nu\,(\nu - 1)}}{\bar{\nu}^2}\ . \tag{6}$$

The value of Γ_2 is approximated as 0.8.[8] The value of S is found using the empirical constant of 43.48 fissions/s/kg for the CRAC experiments.[9] The source strength for the six bottle array containing $U(5\%)O_2F_2$ has been calculated with an empirical constant. This empirical constant is 17.33 ± 0.66 fissions/s/liter which gives an S of 2496.0 ± 95.0 fissions/s for the six bottle array.[21] The mean neutron lifetime is 3.7×10^{-5} sec which is the same as the generation time because the system is assumed to be near critical. The assumed value of ν is 2.43 neutrons/fission.

The delay time is the time it takes for the excursion to initiate. The expected value of the delay time is found from equation 7 and the standard deviation of the delay time is calculated with equation 8.[8]

$$\langle t_1 \rangle = \sqrt{\frac{\pi \bar{\nu} \Gamma_2}{4 \alpha S}} \quad (7)$$

$$\sigma_1 = \sqrt{(1-\frac{\pi}{4})\frac{\bar{\nu} \Gamma_2}{\alpha S}} \quad (8)$$

where

α = ramp reactivity insertion rate ($\Delta k/k/s$).

Table 2 shows the results of calculations done using equations 7 and 8.

Table 2: Values of the Delay time and the Standard Deviation of the Delay Time for Various Reactivity Insertion Rates

α	$< t_1 >$	σ_1
0.5 $/sec	0.40 sec	0.2
1.0 $/sec	0.28 sec	0.15
2.0 $/sec	0.20 sec	0.10
35.0 $/sec	0.0054 sec	0.0023

Thermodynamics

Thermodynamic Models

Two thermodynamic models were developed to describe the hypothetical excursion of the six bottle array; the Closed/Open System (COS) model, and the Open System (OS) model.

The Closed/Open System Model

The thermodynamic system in this model is defined as the UO_2F_2 solution including the air space at the top of a polyethylene bottle. This definition does not

include the bottle itself.

Initially, the solution is assumed to be a two phase mixture at room temperature (20°C). The fluid could be in this condition if the bottles are filled with a hot liquid and then the bottle is capped and the solution cools to room temperature. This is indicated by point 1 on Figure 3. Then as the power increases, the temperature and the pressure inside the bottle also increase. When the pressure reaches 0.345 MPa (point 2 on Figure 3), the bottle is assumed to rupture.[2] Approximately one fourth of the solution flashes to steam and leaves the bottle. The pressure drops to atmospheric (0.10135 MPa) and the temperature falls to saturation for atmospheric pressure (100°C) which is point 3 on Figure 3.[23,24]

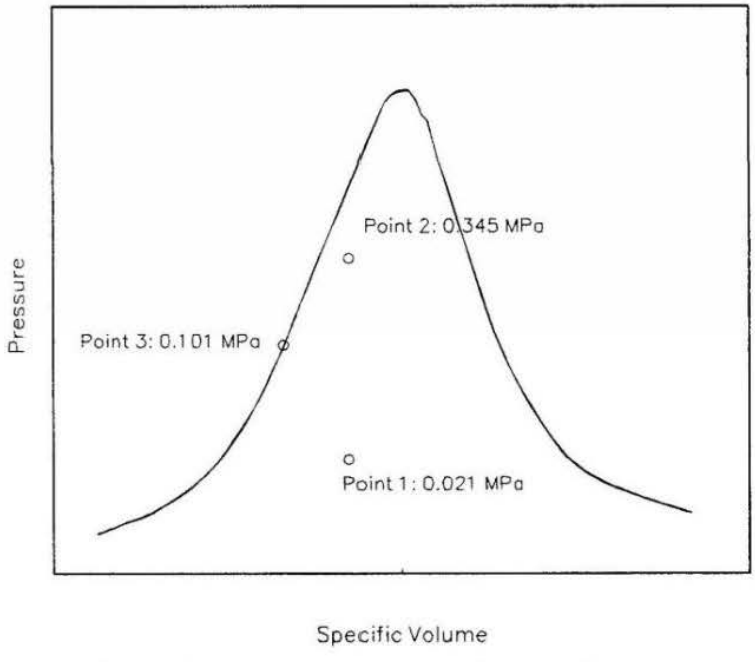

Figure 3: Pressure-Volume Diagram for a Single Bottle in the COS Model

The assumed process between points 1 and 2 is one of constant specific volume while the fluid within the bottle is a two phase mixture.[22] The fact that the bottle is closed justifies the constant volume assumption. No mass leaves the bottle and thus the system volume will not change assuming that the container is rigid. The fact that the system is initially at saturation has minimal effect neutronically because the reactivity feedback from steam production is assumed to be nil until Point 2 on Figure 3 is reached. In addition, the reactivity feedback due to pressure was calculated (calculations shown in Appendix A) and found to be much less than temperature feedback.

The reason for choosing this model comes from the fact that one cannot be certain of the phase of the fluid inside the bottle when going from the actual initial state (subcooled fluid) to the second state (unknown state; fluid could be saturated, superheated, subcooled, or all three phases). This is because the pressure is increasing while the temperature is increasing which means that the second state will be uncertain. The second state is important in determining such factors as steam feedback reactivity which will significantly affect the power as a function of time.[22,23]

The Open System Model

The thermodynamic system discussed in this section consists of only the UO_2F_2 solution contained in a bottle. This definition does not include the bottle or the air space at the top of the bottle. For this model the solution is initially a subcooled liquid at atmospheric pressure. The fluid remains at atmospheric pressure throughout the transient. The path by which the fluid goes from subcooled to saturated is a linear function based

on starting the transient at 20°C and 0.10135 MPa and assuming the fluid ends up as a saturated liquid at 100°C and 0.10135 MPa.

Bulk Thermal-hydraulic Model

The thermodynamic calculations are performed for each individual unit in the array. Each bottle is initially closed for the COS model. An overall energy balance for a closed bottle is shown by the following equation:

$$\frac{dU_{syst}}{dt} = \dot{Q}_{gen} - \dot{Q}_{ht} \qquad (9)$$

where

U_{syst} = internal energy (joules)
$\dot{Q}_{gen}$ = rate of heat generation due to fission (joules/sec)
$\dot{Q}_{ht}$ = rate of heat loss (joules/sec).

Heat generation occurs as a result of the fission process. Heat generation is assumed to be spatially uniform within a bottle. A power fraction factor distributes the array power computed by point kinetics appropriately to each unit in the array. The factor, f, is based on the initial power shape function which is presented later. Thus the time rate of change of the energy generated may be represented as:

$$\dot{Q}_{gen} = \varepsilon f n(t) \qquad (10)$$

where

f = power fraction for each array unit[26]
ε = constant to convert fission power to joules (joules/fission).

The heat loss from the bottle occurs as a result of conduction through the bottle walls and free convection to the surroundings. Two models which calculate the heat loss term were developed. The first heat loss model uses an empirical correlation and the

second model utilizes a numerical approximation to the one-dimensional general heat conduction equation. The first model, referred to herein as the empirical model, is shown by following equations:[4,27,28]

$$\dot{Q}_{ht} = U\,A\,(T_{bulk} - T_{\infty}) \qquad (11)$$

with

$$U = \frac{1}{\left[\frac{0.13\,K_{air}}{H_c}\,(Ra^{\frac{1}{3}})\right]^{-1} + \frac{\Delta r}{K_{wall}}}, \qquad (12)$$

where

A = average surface area (m^2)
T_{bulk} = bulk temperature (°C)
T_{∞} = ambient temperature (°C)
H_c = height of the cylinder (m)
Δr = bottle wall thickness (m)
U = overall heat transfer coefficient (joules/°C/sec/m^2)
K_{air} = thermal conductivity of the air (joules/°C/sec/m)
K_{wall} = thermal conductivity of the container wall (joules/°C/sec/m)
Ra = Raleigh number.

Substituting equations 10 and 11 back into equation 9 yields:

$$\frac{dU_{syst}}{dt} = \varepsilon\,f\,n(t) - U\,A\,(T_{bulk} - T_{\infty})\,. \qquad (13)$$

The T_{bulk} term is unknown at the present time step, t. Therefore, T_{bulk} is lagged one time step. In other words, T_{bulk} becomes a known quantity if it is evaluated using steam table correlations based on the energy and the specific volume at the previous time step, t-1.

The second model, referred to as the analytical model, is characterized by the following equations:

$$\dot{Q}_{ht} = \frac{k_{wall}\, A\, (T_{bulk} - T_s)}{\Delta x} \qquad (14)$$

and

$$\frac{dU_{syst}}{dt} = \varepsilon\, f\, n(t) - \frac{k_{wall}\, A\, (T_{bulk} - T_s)}{\Delta x} \,. \qquad (15)$$

The T_{bulk} and T_s terms are unknown terms at the present time step, t. Therefore, T_{bulk} and T_s are lagged one time step. The term, T_{bulk}, becomes a known quantity if it is evaluated using steam table correlations based on the energy and the specific volume at the previous time step, t-1. T_s is related to T_{bulk} as shown by the following analytical heat transfer model.

Consider the general heat-conduction equation as shown below:[27]

$$\frac{\partial T}{\partial t} = \alpha\, \frac{\partial^2 T}{\partial x^2} \,, \qquad (16)$$

where

α = thermal diffusivity (m^2/sec).

Numerical approximations for the partial derivatives are then made according to the following:[27]

$$\frac{\partial^2 T}{\partial x^2}\Big]_{t-1} \cong \frac{T_{wall}^{t-1} - 2\, T_s^{t-1} + T_{bulk}^{t-1}}{\Delta\, x^2} \qquad (17)$$

where

Δx = distance between nodes, Figure 4 (m)
T_s = wall centerline temperature, Figure 4 (°C)
T_{wall} = wall temperature, Figure 4 (°C).

The temperature of the solution is assumed to be uniform with respect to space. Therefore, the inside bottle wall temperature is the bulk temperature of the solution as shown in Figure 4. Convection boundary conditions are applied as shown below:[27]

$$-K_{wall}\, A\, \frac{\partial T}{\partial x}\Big]_{wall} = h_{fc}\, A\, (T_{wall} - T_{\infty})\ , \qquad \textbf{(19)}$$

where

h_{fc} = free convection heat transfer coefficient (joules/sec/°C/m^2).

Using a numerical approximation evaluated at t-1, equation 19 becomes:[27]

$$-\frac{K_{wall}}{\Delta x}\,(T_{wall}^{\,t-1} - T_s^{\,t-1}) = h_{fc}\,(T_{wall}^{\,t-1} - T_{\infty}) \qquad \textbf{(20)}$$

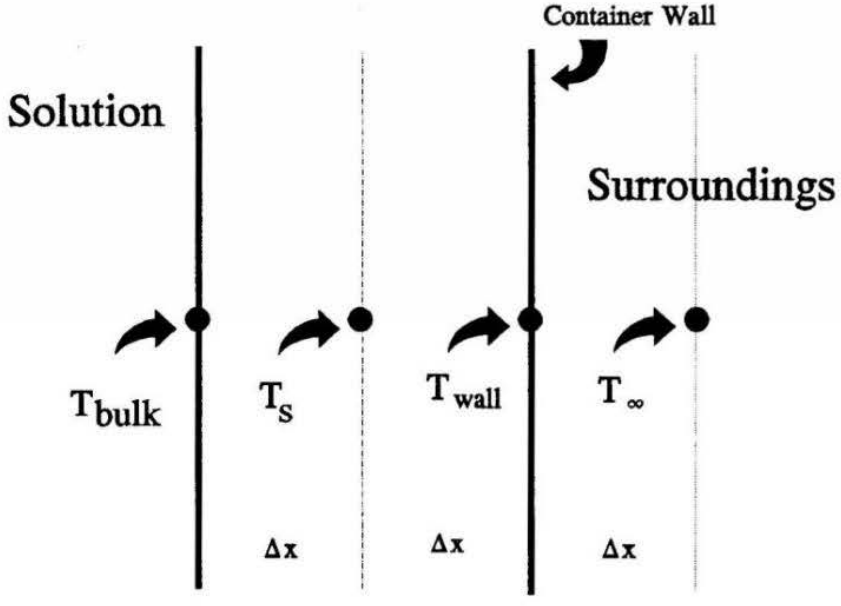

Figure 4: Schematic Used for Numerical Solution of the Unsteady State Analytical Heat Transfer Model with Convection Boundary Conditions

Equation 20 is solved in terms of T_{wall} at t-1 as follows:

$$T_{wall}^{t-1} = \frac{T_s^{t-1} + \frac{h_{fc}\,\Delta x}{K_{wall}}\,T_\infty}{1 + \frac{h_{fc}\,\Delta x}{K_{wall}}} \tag{21}$$

Substituting equations 17,18, and 21 into equation 16 and solving for the wall centerline temperature, T_s^{t-1}, gives:

$$T_s^{t-1} = T_s^{t-2} + \alpha\,\Delta t \frac{\frac{T_s^{t-2} + \frac{h_{fc}\,\Delta x}{k_{wall}}\,T_\infty}{1 + \frac{h_{fc}\,\Delta x}{k_{wall}}} - 2T_s^{t-2} + T_{bulk}^{t-1}}{\Delta x^2} . \tag{22}$$

The following energy balance is used for the OS model for the entire transient and for the COS model only after bottle pressure reaches 0.345 MPa.

$$\frac{dH_{syst}}{dt} = \dot{Q}_{gen} - \dot{Q}_{ht} - \dot{E}_{out} . \tag{23}$$

where

H_{syst} = enthalpy of a bottle (joules)
$\dot{E}_{out}$ = energy loss associated with the mass leaving the open bottle (joules/sec).

The $\dot{E}_{out}$ term in equation 21 is made up of several terms as shown below:[13]

$$\dot{E}_{out} = w_O\,h_O + w_H\,h_H + w_F\,h_F + w_{steam}\,h_{steam} , \tag{24}$$

where

w_O = mass flow rate of the oxygen leaving the bottle (kg/sec)
h_O = specific enthalpy of the oxygen (joules/kg)
w_{steam} = mass flow rate of the steam leaving the bottle (kg/sec)
h_{steam} = specific enthalpy of the steam (joules/kg)
h_H = specific enthalpy of the hydrogen (joules/kg)
w_H = mass flow rate of the hydrogen leaving the bottle (kg/sec)

h_F = specific enthalpy of the fluorine (joules/kg)
w_F = mass flow rate of the fluorine leaving the bottle (kg/sec).

The total mass of gas produced is calculated as follows:

$$w^t_{gas} = w^1_{gas} + w^2_{gas} , \tag{25}$$

where

w^t_{gas} = total production rate of gas (kg/sec)
w^1_{gas} = production rate of radiolytic gas (kg/sec)
w^2_{gas} = production rate of fission gas (kg/sec).

The mass of radiolytic gas produced (H_2 and O_2 as a result of radiolysis of water) is calculated using the following equation:[11]

$$w^1_{gas} = G\, f\, n(t) \tag{26}$$

where

G = empirically derived constant to relate the rate of radiolysis to fission power (kg of radiolytic gas/fission).

The radiolytic gas is separated into its constituents as shown below:[23]

$$w^1_H = w^1_{gas} \frac{(Atomic\ Weight\ H_2)}{(Atomic\ Weight\ H_2O)} \tag{27}$$

$$w^1_O = w^1_{gas} \frac{(Atomic\ Weight\ O_2)}{(Atomic\ Weight\ H_2O)} \tag{28}$$

where

w^1_H = production rate of radiolytic hydrogen (kg/sec)
w^1_O = production rate of radiolytic oxygen (kg/sec).

Each time a fission occurs the UO_2F_2 molecule breaks up forming O_2 and F_2. This is approximated by the following equation:

$$w^2_{gas} = w^2_O + w^2_F \tag{29}$$

where

w^2_F = production rate of fluorine gas from fission (kg/sec)
w^2_O = production rate of oxygen gas from fission (kg/sec).

The production rate is dependent on the number of fissions. One fission results in the liberation of one molecule of F_2 and one molecule of O_2. The production rate of the individual components (O_2 and F_2) is:

$$w_O^2 = \frac{(\ Atomic\ Weight\ O_2\ )\ f\ n(t)}{6.02 \times 10^{23}} \tag{30}$$

$$w_F^2 = \frac{(\ Atomic\ Weight\ F_2\ )\ f\ n(t)}{6.02 \times 10^{23}} \ . \tag{31}$$

The production rates of hydrogen, oxygen, and fluorine are used to find the total volumetric production rate of gas through application of the ideal gas law as described below:[23]

$$\dot{V}_H = \frac{w_H^1\ R_H\ T_{bulk}}{P_{syst}} \tag{32}$$

$$\dot{V}_O = \frac{(\ w_O^1 + w_O^2\ )\ R_O\ T_{bulk}}{P_{syst}} \tag{33}$$

$$\dot{V}_F = \frac{w_F^2\ R_F\ T_{bulk}}{P_{syst}} \tag{34}$$

$$\dot{V}_{gas} = \dot{V}_H + \dot{V}_O + \dot{V}_F \tag{35}$$

where

$\dot{V}_H$ = volumetric production rate of hydrogen (m^3/sec)
T_{bulk} = bulk temperature of the solution (Kelvin)
P_{syst} = system pressure (MPa)
R_H = gas constant for hydrogen (joules/kg/mole/Kelvin)
$\dot{V}_O$ = volumetric production rate of oxygen (m^3/sec)
R_O = gas constant for oxygen (joules/kg/mole/Kelvin)
$\dot{V}_F$ = volumetric production rate of fluorine (m^3/sec)
R_F = gas constant for fluorine (joules/kg/mole/Kelvin)

$\dot{V}_{gas}$ = total volumetric production rate of gas (m^3/sec).

Other models like those used by CRITEX and CREST assume that O_2 and F_2 react and, therefore, do not contribute to gas production feedback reactivity[12,13]. Three variations of the gas production model described by the above equations are considered in this study. One variation considers the reactivity effects of all three gases (H_2, F_2, and O_2). Another variation assumes only the reactivity contribution of H_2. The last variation neglects the effects of gas production altogether. The results and comparisons between these three variations are presented in Chapter III.

Quenching Coefficient Model

Quenching coefficients can be used to represent the negative reactivity feedback associated with the thermal-hydraulics of a fissile solution. The quenching coefficient feedback reactivity is calculated with the following equation:

$$\rho_{fb} = \int_0^t b\, n(t')\, dt' , \tag{36}$$

where

b = quenching coefficient, ($\Delta k/k$/fission)
ρ_{fb} = reactivity feedback associated with the thermal-hydraulics ($\Delta k/k$).

The total reactivity for the quenching coefficient model is calculated as follows:

$$\rho_{tot} = \rho_{ext} + \rho_{fb} \tag{37}$$

The quenching coefficients used herein were originally found by fitting a curve to CRAC excursion data.[9] The resultant equation for the curve is:

$$b = 7.54\times10^{-18}\ V^{-1.47} , \tag{38}$$

where

V = solution volume (m^3).

The CRAC excursion experiments involved highly enriched uranyl nitrate and are not necessarily valid for the low-enriched UO_2F_2 solution in this work. Results for the six bottle array based on quenching coefficients are presented for information only.

Reactivity

External Reactivity

The external reactivity addition rate is determined by the speed at which the bottles move together. The external reactivity is the most dominant factor in determining the magnitude and timing of the initial power pulse as well as the total energy release. Several ramp insertion rates were investigated and the results are shown later in this thesis.

Temperature Feedback Reactivity

The temperature feedback coefficient of reactivity can be attributed to changes in the cross sections (doppler effect), thermal expansion of the fluid, and spectral changes. Two reactivity feedback models are investigated in this research. In the first model all three effects are combined to create one feedback coefficient. The second feedback model treats the effects separately.

The reactivity feedback due to temperature for first model (combined feedback coefficients) is found by the following equation:

$$\rho_{temp} = \alpha_T \left(T_{bulk} - T_0 \right) , \tag{39}$$

where

α_T = temperature coefficient of reactivity ($\Delta k/k/°C$)
ρ_{temp} = reactivity feedback due to temperature ($\Delta k/k$).

The reactivity feedback due to temperature for second model (separated feedback coefficients) is found by the following equations:

$$\rho_{temp} = \rho_{te} + \rho_{dopp} \tag{40}$$

$$\rho_{dopp} = \alpha_{dopp} \left(T_{bulk} - T_0 \right) \tag{41}$$

$$\rho_{te} = \alpha_{te} \left(D_{bulk} - D_0 \right) , \tag{42}$$

where

α_{dopp} = reactivity coefficient due to the doppler effect ($\Delta k/k/°C$)
α_{te} = reactivity coefficient due to thermal expansion ($\Delta k/k/m^3$)
D_{bulk} = bulk density of the fluid (kg/m^3)
D_0 = initial density of the fluid (kg/m^3)
ρ_{dopp} = reactivity feedback due to the doppler effect ($\Delta k/k$)
ρ_{te} = reactivity feedback due to thermal expansion ($\Delta k/k$).

Radiolytic Gas Feedback Reactivity

The production and subsequent release of radiolytic gas provides the driving force for the power pulses which occur after the initial power pulse. Realistically, the first power pulse has the most significant effect on the total energy release, but subsequent pulses can still cause significant radiation exposures if personnel are nearby.

The reactivity feedback from gas production is not well understood.[12] Operational experience with power reactors indicates that radiolytic gas is produced under a neutron flux and this gas will recombine to form water under a gamma flux. In a criticality

accident, such as hypothesized here, a relatively small amount of fission products are produced (as compared to a power reactor), so recombination is not a factor. The gases produced are somewhat soluble and should remain in solution until a particular threshold is reached. For the purposes of this study, the threshold is $1x10^{-4}$ grams of radiolytic gas per gram of solution.[11] An alternate approach is to base this threshold on the fission density.[12] The threshold based on the fission density assumes a flux shape and the radiolytic gas is released based on the fission density in a particular area of the system. This approach is not appropriate for the bulk averaged thermal-hydraulic model used in this study since a multi-node thermal-hydraulic model would be required.

The rate at which the radiolytic gas comes out of solution once the threshold is reached has a profound effect on the magnitude, duration and timing of the subsequent pulses. The model developed in this work makes use of a factor referred to as a volume reduction factor which controls the rate at which dissolved gases leave the solution. This factor is related to the bubble velocity used by other models.[12,13] The volume of gas released is approximated by the following equation:

$$V_{released} = \frac{\dot{V}_{gas}}{VRF} , \tag{43}$$

where

$V_{released}$ = volume of gas released (m^3)
VRF = volume reduction factor (sec^{-1}).

The total volume of gas in solution at a particular time is calculated as:

$$V_{gas}]_t = V_{gas}]_{t-1} + V_{produced} - V_{released} , \tag{44}$$

where

$V_{gas}]_t$ = volume of gas in solution at time t (m^3)
$V_{gas}]_{t-1}$ = volume of gas in solution at time t-1 (m^3)
$V_{produced}$ = volume of gas produced between t-1 and t (m^3).

The reactivity feedback is calculated by:

$$\rho_{gas} = \beta_{gas} (V_{gas}]_t - V_0) \quad (45)$$

where

β_{gas} = gas reactivity feedback coefficient ($\Delta k/k/m^3$).

The term, β_{gas} is calculated using XSDRNPM as shown in Appendix A.

The volume of gas produced during a time step and used in equation 46 is found by:

$$V_{produced} = \dot{V}_{gas} \Delta t \quad (46)$$

The volume of gas released is used to find the mass of gas released because the threshold for gas release is based on the ratio of the mass of the solution in the bottle to the mass of gas in solution. Therefore, the mass of the solution is recalculated at each time step in order to recalculate the threshold for gas release. The mass of gas in solution and the total mass of the solution in the bottle are given by the following equations:

$$m_{gas}]_t = m_{gas}]_{t-1} + m_{produced} - m_{released} \quad (47)$$

$$m_{solution}]_t = m_{solution}]_{t-1} - m_{released} - m_{steam}]_{t-1} , \quad (48)$$

where

$m_{gas}]_t$ = mass of gas in solution at time t (kg)
$m_{gas}]_{t-1}$ = mass of gas in solution at time t-1 (kg)
$m_{produced}$ = mass of gas produced between t-1 and t (kg)
$m_{released}$ = mass of gas released between t-1 and t (kg)
m_{steam} = mass of steam produced (kg)
$m_{solution}]_t$ = mass of solution at time t (kg)

$m_{solution}]_{t-1}$ = mass of solution at time t-1 (kg).

The mass of gas produced is given by:

$$m_{produced} = w^{t}_{gas} \, \Delta t \ . \tag{49}$$

The mass of gas released is calculated by the following ideal gas relationship:

$$m_{released} = \frac{V_{released} \, P_{syst}}{R_{ave} \, T_{bulk}} \ , \tag{50}$$

where

R_{ave} = average gas constant for the gas in solution (joules/kg · mole · Kelvin).

Steam Feedback Reactivity

The production and subsequent release of steam significantly affects the power production. Steam production can introduce a significant amount of negative reactivity. For this study the steam does not buildup in the solution. The steam produced in a particular time step only contributes to total reactivity in that time step and is released from solution in the next time step. The mass of steam produced during Δt is approximated using the following equation:

$$m_{steam} = \frac{H_{syst} - H_{f}}{h_{fg}} \ , \tag{51}$$

where

H_{syst} = enthalpy of the system (joules)
H_f = enthalpy of the saturated liquid (joules)
h_{fg} = heat of vaporization of the fluid (joules/kg).

The volume of steam produced is given by:

$$V_{steam} = m_{steam} \, v_{steam} \ , \tag{52}$$

where

V_{steam} = volume of steam produced (m^3)
v_{steam} = specific volume of the steam (m^3/kg).

The reactivity feedback due to steam production is then calculated using the following equation:

$$\rho_{steam} = \beta_{steam} V_{steam} , \quad (53)$$

where

β_{steam} = steam reactivity feedback coefficient ($\Delta k/k/m^3$).

The term, β_{steam}, is calculated using XSDRNPM as shown in Appendix A.

LSODE Considerations

LSODE is the differential equation solver used in this work. LSODE uses the Gear Method to solve the equations.[5] An explicit "F" subroutine is written by the user to define the differential equations and any calculations which are coupled to the differential equations. Many of the previous equations are solved within LSODE which means that such calculations are performed inside the "F" subroutine. Originally everything was solved within or by LSODE, but the run time was so long that adjustments had to be made. Slowly, equations were backed out of LSODE until, for the six bottle array, 14 differential equations were solved by LSODE. The differential equations solved by LSODE are the point kinetics equations, the total energy release, and the six differential energy balances for the six bottle array. The analytical heat transfer model, the steam table evaluations, and gas production are the only calculations performed outside of LSODE. All other equations are treated within the "F" subroutine. The size of the LSODE edit time step varies from 0.01 seconds for the 0.5 $/sec ramp to 0.00005 seconds for the 35.0 $ step.

Numerical Solution Procedure

The general procedure used in the solution of the equations begins with the initial conditions which are

T_{bulk} = 20.0°C

P_{syst} = 0.021 MPa

$n(t)$ = 2496.0 fissions/sec

C_i = $\beta_i + n(t)/(\lambda_i \Lambda_i)$

t = 0.0 sec

U_{syst} = 83.93121 KJ (closed system)

H_{syst} = 83.93525 KJ (open system)

v_{syst} = 1/288.38097 m^3/kg

V_{gas} = V_0

V_{steam} = 0.0 m^3.

The initial conditions are input into LSODE along with fourteen equations: namely, equations 1, 2 (which really represents six equations), 4, and six energy balance equations (either equation 9 or 23). The Q_{ht} and E_{out} terms in the heat balance equations involve T_{bulk} which is an unknown quantity at time, t. However, T_{bulk} is a known quantity at time t-1 because it is evaluated at t-1 using steam table correlations based on the energy and the specific volume which is known at t-1. Thus, T_{bulk} is lagged one time step. After LSODE returns values of $n(t)$, $C_i(t)$, $P_{fiss}(t)$, and either $U_{syst}(t)$, or $H_{syst}(t)$, then the bulk temperature is evaluated at time t using steam table correlations, and LSODE is called again to perform calculations for the next time step. The transients were computed using a DEC model 3100 VAX workstation located in the Nuclear Engineering Department of the University of Tennessee-Knoxville.

CHAPTER III

Results

Reactivity Effects

Five reactivity effects are considered in this work. The reactivity effects are the external driving force, temperature, pressure, gas production, and steam production. Another feedback effect which is referred to as cavitation is not considered.[29]

The external reactivity addition rate is dependent on the surface separation distance of the bottles. In this study the worst case is used in which the final separation distance is zero. The system is subcritical at and beyond a separation distance of 2 cm (0.8 inches) as shown in Appendix A. The point at which the system goes critical can also be observed from the experiments performed by E. B. Johnson and described earlier.[2] The external reactivity addition rate is also dependent on the speed at which the bottles move together. Table 3 illustrates the relationship between external reactivity and the speed at which the bottles move. These calculations were performed to assess the feasibility of the postulated external reactivity addition rates. As can be observed, all of the ramp rates are possible. The results for various postulated reactivity addition rates are shown later in this chapter.

Table 3: Reactivity Addition Rate vs. Bottle Speed

Reactivity Addition Rate ($/sec)	Calculated Speed (cm/sec)
0.5	0.03
1.0	0.05
2.0	0.11
5.0	0.37
35.0	1.86

All feedback coefficients in this work were calculated using XSDRNPM.[30] The six bottle array was modeled in XSDRNPM as a multi-region one-dimensional slab as shown in Figure 5.

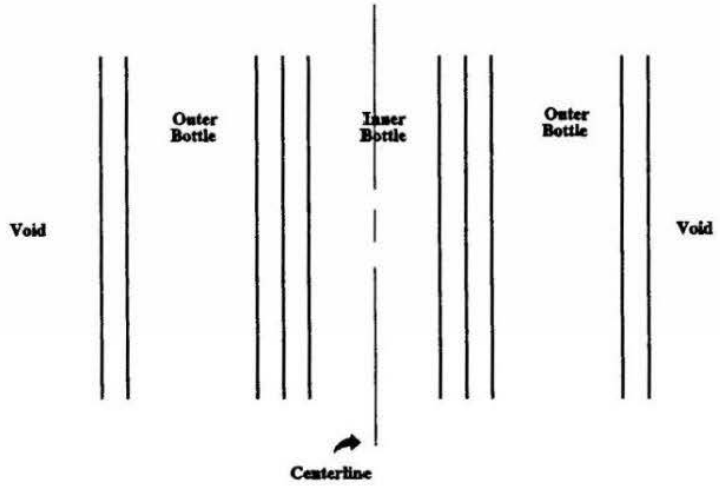

Figure 5: XSDRNPM Model

The results of the XSDRNPM calculations and some associated hand calculations are shown in Appendix A. The values of the reactivity feedback coefficients which were used in SKINATH-AR for the six bottle array (both the inner and outer bottles as shown in Figures 2 and 5) are shown in Table 4.

Table 4: Reactivity Feedback Coefficients for the Six Bottle Array

	α_T $\Delta k/k/°C$	β_{gas} $\Delta k/k/m^3$	β_{steam} $\Delta k/k/m^3$
Six Bottle Array (Outer Bottle)	-3.0×10^{-4}	-39.1	-29.3
Six Bottle Array (Inner Bottle)	-8.4×10^{-5}	-34.5	-25.0

Generation Time Data

As stated previously, the mean generation time was calculated by KENO.[20] The KENO results and comparisons with other calculations are shown in the Table 5.

Table 5: Generation Time Data

	KENO (sec)	CREST (sec)	CRITEX (sec)	Reference 9 (sec)
CRAC 05	3.66×10^{-5}	3.7×10^{-5}	3.7×10^{-5}	2.0×10^{-4}
CRAC 09	3.28×10^{-5}	N/A	Unknown	2.0×10^{-4}
CRAC 10	3.11×10^{-5}	N/A	3.1×10^{-5}	2.0×10^{-4}
CRAC 12	3.14×10^{-5}	N/A	3.1×10^{-5}	2.0×10^{-4}
CRAC 13	3.04×10^{-5}	N/A	3.1×10^{-5}	2.0×10^{-4}
CRAC 16	3.58×10^{-5}	Unknown	N/A	2.0×10^{-4}
CRAC 19	2.98×10^{-5}	N/A	3.05×10^{-5}	2.0×10^{-4}
SHEBA	3.27×10^{-5}	N/A	Unknown	N/A
Six Bottle Array	3.33×10^{-5}	N/A	N/A	N/A

Initial Shape Function Calculation

The shape function is important in determining the power distribution in the system.[26] This calculation was performed with XSDRNPM using the slab model discussed previously. Figure 6 shows the normalized power as a function of position.

XSDRNPM was used primarily because of low computing costs. This shape was calculated at t=0 and is assumed to be constant throughout the transient.

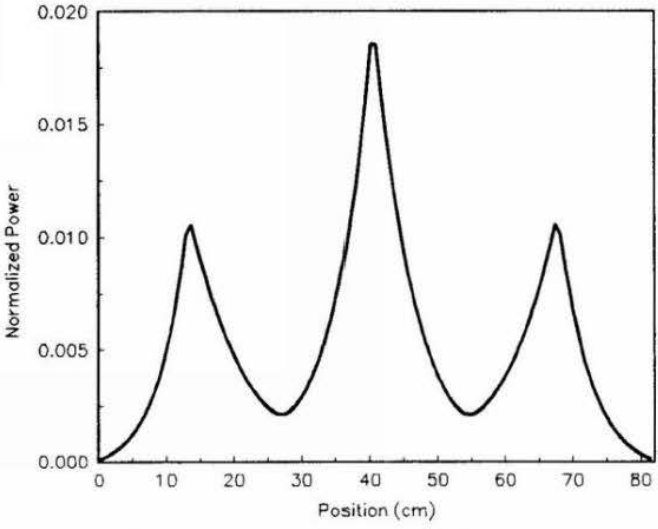

Figure 6: Initial Power Calculation

Transient Results

References Cases

The transient results for the six bottle array are presented in Table 6. OS is the model in which the bottle remains open to the atmosphere throughout the transient. COS is the model in which the bottle is initially closed and becomes an open system when the internal pressure reaches 0.345 MPa. QC represents results obtained using quenching coefficients.

The models which are used in computing the results shown for the COS model were selected based on sensitivity studies which follow. These cases which are referred to as reference cases use; the gas production model which considers only H_2 contribution

to reactivity, the start from delayed critical approach, an initial power of 2496.0 fissions/sec, feedback coefficients as calculated by XSDRNPM, the empirical heat transfer model, and the combined temperature feedback coefficient model. Delay times were not used because they were so small in magnitude.

The OS model uses the same reference cases as are used in computing the COS model results. The only difference is the use of the OS thermal-hydraulic model instead of the COS model.

Table 6: Results for the Six Bottle Array System using the Three Models

Reactivity Insertion Rate	Method	Time of Peak	Peak Power (fissions/sec)	Total Energy (fissions)
0.5 $/sec Ramp	QC	2.60	1.4×10^{17}	2.0×10^{17}
	COS	2.57	3.1×10^{16}	3.3×10^{16}
	OS	2.65	2.2×10^{17}	4.2×10^{17}
1.0 $/sec Ramp	QC	1.45	8.9×10^{17}	4.5×10^{17}
	COS	1.46	5.4×10^{16}	6.1×10^{16}
	OS	1.55	3.5×10^{18}	5.4×10^{17}
2.0 $/sec Ramp	QC	0.90	3.7×10^{18}	9.4×10^{17}
	COS	0.85	1.2×10^{17}	1.3×10^{17}
	OS	0.90	8.2×10^{18}	1.0×10^{18}
5.0 $/sec Ramp	QC	0.50	7.7×10^{18}	2.4×10^{18}
	COS	0.44	3.1×10^{17}	8.7×10^{17}
	OS	0.50	8.4×10^{18}	3.1×10^{18}
35.0 $/sec Ramp	QC	0.30	4.5×10^{19}	4.0×10^{18}
	COS	0.12	8.7×10^{17}	1.1×10^{18}
	OS	0.13	6.8×10^{19}	4.2×10^{18}
35.0 $ Step	QC	0.01	4.7×10^{21}	7.7×10^{18}
	COS	0.01	1.9×10^{22}	3.2×10^{18}
	OS	0.01	1.2×10^{20}	4.5×10^{18}

The COS model is believed to be more realistic thermal-hydraulically than the OS models, but the OS model gives a higher peak power and higher total energy release for all reactivity insertion rates with the exception of the peak power results for the 35.0 $ step. The OS thermal-hydraulic model also has the advantage of being validated by comparison with experimental results and has shorter computing times when compared with similar COS transients. Thus, the OS model was selected for use in the sensitivity studies which follow. The 1.0 $/sec ramp was selected for the following sensitivity studies in order to avoid long computing times.

The transient results for the three models are shown in figures 7, 8, and 9. For the 0.5 $/sec ramp using the COS model, the power drops sharply from about 10^{15} to 10^{14} fissions/sec at about 5 sec. This is the point where three of the six bottles rupture. For the 0.5 $/sec ramp using the OS model, the power drops sharply from about 10^{17} to 10^{14} fissions/sec at approximetely 16 sec. This is the point where the fluid inside three of the six bottles begins to boil. These processes are repeated at various times, depending on the external reactivity addition rate, in all of the results contained in this chapter.

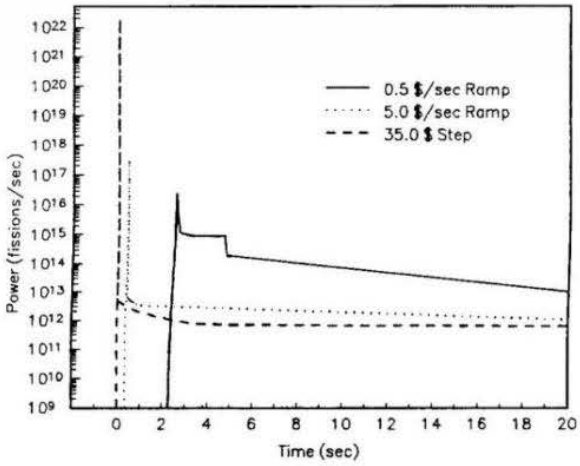

Figure 7: Reference Case Results for Three Postulated Reactivity Addition Rates for the Six Bottle Array using the COS Model

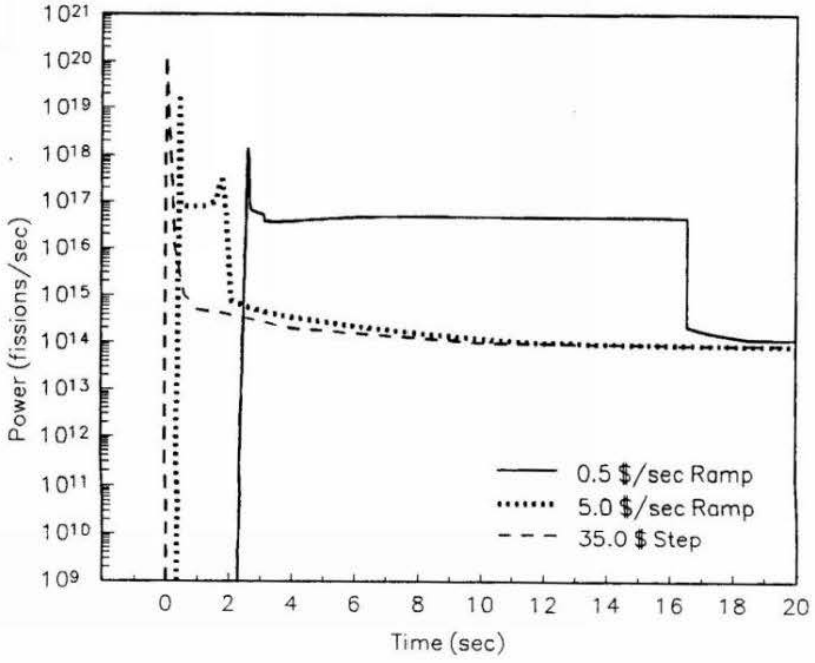

Figure 8: Reference Case Results for three Postulated Reactivity Addition Rates for the Six Bottle Array using the OS Model

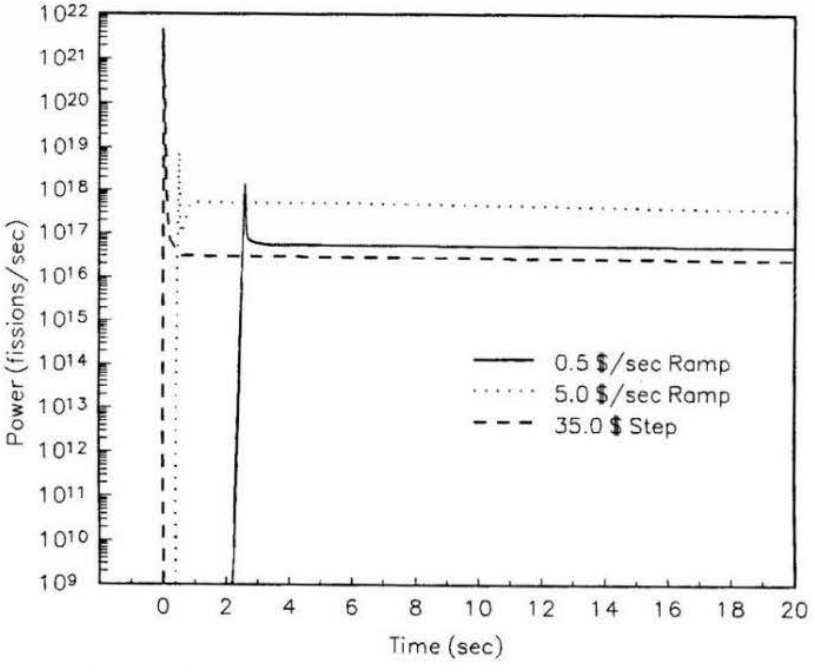

Figure 9: Results for three Postulated Reactivity Addition Rates for the Six Bottle Array using the QC Model

Figures 10, 11, and 12 show the power as a function of time along with the corresponding total energy release for the COS, OS, and QC models for a 1.0 $/sec ramp. The OS model results in the largest total energy release and the highest peak power.

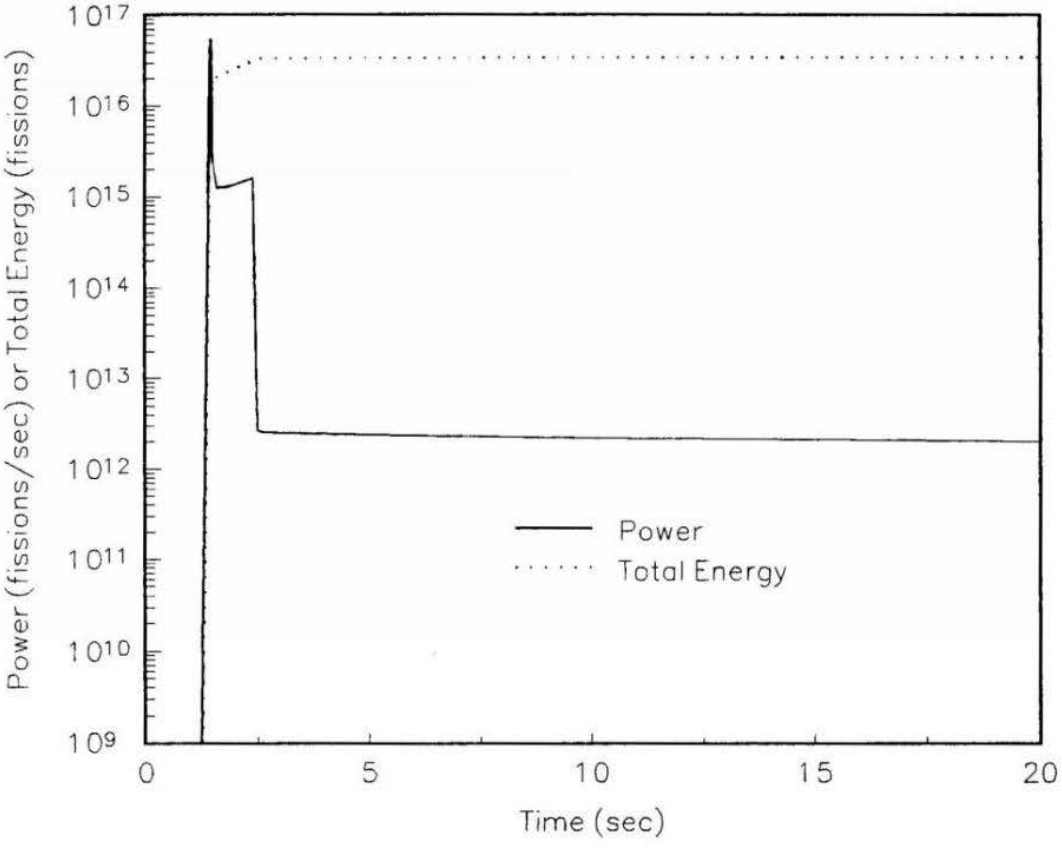

Figure 10: Power vs. Time for a Ramp of 1.0 $/sec using the COS Model (Reference Case Results)

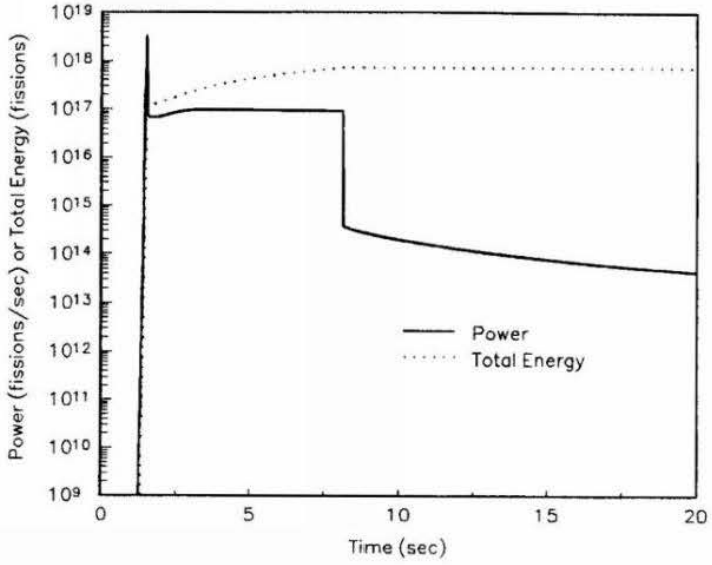

Figure 11: Power vs. Time for a Ramp of 1.0 $/sec using the OS Model (Reference Case Results)

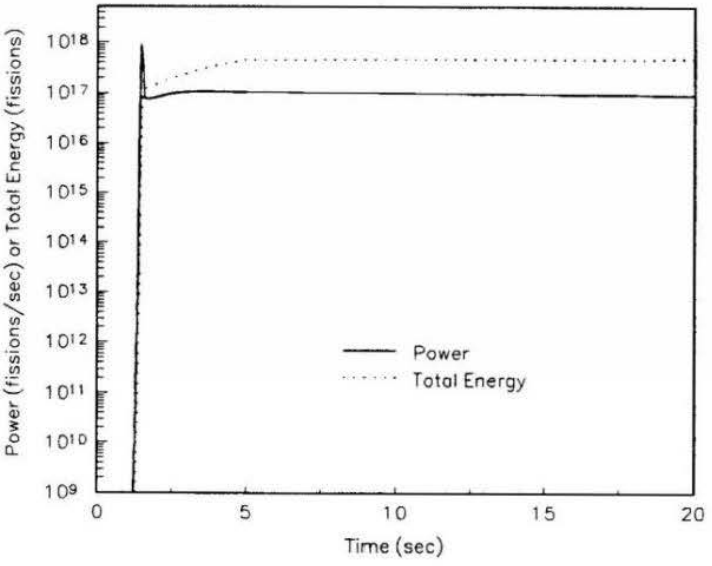

Figure 12: Power vs. Time for a Ramp of 1.0 $/sec using the QC Model

Figures 13 and 14 show the bulk bottle temperature as a function of time for the six bottle array with a 1.0 $/sec ramp using the COS and OS models. Both the inner and

outer bottle temperatures are shown. The majority of the energy is produced in the inner bottles. As can be seen from figures 13 and 14, the resulting temperature is significantly higher in the inner bottles.

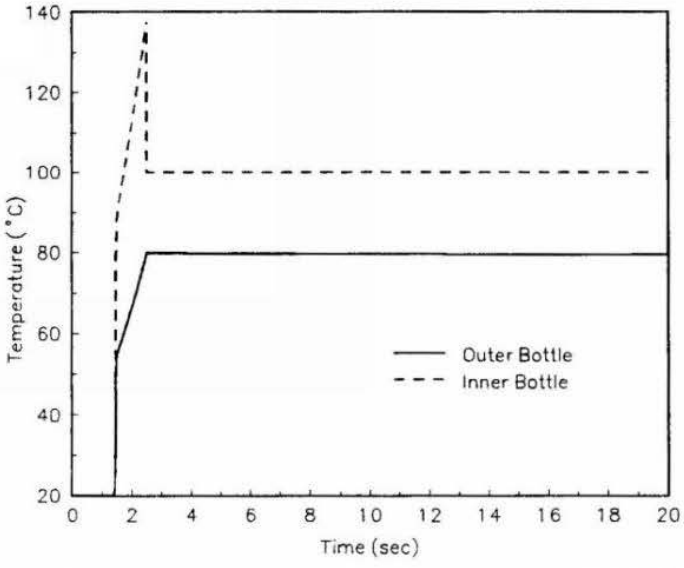

Figure 13: Temperature vs. Time for a Ramp of 1.0 $/sec using the COS Model (Reference Case Results)

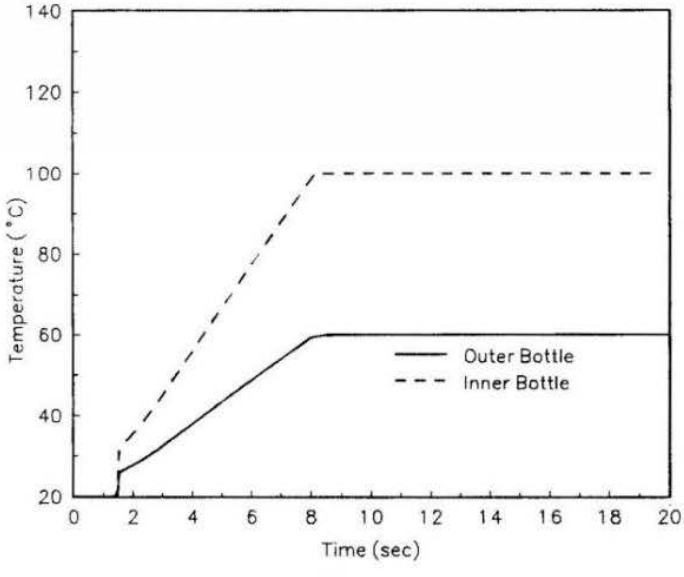

Figure 14: Temperature vs Time for a Ramp of 1.0 $/sec using the OS Model (Reference Case Results)

Figures 15 and 16 show the pressure as function of time for the six bottle array with various reactivity insertion rates using the COS model, both inner and outer bottles. Again the most energetic transient is the 35.0 $ step. When the pressure drops to 0.101 MPa, the bottles have ruptured. For the 35.0 $ step all six bottles rupture near the power peak. For some of the more energetic transients (the 35.0 $ step) the pressure may exceed 0.345 MPa. This is due to the numerical nature of the solution technique and, therfore meaningless. For the 5.0 and 0.5 $/sec ramps only the inner bottles rupture.

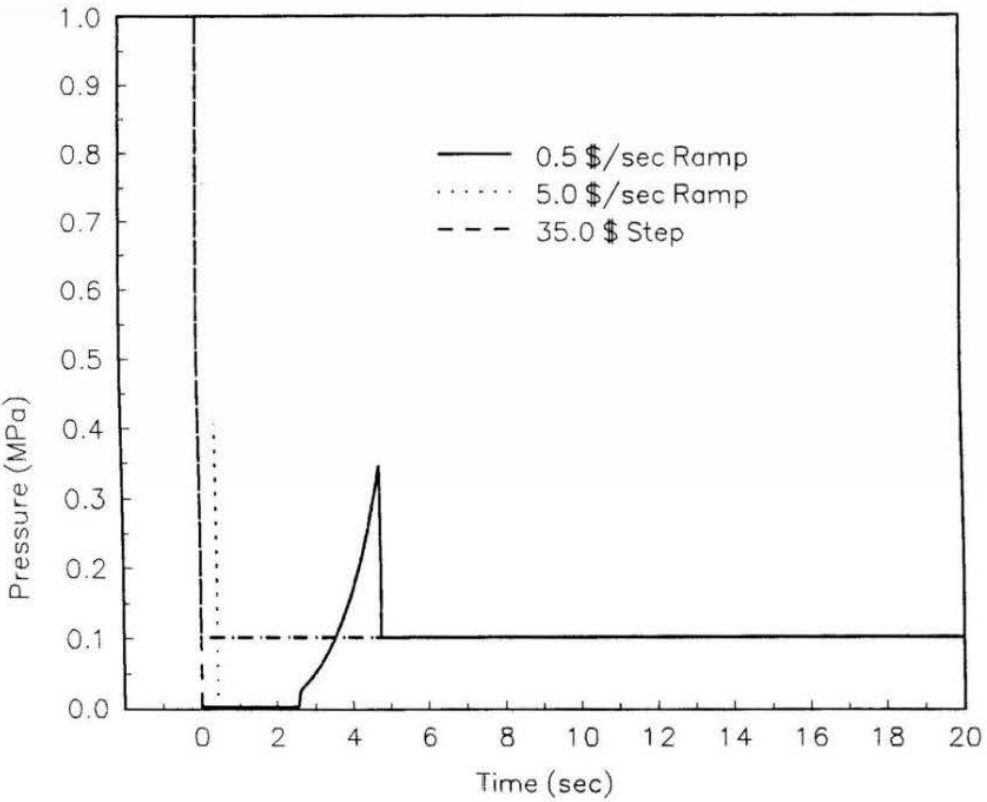

Figure 15: Pressure vs. Time for a Ramp of 1.0 $/sec using the COS Model (Inner Bottle): Reference Case Results

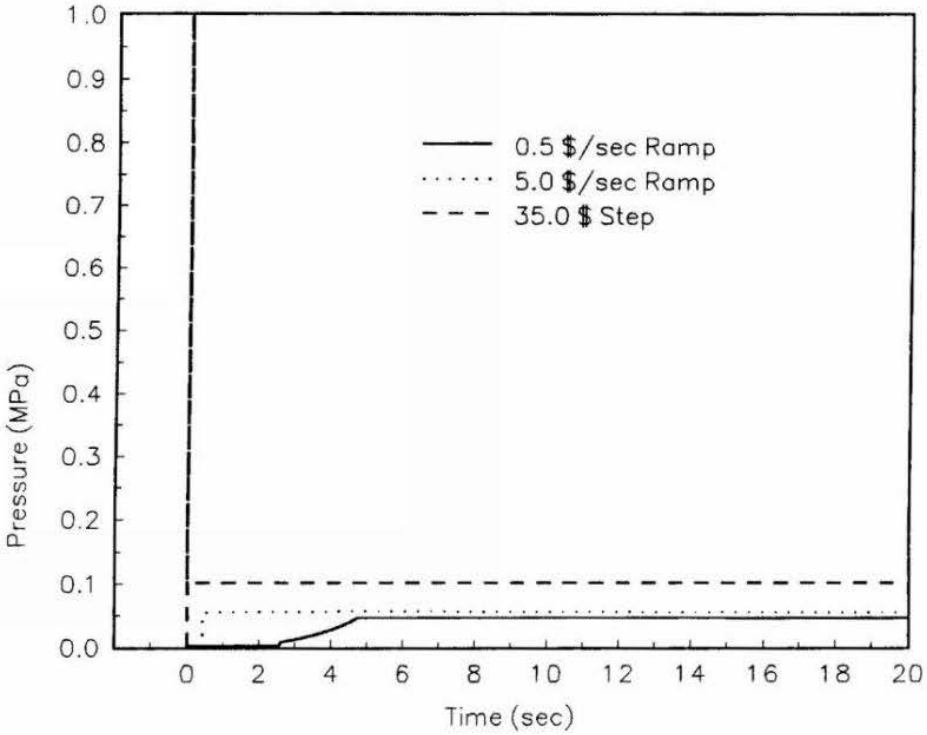

Figure 16: Pressure vs. Time for a Ramp of 1.0 $/sec using the COS Model (Outer Bottle): Reference Case Results

Heat Transfer Models

This section shows the difference in results obtained with the analytical heat transfer model and the empirical heat transfer model. Results are presented for CRAC 05 and the six bottle array using the OS model and a 1.0 $/sec ramp. These two heat transfer models were discussed in Chapter III. The heat transfer is only significant when the transient is slow.[12] The CRAC 05 experiment is considered to be a slow transient because the initial power peak occurs at more than 10 seconds after the transient begins, and the six bottle array is a fast transient because the initial power peak occurs at less than 5 seconds after the transient begins. The results of this study show that the choice

of heat transfer models is not really important for analysis of the six bottle array.

Figure 17 shows the power as a function of time using the two heat transfer models for CRAC 05. The peak power using the analytical heat transfer model is 4.0×10^{16} fissions/sec and the total energy release is 3.1×10^{16} fissions. The peak power using the empirical heat transfer model is 5.5×10^{16} fissions/sec and the total energy release is 5.8×10^{16} fissions. As can be seen from figure 17, the second power pulse using the analytical model lags slightly behind the empirical model and the experiment. The empirical heat transfer model gives better agreement with the experiment (with regard to power and total energy release) and it also has the advantage of having a significantly shorter computer time. Therefore, the empirical heat transfer model was selected for use in the remaining studies presented in this work.

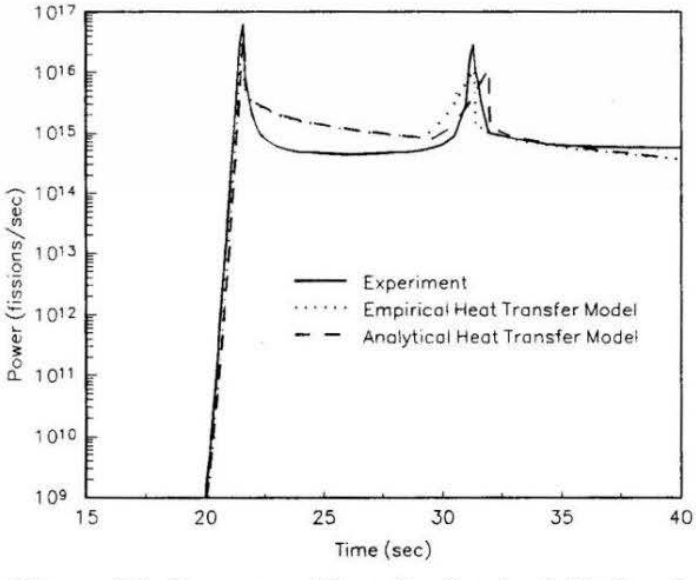

Figure 17: Power vs. Time for the Analytical and Empirical Heat Transfer Models for CRAC 05

Figure 18 shows the power as a function of time for the six bottle array using a 1.0 \$/sec ramp with both the empirical and analytical heat transfer models. The peak power using the analytical heat transfer model is 3.4×10^{18} fissions/sec and the total energy release is 5.3×10^{17} fissions. The peak power using the empirical heat transfer model is 3.5×10^{18} fissions/sec and the total energy release is 5.4×10^{17} fissions. For the six bottle array, the difference between heat transfer models appears to be so slight that it does not matter which model is used.

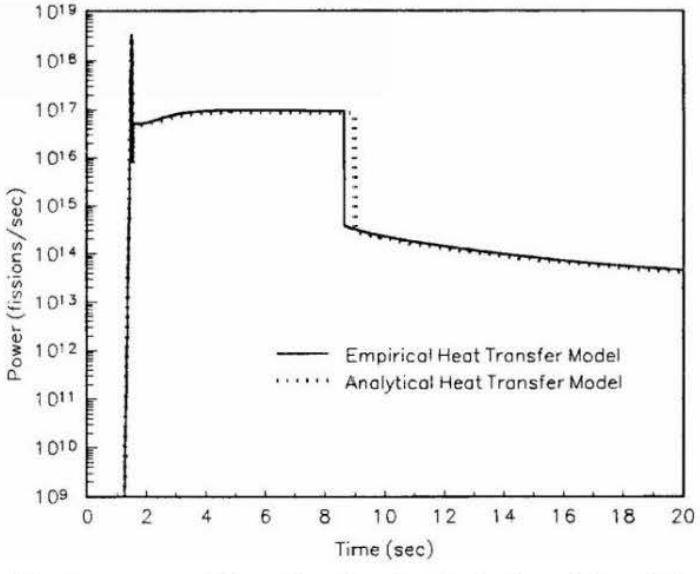

Figure 18: Power vs. Time for the Analytical and Empirical Heat Transfer Models for a 1.0 \$/sec Ramp using the OS Model

Gas Production Models

This section illustrates the difference in results obtained with three variations of the gas production models for CRAC 05. The three variations discussed here were described previously. The first variation (labeled "Hydrogen Only" on Figure 19) considers only hydrogen reactivity feedback effects and neglects all other gases. The

second variation (labeled "Hydrogen, Oxygen, and Nitrogen" on figure 19) considers hydrogen, oxygen, and nitrogen reactivity feedback effects. The third variation (labeled "No Gas" on figure 19) neglects the reactivity feedback of any gas which is produced.

The peak power using the hydrogen only variation is 5.5×10^{16} fissions/sec and the total energy release is 5.8×10^{16} fissions. The peak power using the hydrogen, oxygen, and nitrogen variation is 5.4×10^{16} fissions/sec and the total energy release is 5.5×10^{16} fissions. Using the no gas variation, the peak power is 5.5×10^{16} fissions/sec and the total energy release is 5.9×10^{16} fissions. The variation which considers only hydrogen contribution to reactivity has the best agreement with the experiment. The array system was not considered in this parametric study because feedback from radiolytic gas production is not well understood and there are no experimental results with which to compare.

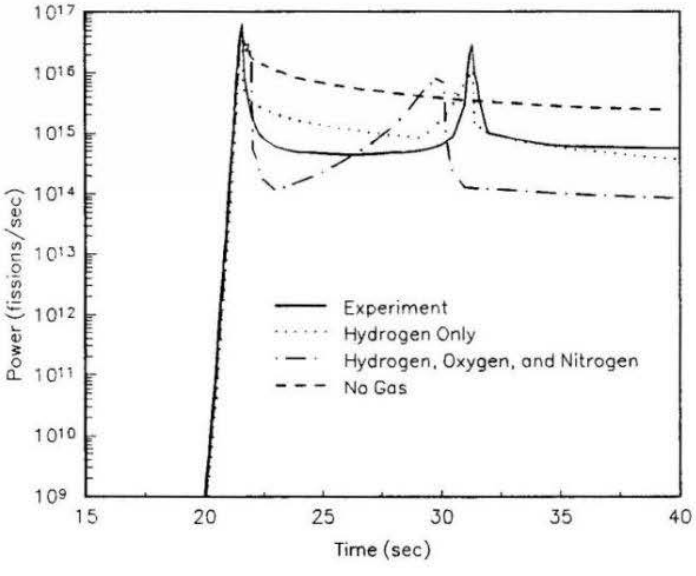

Figure 19: Power vs. Time for the Different Gas Production Models for CRAC 05

Initial Power Sensitivity

In this section the effect of changing the initial power is observed. The initial power was varied between 1.0 and 10^9 fissions/sec. The initial power has only a slight effect on the peak power and the total energy released, but it does affect the timing of the subsequent power pulses.

The results of this study for CRAC 05 are shown in figure 20. For an initial power of 1.0 fissions/sec, the peak power is 6.6×10^{16} fissions/sec and the total energy release is 6.4×10^{16} fissions. For 123.0 fissions/sec, the peak power is 5.5×10^{16} fissions/sec and the total energy release is 5.8×10^{16} fissions. For 10^9 fissions/sec, the peak power is 2.0×10^{16} fissions/sec and the total energy release is 1.8×10^{16} fissions.

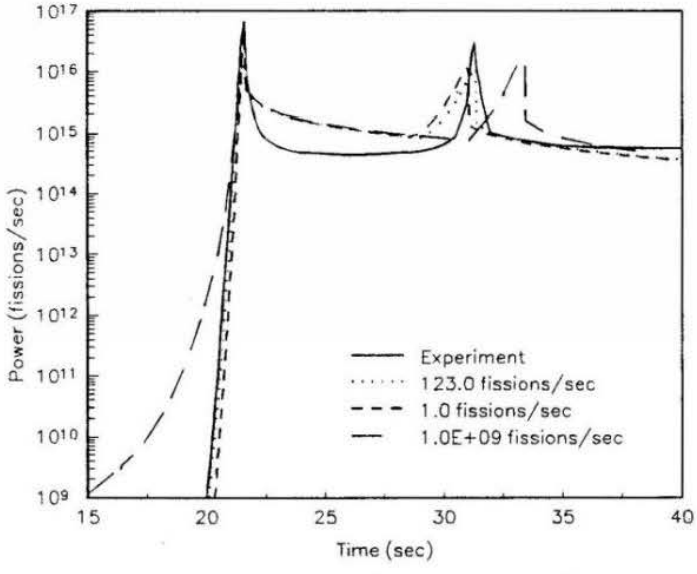

Figure 20: Power vs. Time for the Different Initial Powers for CRAC 05

The results of this study for the six bottle array are shown in figure 21. For an initial power of 1.0 fissions/sec, the peak power is 1.9×10^{18} fissions/sec and the total energy release is 4.0×10^{17} fissions. For 2496.0 fissions/sec, the peak power is 3.5×10^{18}

fissions/sec and the total energy release is 5.4×10^{17} fissions. For 10^{9} fissions/sec, the peak power is 1.4×10^{18} fissions/sec and the total energy release is 9.1×10^{16} fissions.

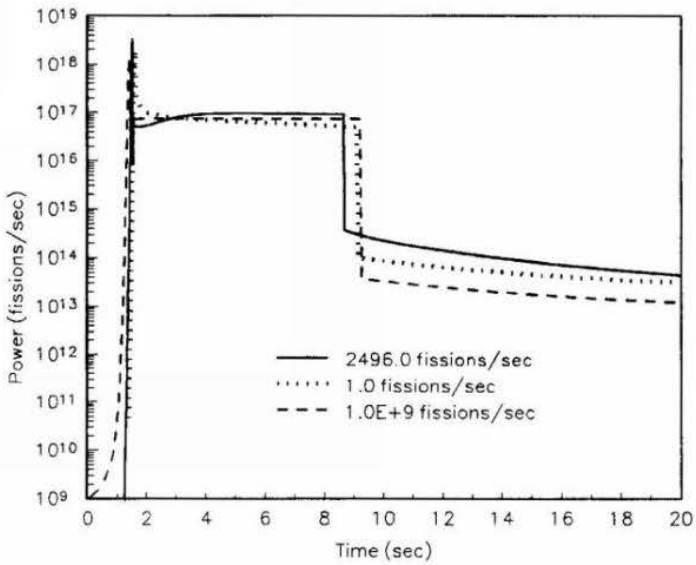

Figure 21: Power vs. Time for the Different Initial Powers for a 1.0 $/sec Ramp using the OS Model

Effect of Starting at Subcritical

In this section the effect of beginning the transient at subcritical with a source present vs. delayed critical without a source is observed. The calculations were performed as in reference 15. The source for the CRAC 05 study is 123.0 neutrons/sec. The source for the six bottle array is 2496.0 neutrons/sec. This parametric study was conducted for both CRAC 05 and the six bottle array.

The results of this study for CRAC 05 are shown in figure 22. For the delayed critical situation, the peak power is 5.5×10^{16} fissions/sec and the total energy release is 5.8×10^{16} fissions. For the subcritical situation, the initial power is 0.1 neutrons (corresponds to 689.1 fissions/sec) and the source strength is 123.0 neutrons/sec.[15] The

peak power is 5.0×10^{16} fissions/sec and the total energy release is 4.1×10^{16} fissions. The subcritical case was shifted to show the comparisons in figure 22. The initial peak occurred at 34.6 sec as compared with 21.6 sec for the experiment and the delayed critical cases.

The results of this study for the array system are shown in figure 23. For the delayed critical situation, the peak power is 3.5×10^{18} fissions/sec and the total energy release is 5.4×10^{17} fissions. For the subcritical situation, the initial power is 0.1 neutrons (corresponds to 689.1 fissions/sec) and the source strength is 2496.0 neutrons/sec.[15] The corresponding peak power is 3.3×10^{18} fissions/sec and the total energy release is 5.3×10^{17} fissions. The peak power for the subcritical case lags behind the delayed critical case. The differences are small, but the delayed critical case requires much less computer time and was used for all further studies.

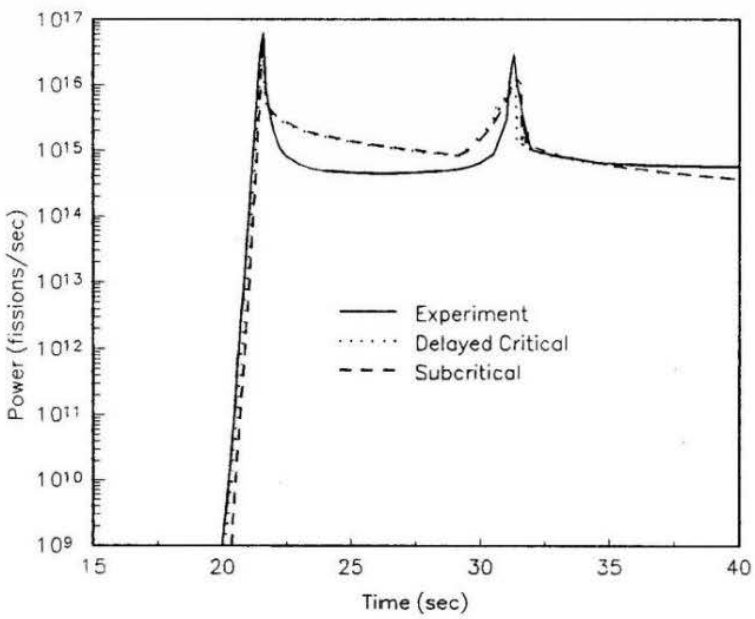

Figure 22: Power vs. Time for Starting at Delayed Critical and Starting at Subcritical for CRAC 05

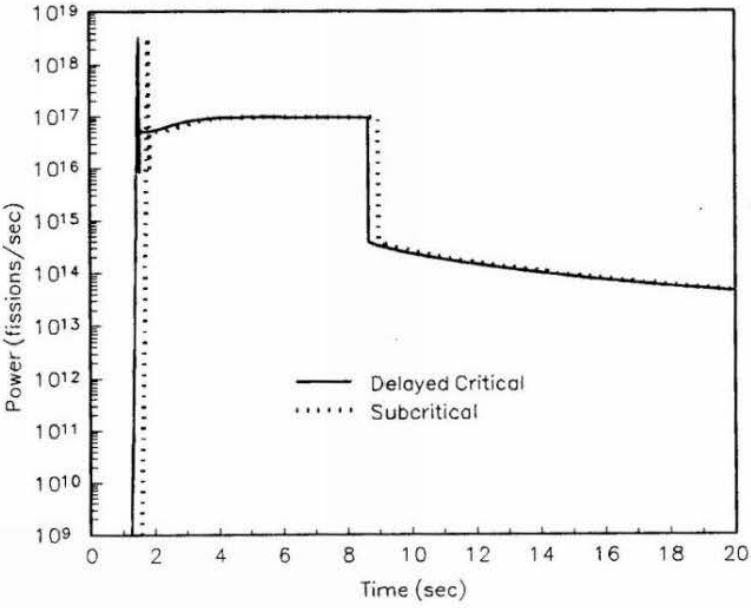

Figure 23: Power vs. Time for Starting at Delayed Critical and Starting at Subcritical for a 1.0 $/sec Ramp using the OS Model

Feedback Coefficient Sensitivity

In this section the effect of changing the reactivity feedback coefficients is evaluated. Temperature feedback coefficients were varied for both CRAC 05 and the array system and gas feedback coefficients were varied for CRAC 05 only for the same reasons as before. Steam feedback coefficients were not varied because there is no way to verify or validate the results.

The results are shown in figure 24 and Table 7. The temperature feedback coefficient (α_T) was varied between -9.0×10^{-5} and -1.0×10^{-3} $\Delta k/k/°C$ for CRAC 05. Numerical difficulties were encountered when α_T was less than -9.0×10^{-5} $\Delta k/k/°C$. When α_T is -7.1×10^{-4} $\Delta k/k/°C$ (value calculated by XSDRNPM) there is good agreement with the experiment with regard to the peak power and total energy release.

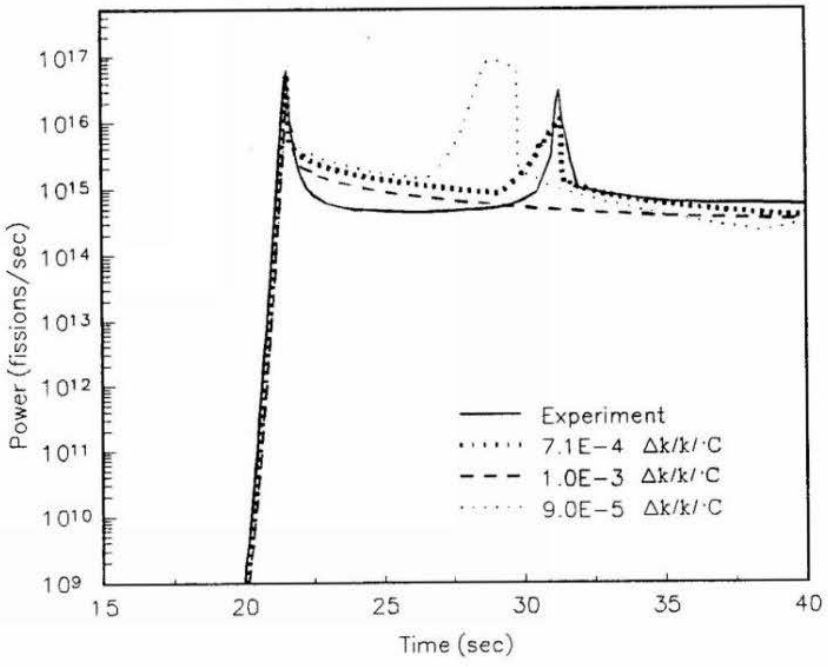

Figure 24: Power vs. Time for Various Values of α_T for CRAC 05

Table 7: Results of SKINATH-AR for Different Values of α_T

CRAC 05			
α_T ($\Delta k/k/°C$)		Peak Power (fissions/sec)	Total Energy Release (fissions)
-9.0×10^{-5}		4.4×10^{16}	1.4×10^{17}
-7.1×10^{-4}		5.5×10^{16}	5.8×10^{16}
-1.0×10^{-3}		1.6×10^{16}	1.7×10^{16}
Six Bottle Array			
Inner	Outer		
-5.0×10^{-5}	-1.0×10^{-4}	3.1×10^{18}	4.2×10^{17}
-8.9×10^{-5}	-3.0×10^{-4}	3.5×10^{18}	5.4×10^{17}
-1.0×10^{-4}	-1.0×10^{-3}	1.9×10^{17}	5.1×10^{17}

For the array, α_T was varied between -1.0×10^{-4} and -1.0×10^{-3} $\Delta k/k/°C$ for an outer bottle and between -5.0×10^{-5} and -5.0×10^{-4} $\Delta k/k/°C$ for an inner bottle. The results are shown in figure 25 and in Table 7.

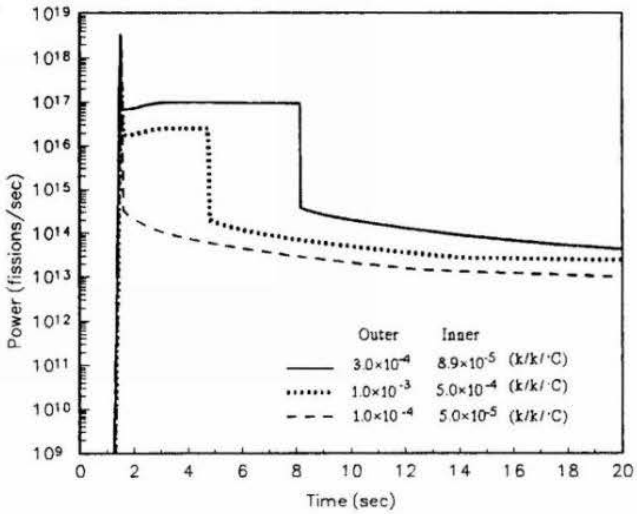

Figure 25: Power vs. Time for Various Values of α_T for a 1.0 \$/sec Ramp using the OS Model

The gas feedback coefficient (β_{gas}) was varied between -10.0 and -50.0 $\Delta k/k/m^3$ for CRAC 05. As seen in figure 26 and Table 8, when β_{gas} is -35.3 $\Delta k/k/m^3$ (value calculated by XSDRNPM) there is good agreement with the experiment.

Table 8: Results of SKINATH-AR for Different Values of β_{gas}

CRAC 05		
β_{gas} ($\Delta k/k/m^3$)	Peak Power (fissions/sec)	Total Energy Release (fissions)
-35.3	5.5×10^{16}	5.8×10^{16}
-10.0	4.9×10^{16}	6.3×10^{16}
-50.0	3.3×10^{16}	1.4×10^{16}
Experiment	6.3×10^{16}	6.3×10^{17}

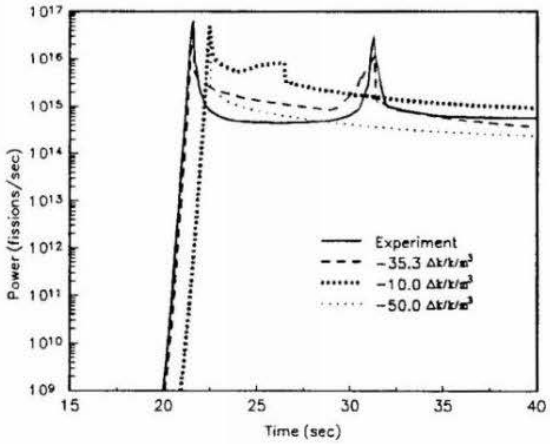

Figure 26: Power vs. Time for Various Values of β_{gas} for CRAC 05

Temperature Feedback Models

In this section results are presented for the two temperature feedback models discused previously. Results are presented only for CRAC 05 because the computer time when modeling the six bottle array was too long for the separated temperature feedback coefficients. For the combined model, the peak power is 5.5×10^{16} fissions/sec and the total energy release is 5.8×10^{16} fissions. For the separated model, the peak power is 3.1×10^{16} fissions/sec and the total energy release is 3.0×10^{16} fissions. The combined model has better agreement with the experiment. These results are shown in figure 27.

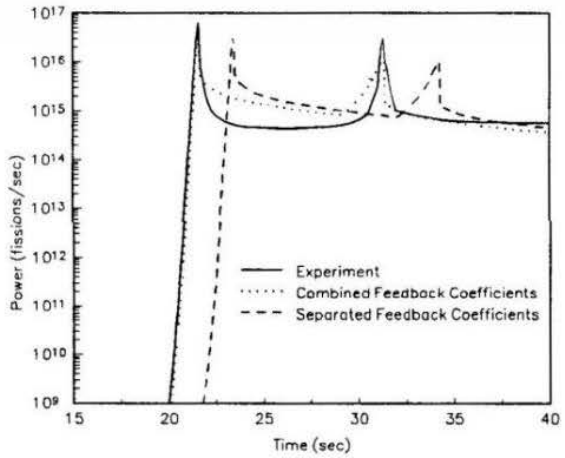

Figure 27: Power vs. Time for the Two Temperature Feedback Models for CRAC 05

The shutdown mechanism for the six bottle array using the COS thermal-hydraulic model occurs when either three or six of the bottles rupture. The UO_2F_2 solution in the bottles is optimally moderated with a H/U^{235} ratio of 496, so with any significant addition or removal of moderator (H_2O), negative reactivity is inserted. When the bottles rupture, approximately one fourth of the moderator (water) in an individual bottle flashes to steam and is removed from the system. A minimum of three bottles undergo this transition. The shutdown occurs rapidly and is irreversible as shown in figure 28.

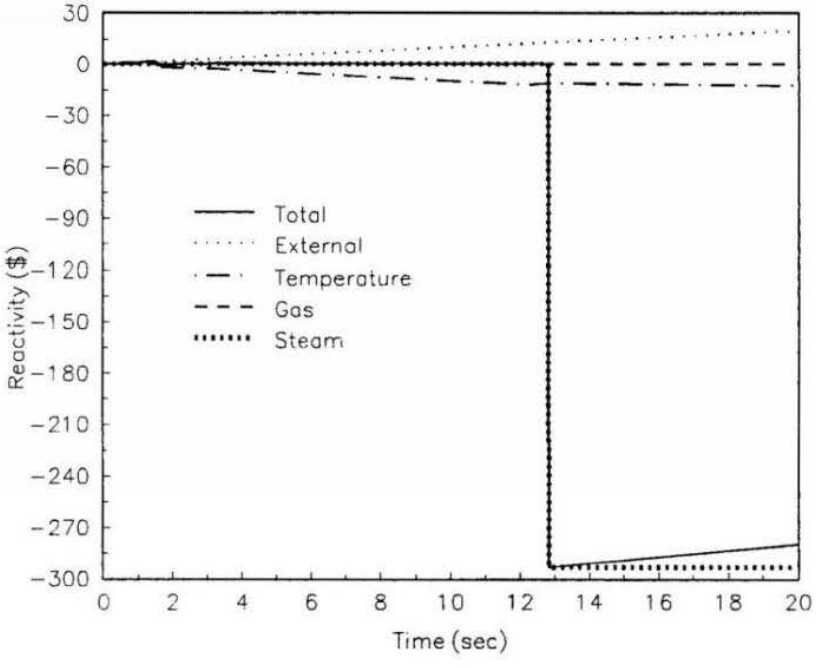

Figure 28: Reactivity vs. Time for a 1.0 $/sec Ramp using the COS Model

The shutdown mechanism for the OS thermal-hydraulic model is a combination of factors. Boiling occurs soon after the initial power peak, and the combination of boiling, temperature, and gas production create a high degree of subcriticality as shown in figures 29 and 30.

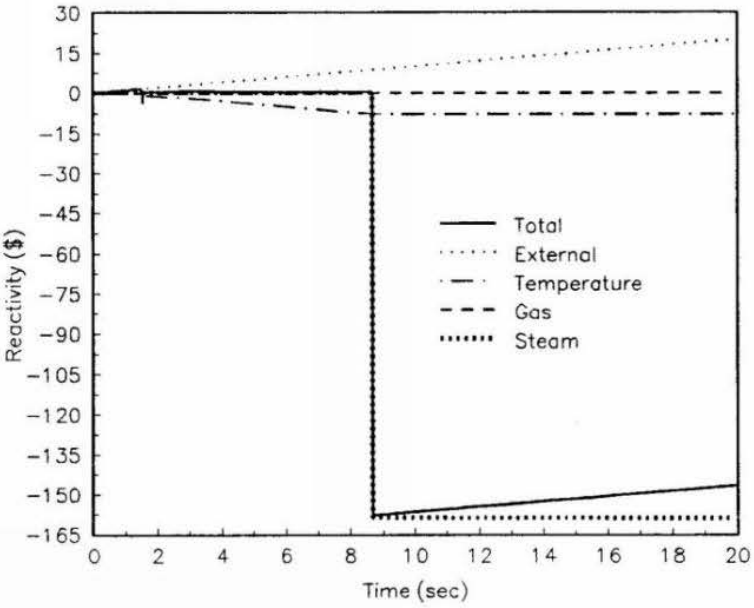

Figure 29: Reactivity vs. Time for a 1.0 $/sec Ramp using the OS Model

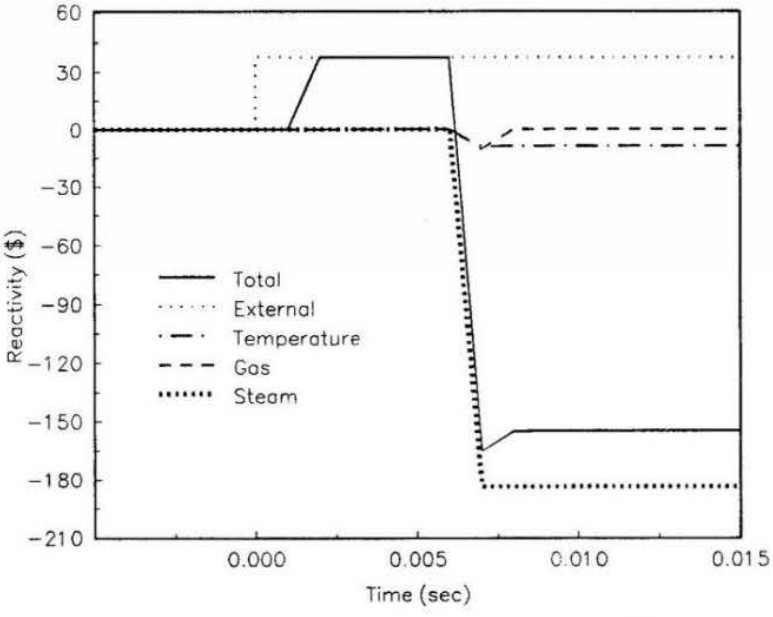

Figure 30: Reactivity vs. Time for a 35.0 $/sec Step using the OS Model

Even though a high degree of subcriticality is seen, the system is still not irreversibly shutdown as shown in figure 29. This is the principle reason why so much care was taken to ensure that the second power pulse could be predicted. In the following section (Validation Efforts), it will be shown that SKINATH-AR can accurately predict the second pulse when modeling experiments. As shown in figure 31, a second pulse will occur using the OS model.

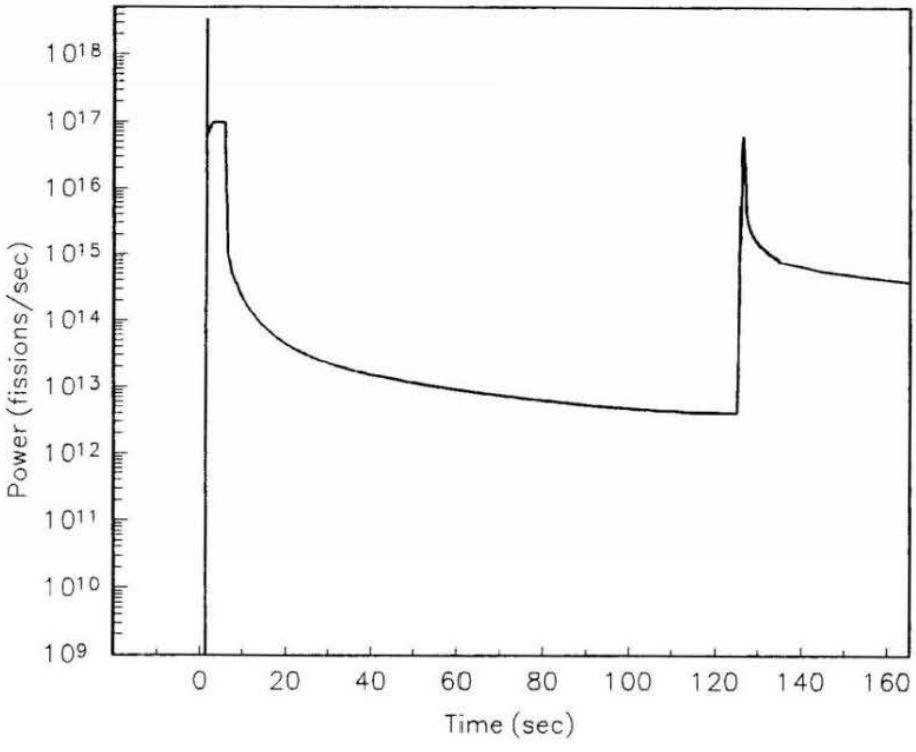

Figure 31: Power vs. Time for a 1.0 $/sec Ramp using the OS Model

CHAPTER IV

Validation Efforts

CRAC Results

The results obtained with SKINATH-AR for several CRAC experiments are presented in this section. Table 9 gives the values of the feedback coefficients used for the seven CRAC experiments studied in this section. Table 10 shows results of SKINATH-AR using the two thermal-hydraulic models described earlier, and SKINATH-AR using quenching coefficients for various CRAC experiments. As can be seen from the table, there is good agreement (within 10 % of the experimental results) between SKINATH-AR and the experiments for the peak power and the total energy release.

The value of the volume reduction factor is adjusted to fit experimental results. The results of SKINATH-AR for a nonadjusted volume reduction factor are presented in Appendix C. Adjusting the volume reduction factor does not affect the peak power or the total energy release, it only affects the timing and magnitude of subsequent power pulses.

Table 9: Reactivity Feedback Coefficients for the Seven CRAC Experiments

	α_T $\Delta k/k/°C$	β_{steam} $\Delta k/k/m^3$	β_{gas} $\Delta k/k/m^3$
CRAC 05	-7.1×10^{-4}	-27.8	-35.3
CRAC 09	-8.3×10^{-4}	-27.8	-35.3
CRAC 10	-7.7×10^{-4}	-27.8	-35.3
CRAC 12	-5.9×10^{-4}	-27.8	-35.3
CRAC 13	-8.6×10^{-4}	-27.8	-35.3
CRAC 16	-6.5×10^{-4}	-27.8	-35.3
CRAC 19	-7.2×10^{-4}	-27.8	-35.3

Table 10: Results of SKINATH-AR for Various CRAC Experiments

	Method	Peak Power (fissions/sec)	Time of Peak (sec)	Total Energy (fissions)
CRAC 05	Experiment	6.3×10^{16}	21.6	6.3×10^{16}
	SKINATH-AR	5.5×10^{16}	21.6	5.8×10^{16}
	SKINATH-AR-QC	5.6×10^{16}	18.3	6.1×10^{16}
CRAC 09	Experiment	2.9×10^{17}	6.4	4.4×10^{16}
	SKINATH-AR	2.0×10^{17}	6.9	2.7×10^{16}
	SKINATH-AR-QC	8.7×10^{16}	7.2	9.5×10^{16}
CRAC 10	Experiment	2.0×10^{17}	6.6	4.3×10^{16}
	SKINATH-AR	1.5×10^{17}	14.3	4.4×10^{16}
	SKINATH-AR-QC	3.7×10^{17}	13.4	8.4×10^{16}
CRAC 12	Experiment	1.0×10^{16}	65.0	3.7×10^{16}
	SKINATH-AR	7.6×10^{15}	58.0	4.5×10^{16}
	SKINATH-AR-QC	8.7×10^{16}	57.6	6.5×10^{16}
CRAC 13	Experiment	5.3×10^{17}	7.5	5.2×10^{16}
	SKINATH-AR	2.7×10^{17}	7.5	8.0×10^{16}
	SKINATH-AR-QC	5.6×10^{16}	18.3	3.2×10^{16}
CRAC 16	Experiment	1.6×10^{16}	11.2	3.6×10^{16}
	SKINATH-AR	1.2×10^{16}	11.2	3.1×10^{16}
	SKINATH-AR-QC	8.7×10^{16}	7.2	7.6×10^{16}
CRAC 19	Experiment	6.7×10^{16}	16.2	3.5×10^{16}
	SKINATH-AR	1.1×10^{17}	16.2	4.1×10^{16}
	SKINATH-AR-QC	3.7×10^{17}	13.4	9.5×10^{16}

Figure 32 shows the power as a function of time for CRAC 05. Comparisons are made between SKINATH-AR and CREST. SKINATH-AR accurately predicts the first and second power pulses, but problems are encountered when predicting the occurrence of pulses beyond the second pulse. The reported results in the figures 32-40 for CRITEX and CREST were obtained from graphs contained in references 4 and 5.

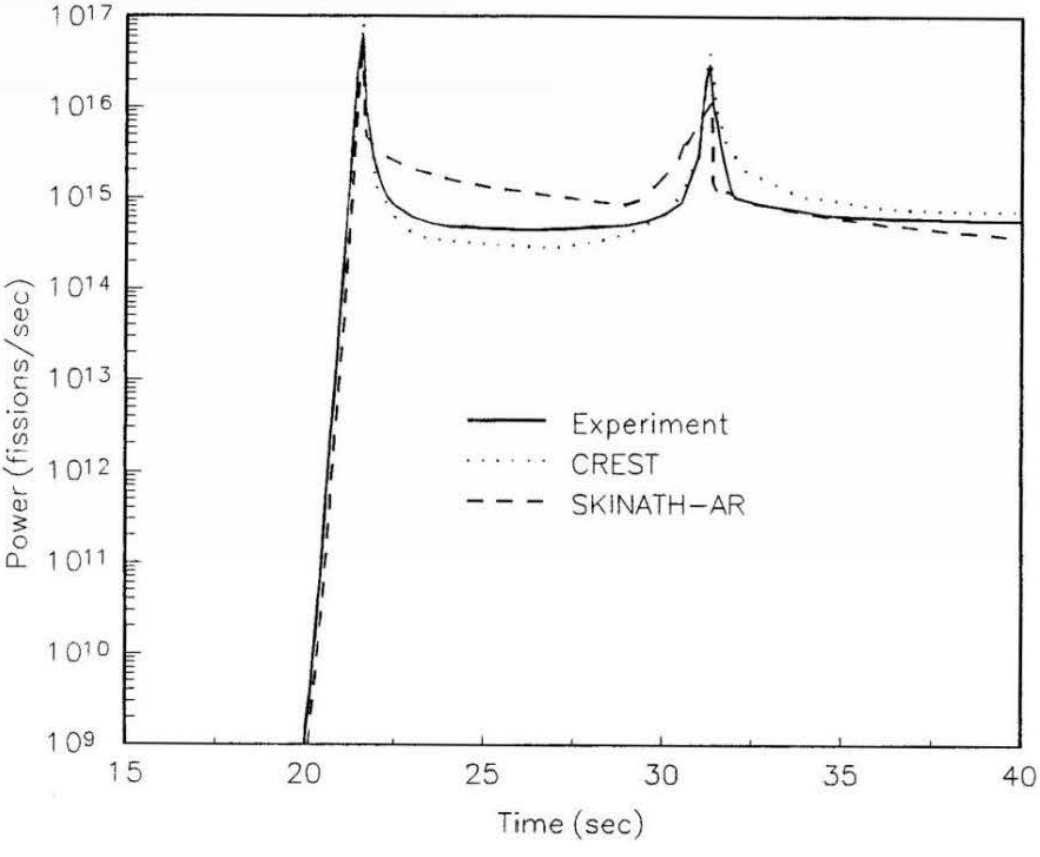

Figure 32: Power vs. Time for SKINATH-AR and CREST for CRAC 05

Figure 33 shows the power and the total energy release as a function of time for CRAC 05 as calculated by SKINATH-AR. Figure 34 shows the temperature as a function of time for CRAC 05 as calculated by SKINATH-AR.

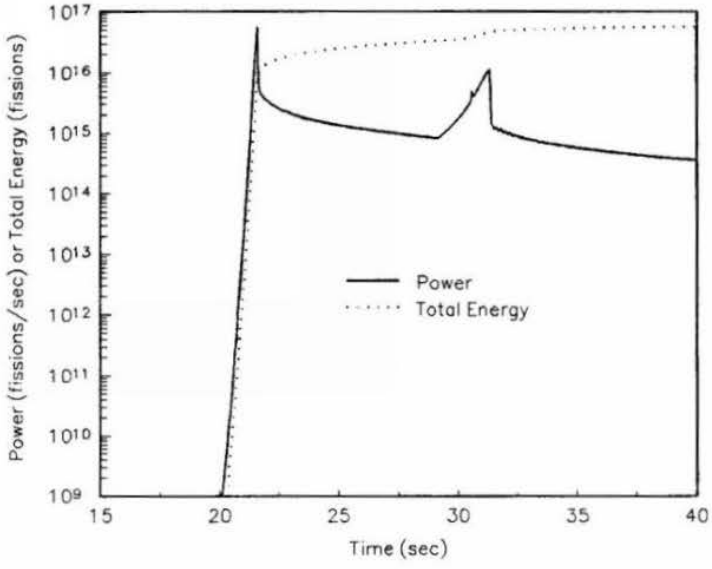

Figure 33: Results of SKINATH-AR for CRAC 05

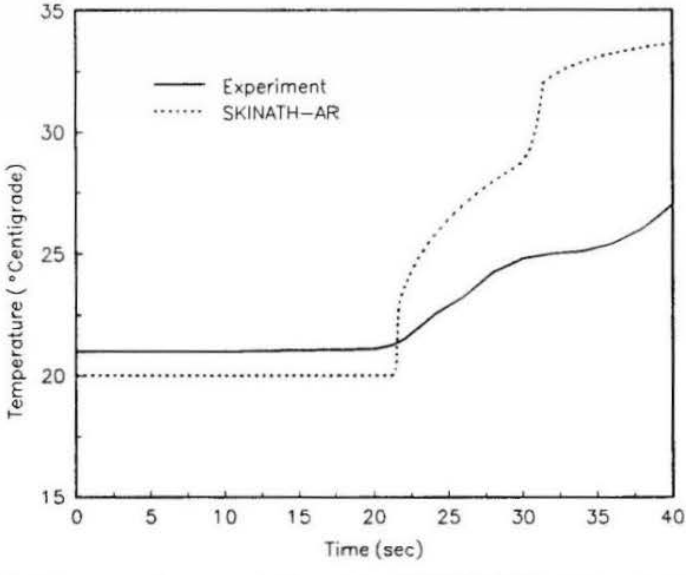

Figure 34: Temperature vs. Time for SKINATH-AR and CRAC 05

Figure 35 shows the power as a function of time for CRAC 16. Comparisons are made between SKINATH-AR and CREST. Again, SKINATH-AR accurately predicts the first and second power pulses. The second power pulse is slightly lower than the experiment, but the timing is almost exact.

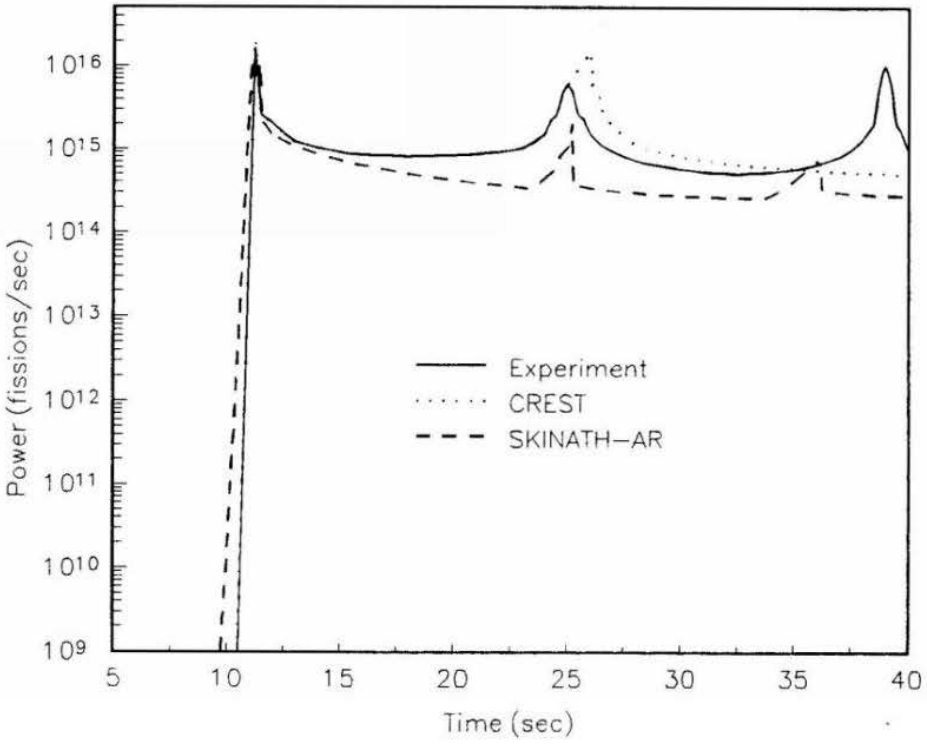

Figure 35: Power vs. Time for SKINATH-AR and CREST for CRAC 16

Figure 36 shows the power as a function of time for CRAC 13. Comparisons are made between SKINATH-AR and CRITEX. Again, SKINATH-AR accurately predicts the first and second power pulses.

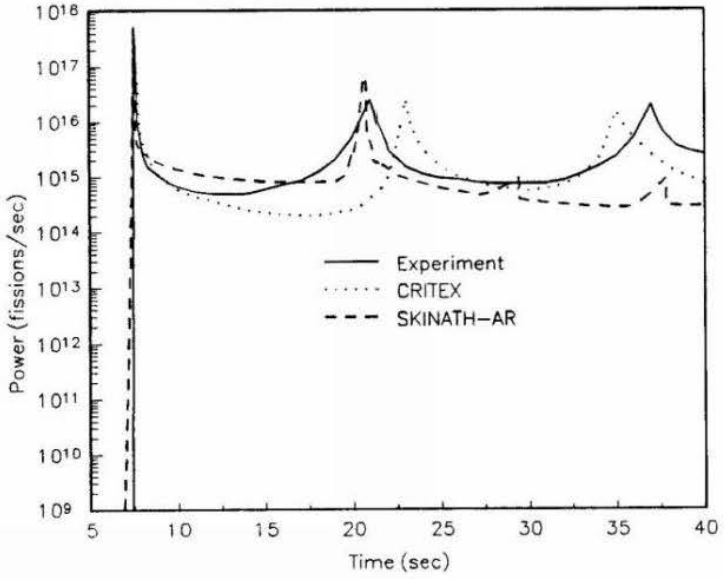

Figure 36: Power vs. Time for SKINATH-AR and CRITEX for CRAC 13

Figure 37 shows the power as a function of time for CRAC 19. Comparisons are made between the experiment, CRITEX, and SKINATH-AR. Again, SKINATH-AR accurately predicts the first and second power pulses.

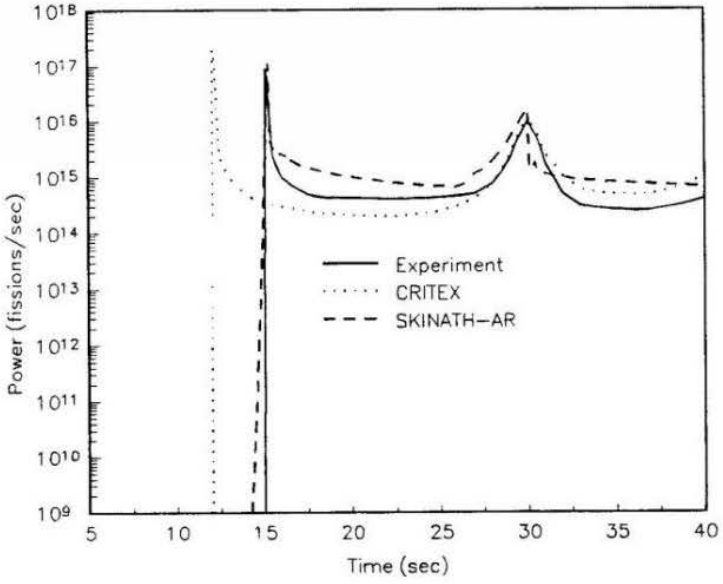

Figure 37: Power vs. Time for SKINATH-AR and CRITEX for CRAC 19

SHEBA Results

The comparisons with the SHEBA experiments are presented in this section. Table 11 gives the feedback coefficients used in calculating the three SHEBA experiments. Table 12 shows the results for three SHEBA experiments as calculated by SKINATH-AR with the models and the parameters which were obtained as a result of the previous parametric studies. The results show good agreement (within 10 % of the experimental results) with experiment.

Table 11: Reactivity Feedback Coefficients for the Three SHEBA Experiments

	α_T $\Delta k/k/°C$	β_{steam} $\Delta k/k/m^3$	β_{gas} $\Delta k/k/m^3$
SHEBA, 0.114 $ Step	-4.1×10^{-4}	-26.7	-36.2
SHEBA, 0.082 $ Step	-3.8×10^{-4}	-26.7	-36.2
SHEBA 0.062 $ Step	-3.1×10^{-4}	-26.7	-36.2

Table 12: Results of SKINATH-AR for Various SHEBA Experiments

	Method	Peak Power (fissions/sec)	Time of Peak (sec)	Energy (fissions)
SHEBA 0.114 $ Step	Experiment	7.7×10^{13}	980	4.5×10^{16}
	SKINATH-AR	5.64×10^{13}	2140	4.2×10^{16}
SHEBA 0.082 $ Step	Experiment	5.4×10^{13}	1300	3.5×10^{16}
	SKINATH-AR	4.41×10^{13}	3170	2.7×10^{16}
SHEBA 0.066 $ Step	Experiment	5.2×10^{13}	1550	3.2×10^{16}
	SKINATH-AR	3.32×10^{13}	4080	2.6×10^{16}

Figures 38, 39, and 40 show the power as a function of time along with comparisons between the experiment, CRITEX, and SKINATH-AR. Agreement is considered to be good (within 10% of the experiment).

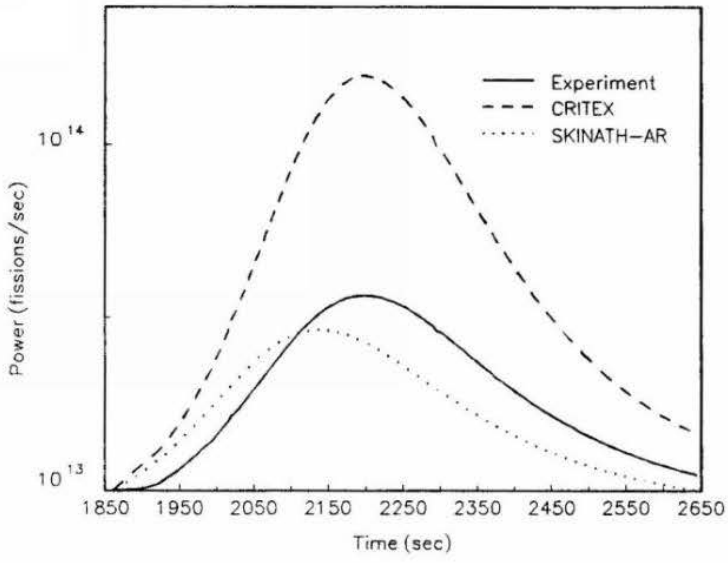

Figure 38: Power vs. Time for SKINATH-AR and CRITEX for SHEBA with a 0.114 $ Step

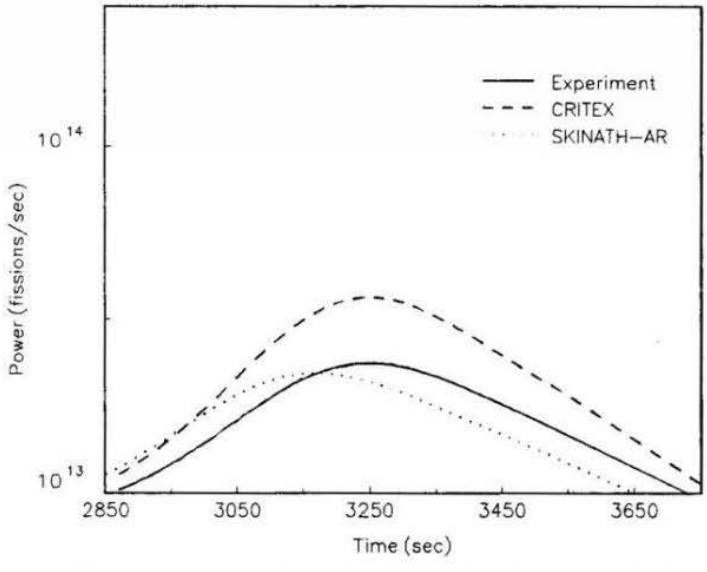

Figure 39: Power vs. Time for SKINATH-AR and CRITEX for SHEBA with a 0.082 $ Step

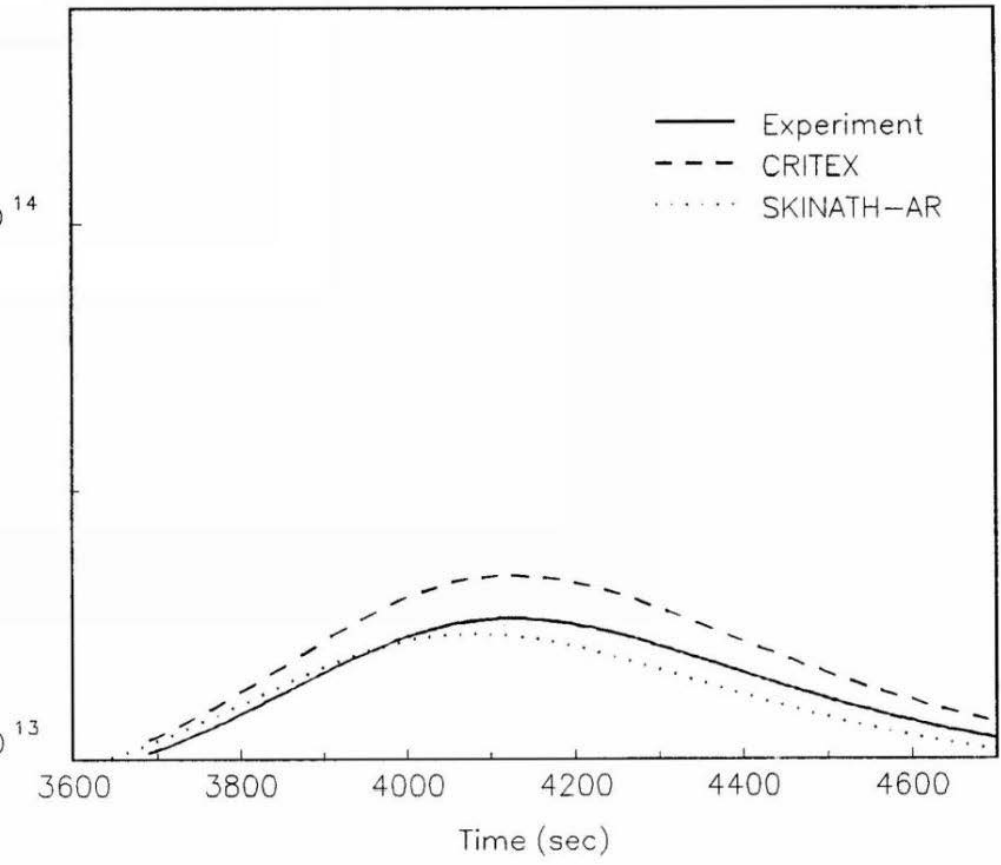

Figure 40: Power vs. Time for SKINATH-AR and CRITEX for SHEBA with a 0.066 $ Step

CHAPTER V

Conclusions and Future Work

Conclusions

The model developed in this work calculates the power history, the total energy release, and various thermal-hydraulic parameters for a criticality accident involving an array of six polyethylene bottles each containing a low-enriched UO_2F_2 solution. The model is also used to calculate various CRAC and SHEBA experiments and to compare results with those calculated using other codes, namely CREST and CRITEX. Even though the experiments are single units and not arrays, they are fissile solutions and, therefore, do provide some validation for the model developed here. The agreement with the experiments is considered satisfactory (within 10 % of the experiment).

The open system (OS) model gives the highest energy release for the six bottle array. The peak powers range from 9.2×10^{17} to 1.2×10^{20} fissions/sec while the total energy release varies from 2.2×10^{17} to 4.5×10^{18} fissions, respectively, using the OS model.

For the closed/open system (COS) model, the peak powers range from 3.1×10^{16} to 1.9×10^{22} fissions/sec while the total energy release varies from 30.3×10^{16} to 3.2×10^{18} fissions, respectively. In summary, the array results are within reasonable bounds. The total energy releases are as expected (less than 10^{19} fissions).

Shutdown occurs for the COS model when some or all of the bottles rupture. For the COS model subsequent pulses do not occur, but for the OS model subsequent pulses can occur. The COS model is believed to more closely reflect the thermal-hydraulics of the system. Thus, the shutdown mechanism for the COS model is believed to be more

accurate than the OS model.

As a final comment, Woodcock postulates that storage arrays, like the one studied in this work, could result in a nuclear excursion with a total energy release of 3×10^{22} fissions, but this is not observed in this study.[1] Even though the peak power reaches 1.9×10^{22} fissions/sec, the total energy release is 3.2×10^{18} fissions. The width of the peak is extremely narrow because of the fast acting thermal-hydraulic feedback.

Future Work

Difficulty was encountered beyond the second power pulse when using SKINATH-AR. Since the gas production model is the major contributor for accurate prediction of subsequent power pulses, further improvements should be made in the gas production model. Replacing point neutronics with some type of simple space-time neutronics model might improve the prediction of subsequent power pulses when using the OS model. For the COS model, space-time neutronics is not necessary because the six bottle array shuts down when the bottles change from closed to open systems.

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APPENDICES

APPENDICES

Appendix A: KENO and XSDRNPM Calculations

The results of various KENO and XSDRNPM calculations are presented in this appendix along with hand calculations performed to find coefficients of reactivity. Table 13 shows the KENO results for different numbers of bottles.

Table 13: KENO Results for Different Bottle Arrangements

Number of Bottles	$k_{eff} \pm \sigma$
3	0.912 ± 0.004
4	0.943 ± 0.005
5	0.996 ± 0.004
6	1.263 ± 0.003
7	1.259 ± 0.004

Table 14 shows reactivity as a function of separation distance as determined by KENO. The information presented in Table 14 was used to compute bottle speeds which correspond to the external reactivity addition rates considered in this research (see Table 3 in Chapter III).

Table 14: KENO Results for Various Bottle Spacings in the Six Bottle Array

Distance Between Bottles (cm)	$k_{eff} \pm \sigma$
0.00	1.263 ± 0.003
0.50	1.201 ± 0.004
1.35	1.135 ± 0.004
2.00	1.002 ± 0.005
3.00	0.965 ± 0.005

In Table 15, the temperature of the solution was varied based on the response of the cross-sections to changing temperature. These data are used in determining α_T and α_{dopp}.

Table 15: XSDRNPM Results for Different Solution Temperatures

Temperature Outer Bottle (Kelvin)	Temperature Inner Bottle (Kelvin)	k_{inf}
293	293	1.33133
550	293	1.26759
293	550	1.31283

$$\alpha_{dopp} = \frac{1.33133 - 1.26759}{293 - 550} = -2.5\times10^{-4}\ \frac{\Delta k}{^{\circ}C\ Bottle}$$

$$\alpha_{dopp} = \frac{1.33133 - 1.31211}{293 - 373} = -2.4\times10^{-4}\ \frac{\Delta k}{^{\circ}C\ Bottle}$$

$$\alpha_{dopp} = \frac{1.33133 - 1.31283}{293 - 550} = -7.2\times10^{-5}\ \frac{\Delta k}{^{\circ}C\ Bottle}$$

$$\alpha_{dopp} = \frac{1.33133 - 1.32560}{293 - 373} = -7.2\times10^{-5}\ \frac{\Delta k}{^{\circ}C\ Bottle}$$

In Table 16 the density of the solution was varied to determine α_{te}, α_T, and the reactivity feedback coefficient of pressure. The α_T for the combined feedback model is calculated as follows:

$$\alpha_T = \alpha_{te} + \alpha_{dopp}$$

Table 16: XSDRNPM Results for Different Solution Densities

Density Outer Bottle (kg/m^3)	Density Inner Bottle (kg/m^3)	k_{inf}
1987.5	1987.5	1.33133
2000.0	1987.5	1.33221
1987.5	2000.0	1.33162

The change in density from 1987.5 to 2000.0 is due to a change in pressure from 0.10135 to 33.4 MPa for a solution temperature of 20°C. The change in density from 1987.5 to 2000.0 is also due to a change in temperature from 20.0°C to 3.1°C for a pressure of 0.10135 MPa.

$$\alpha_{te} = \frac{1.33133 - 1.33221}{293.0 - 276.1} = -5.2\times10^{-5}\frac{\Delta k}{°C\ Bottle}$$

$$\alpha_{te} = \frac{1.33133 - 1.33162}{293.0 - 276.1} = -1.7\times10^{-5}\frac{\Delta k}{°C\ Bottle}$$

$$\alpha_{te} = \frac{1.33133 - 1.33221}{0.10135 - 33.4} = 2.6\times10^{-5}\frac{\Delta k}{MPa\ Bottle}$$

$$\alpha_{te} = \frac{1.33133 - 1.33162}{0.10135 - 33.4} = 8.7\times10^{-6}\frac{\Delta k}{MPa\ Bottle}$$

In Table 17 the results of the study to find reactivity feedback coefficients for gas production are shown.

Table 17: XSDRNPM Results for Different Solution H_2 Concentrations

H_2 Concentration Outer Bottle (m^3 of gas/kg of solution)	H_2 Concentration Inner Bottle (m^3 of gas/kg of solution)	k_{inf}
0.0	0.0	1.33133
1.0×10^{-4}	0.0	1.14482
0.0	1.0×10^{-4}	1.16677

$$\beta_{gas} = \frac{1.33133 - 1.14482}{-47.7 \times 10^{-4}} = -39.1 \frac{\Delta k}{m^3\ Bottle}$$

$$\beta_{gas} = \frac{1.33133 - 1.16677}{-47.7 \times 10^{-4}} = -34.5 \frac{\Delta k}{m^3\ Bottle}$$

In Table 18 the results of the study to find reactivity feedback coefficients for steam production are shown.

Table 18: XSDRNPM Results for Different Solution Steam Concentrations

Steam Concentration Outer Bottle (m^3 of steam/kg of solution)	Steam Concentration Inner Bottle (m^3 of steam/kg of solution)	k_{inf}
0.0	0.0	1.33133
1.0×10^{-4}	0.0	1.19157
0.0	1.0×10^{-4}	1.21208

$$\beta_{steam} = \frac{1.33133 - 1.19157}{-47.7 \times 10^{-4}} = -29.3 \frac{\Delta k}{m^3\ Bottle}$$

$$\beta_{steam} = \frac{1.33133 - 1.21208}{-47.7 \times 10^{-4}} = -25.0 \frac{\Delta k}{m^3\ Bottle}$$

Appendix B: Explanation of Gas Release Rate

The volume of gas released from the system is calculated as shown previously using equation 39. The volume reduction factor is based on a simple approximation to the bubble velocity model.

$$w = \rho_H A v$$

$$\textit{Volume Reduction Factor} = \frac{w}{m_{soln}},$$

where

w = average mass flow rate of the gas to the surface once the threshold for gas release is reached (kg/sec)
ρ_H = density of the hydrogen (kg/m^3)
A = cross-sectional area of the bottle (m^2)
v = assumed average bubble velocity of the gas once the threshold for gas release is reached (m/sec)
m_{soln} = initial mass of the solution (kg).

Appendix C: SKINATH-AR Results Using the Calculated Volume Reduction Factor

In this appendix, the results of SKINATH-AR are presented for a volume reduction factor of 1.0×10^{-9} sec^{-1} (nonadjusted volume reduction factor as discussed in Chapter III). This value was calculated using the formulas given in Appendix B. The volume reduction factor has no effect on the timing or magnitude of the initial power peak. It does significantly affect the timing and magnitude of the subsequent pulses.

Figure 41 gives the results for the CRAC 05 experiment.

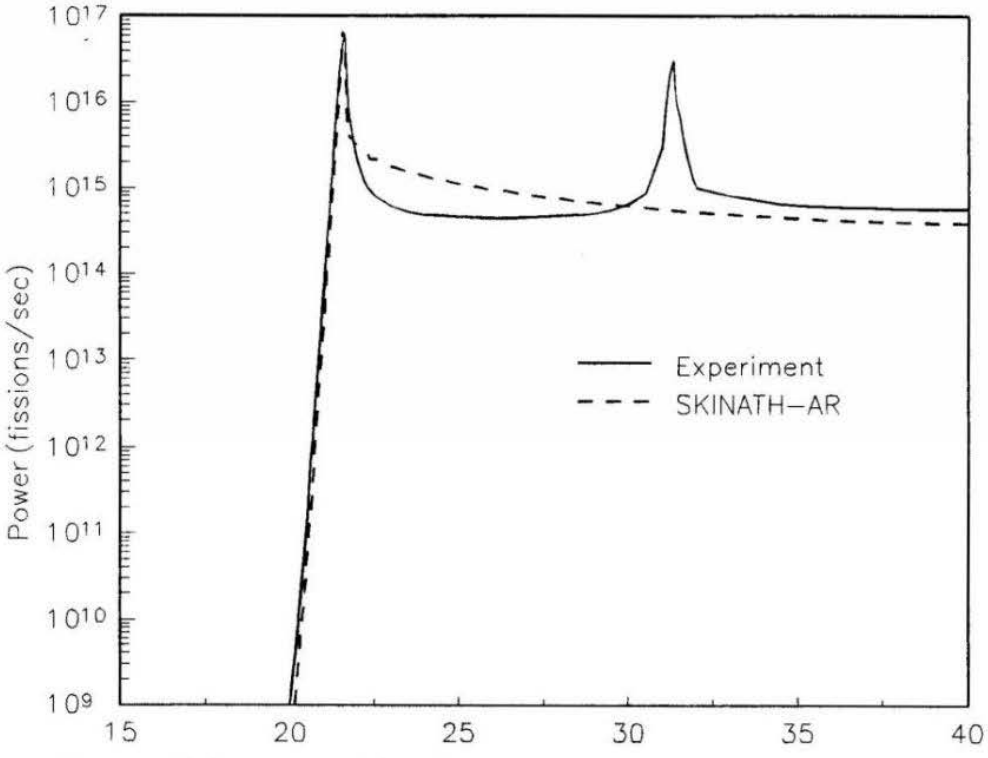

Figure 41: Power vs. Time for SKINATH-AR and for CRAC 05

Figure 42 gives the results for the CRAC 13 experiment.

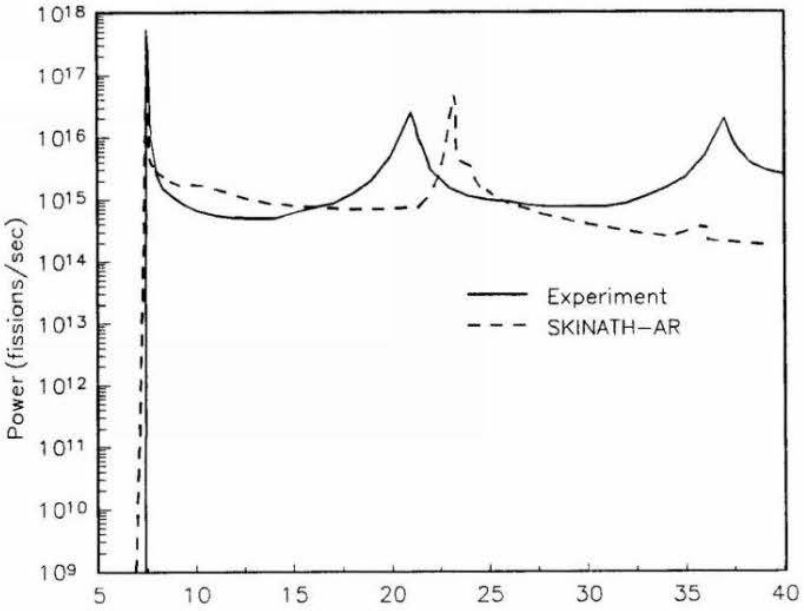

Figure 42: Power vs. Time for SKINATH-AR and for CRAC 13

Figure 43 gives the results for the CRAC 16 experiment.

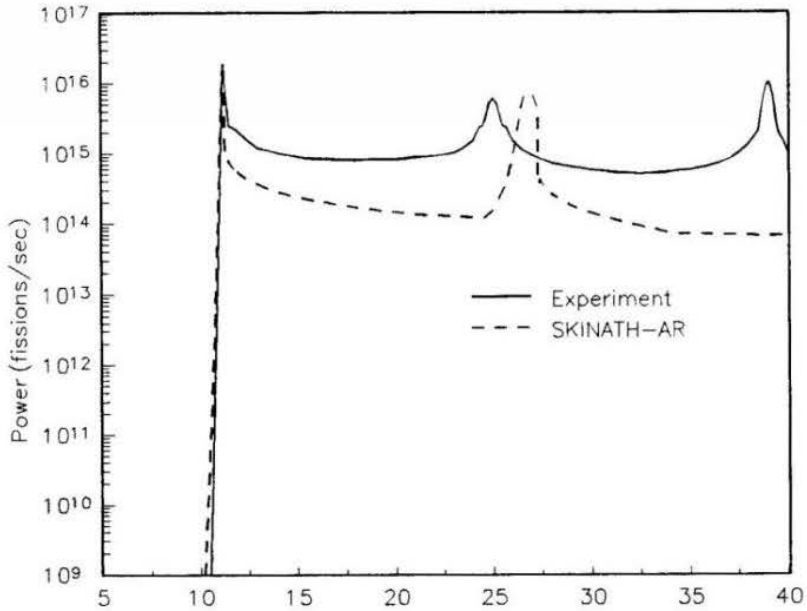

Figure 43: Power vs. Time for SKINATH-AR and for CRAC 16

Figure 44 gives the results for the CRAC 19 experiment.

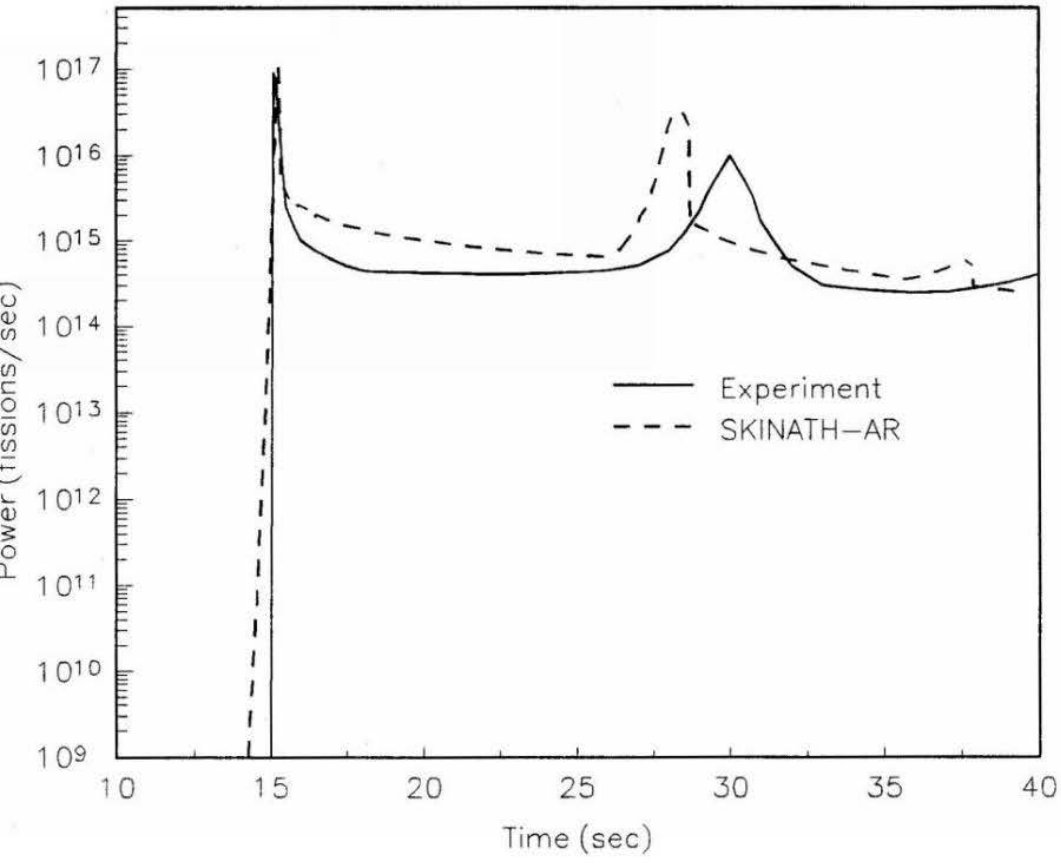

Figure 44: Power vs. Time for SKINATH-AR and for CRAC 19

Appendix D: Code Listing

```
      PROGRAM SKINATH_AR
      IMPLICIT NONE
********************** VARIABLE DESCRIPTION************************
* TOUT     : EDIT TIME                                             *
* TSTOP    : TIME AT WHICH THE TRANSIENT STOPS                     *
* DT       : SIZE OF THE TIME STEP                                 *
* TSUM     : DELAY TIME                                            *
* T        : LSODE TIME                                            *
* QHTRANS: RATE OF HEAT TRANSFER                                   *
* QGEN     : HEAT GENERATED FROM FISSION                           *
* POLY1    : CONSTANT, CONVERTS FISSIONS TO JOULES                 *
* TBULK    : BULK TEMPERATURE                                      *
* TAMB     : AMBIENT TEMPERATURE                                   *
* TWALL    : INSIDE CYLINDER WALL TEMPERATURE                      *
* RTOL     : RELATIVE TOLERANCE, LSODE                             *
* ATOL     : ABSOLUTE TOLERANCE, LSODE                             *
* FRGAS    : FEEDBACK REACTIVITY DUE TO GAS PRODUCTION             *
* FRTEMP   : FEEDBACK REACTIVITY DUE TO TEMPERATURE                *
* Y(1)     : TOTAL FISSIONS                                        *
* Y(2)     : INSTANTANEOUS FISSION POWER                           *
* Y(3)     : DELAYED NEUTRON PRECURSOR GROUP 1 CONC.               *
* Y(4)     : DELAYED NEUTRON PRECURSOR GROUP 2 CONC.               *
* Y(5)     : DELAYED NEUTRON PRECURSOR GROUP 3 CONC.               *
* Y(6)     : DELAYED NEUTRON PRECURSOR GROUP 4 CONC.               *
* Y(7)     : DELAYED NEUTRON PRECURSOR GROUP 5 CONC.               *
* Y(8)     : DELAYED NEUTRON PRECURSOR GROUP 6 CONC.               *
* Y(9)     : ENERGY BALANCE, FIRST BOTTLE                          *
* Y(10)    : ENERGY BALANCE, SECOND BOTTLE                         *
* Y(11)    : ENERGY BALANCE, THIRD BOTTLE                          *
* Y(12)    : ENERGY BALANCE, FOURTH BOTTLE                         *
* Y(13)    : ENERGY BALANCE, FIFTH BOTTLE                          *
* Y(14)    : ENERGY BALANCE, SIXTH BOTTLE                          *
* Y(15)    : MASS OF SOLUTION IN THE FIRST BOTTLE                  *
```

```
* Y(16)      : MASS OF SOLUTION IN THE SECOND BOTTLE                    *
* Y(17)      : MASS OF SOLUTION IN THE THIRD BOTTLE                     *
* Y(18)      : MASS OF SOLUTION IN THE FOURTH BOTTLE                    *
* Y(19)      : MASS OF SOLUTION IN THE FIFTH BOTTLE                     *
* Y(20)      : MASS OF SOLUTION IN THE SIXTH BOTTLE                     *
* L          : LOOP COUNTER                                             *
* NBOT       : NUMBER OF BOTTLES                                        *
* UNOW       : SYSTEM INTERNAL ENERGY                                   *
* RWORK      : REAL WORK ARRAY, LSODE                                   *
* GEN        : MEAN GENERATION TIME                                     *
* BT         : TOTAL DELAYED NEUTRON FRACTION                           *
* B(1)       : DELAYED NEUTRON FRACTION, GRP 1                          *
* B(2)       : DELAYED NEUTRON FRACTION, GRP 2                          *
* B(3)       : DELAYED NEUTRON FRACTION, GRP 3                          *
* B(4)       : DELAYED NEUTRON FRACTION, GRP 4                          *
* B(5)       : DELAYED NEUTRON FRACTION, GRP 5                          *
* B(6)       : DELAYED NEUTRON FRACTION, GRP 6                          *
* AMDA(1)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 1             *
* AMDA(2)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 2             *
* AMDA(3)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 3             *
* AMDA(4)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 4             *
* AMDA(5)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 5             *
* AMDA(6)    : DELAYED NEUTRON PRECURSOR DECAY CONST, GRP 6             *
* HEIGHT     : HEIGHT OF THE CYLINDER                                   *
* AREACYL: SURFACE AREA OF THE CYLINDER                                 *
* THICKNESS: THICKNESS OF THE CYLINDER                                  *
* DIAMCYL: DIAMETER OF THE CYLINDER                                     *
* RHOTEMP: TEMPERATURE COEFFICIENT OF REACTIVITY                        *
* RHOGAS     : COEFFICIENT OF REACTIVITY FROM GAS PROD.                 *
* RHOEXT     : EXTERNAL DRIVING FORCE                                   *
* KPOLY      : THERMAL CONDUCTIVITY OF THE CYLINDER                     *
* HBAR       : OVERALL HEAT TRANSFER COEFFICIENT                        *
* ALPHA      : THERMAL DIFFUSIVITY COEFFICIENT                          *
* M1         : SOLUTION MASS ADDITION RATE                              *
* GG1        : EMPIRICAL CONSTANT, DERIVES MASS GAS PRODUCED            *
```

```
*  NUCLEATION: MASS OF GAS / MASS OF SOLUTION                          *
*  MOUT     : MASS LEAVING THE SYSTEM                                  *
*  MASS1O2  : MASS OF OXYGEN PRODUCED FROM FISSION                     *
*  MASSH2   : MASS OF HYDROGEN PRODUCED FROM FISSION                   *
*  MASSN2   : MASS OF NITROGEN PRODUCED FROM FISSION                   *
*  MSTEAM   : MASS OF STEAM PRODUCED                                   *
*  VOLGAS   : VOLUME OF GAS PRODUCED                                   *
*  VOLN2    : VOLUME OF NITROGEN PRODUCED                              *
*  VOLO2    : VOLUME OF OXYGEN PRODUCED                                *
*  VOLH2    : VOLUME OF HYDROGEN PRODUCED                              *
*  WO2      : MASS FLOW RATE OF OXYGEN                                 *
*  WN2      : MASS FLOW RATE OF NITROGEN                               *
*  WH2      : MASS FLOW RATE OF HYDROGEN                               *
*  WSTEAM   : MASS FLOW RATE OF STEAM                                  *
*  TOTALREAC: TOTAL REACTIVITY                                         *
*  PI       : PI, 3.1416                                               *
*  G        : ACCELERATION OF GRAVITY                                  *
*  Q1       : QUENCHING COEFFICIENT                                    *
*  R1       : REACTIVITY ADDITION RATE                                 *
*  EOUT     : DUMMY VARIABLE                                           *
*  TEMP1    : DUMMY VARIABLE                                           *
*  EIN      : DUMMY VARIABLE                                           *
*  PRESS    : SYSTEM PRESSURE                                          *
*  NEQ      : NUMBER OF EQUATIONS SUBMITTED TO LSODE                   *
*  ITOL     : FLAG TO DESIGNATE ATOL AS A SCALAR OF ARRAY              *
*  ITASK    : TASKS, LSODE                                             *
*  ISTATE   : LSODE STATE                                              *
*  IOPT     : FLAG TO DESIGNATE LSODE OPTIONAL INPUTS                  *
*  LRW      : LENGTH OF THE RWORK ARRAY                                *
*  LIW      : LENGTH OF THE IWORK ARRAY                                *
*  MF       : LSODE METHOD                                             *
*  JEX      : INPUT JACOBIAN MATRIX FOR LSODE                          *
*  I        : LOOP COUNTER                                             *
*  IWORK    : INTEGER WORK ARRAY, LSODE                                *
************************************************************************
```

```
 REAL*8 TOUT,TSTOP,DT,TSUM,AEDIT,BEDIT,NUCLEATION,MGAS(6),
1POLY1,TBULK(6),PSUM,RTOL,ATOL,T,FRGAS(6),FRTEMP(6), Y(14),
2YDOT(14),RWORK(344),TF1(6),TF2(6),MOUT(6),GEN,BT,HEIGHT,
3R1,Q1,NUCF(6),MASSH2(6),MASSO2(6),RHOTEMP(6),AREACYL,B(6),
4AMDA(6),THICKNESS,VF,RHOEXT,RHOGAS,KPOLY,ALPHA,GG1,
5TOTALREAC,PI,G,DIAMCYL,P0,RHO1(6),MASS1O2(6),EOUT(6),TEMP1(6),
6HBAR(6),TWALL(6),TAMB,PRESS(6),WO2(6),WH2(6),EO2(6),EH2(6),
7EF2(6),VOLGAS(6),VAR1,VAR2,VOLH2(6),VOLO2(6),VOLF2(6),VGF,NF,
8MASS(6),T1,FRG,FRT,F1(6)
 INTEGERNEQ,ITOL,ITASK,ISTATE,IOPT,IFLG,CNTR,NBOT,LRW,LIW,MF,
1JEX,I,IWORK(34),IFL,J,JT,L,IFLAG(6)
 CHARACTER*70 ERRMSG
 EXTERNAL F
 COMMON/DAT1/DT,POLY1,KPOLY,GG1,RHOGAS,RHOTEMP,TOUT,
1TOTALREAC,RHOEXT,B,AMDA,BT,GEN,PI,G,DIAMCYL,THICKNESS,
2HEIGHT,TBULK,ALPHA,FRGAS,FRTEMP,TWALL,TSUM,RHO1,TEMP1,
3EOUT,AREACYL,HBAR,TAMB,PRESS,Q1,R1,MASS,FRG,FRT,VOLGAS,F1
 COMMON/DAT2/NBOT
 COMMON/ERRORS/ERRMSG
 OPEN(UNIT=21,FILE='A1.IN',STATUS='OLD')
 OPEN(UNIT=30,FILE='A1.DAT',STATUS='NEW')
 OPEN(UNIT=31,FILE='A2.DAT',STATUS='NEW')
 OPEN(UNIT=32,FILE='A3.DAT',STATUS='NEW')
 OPEN(UNIT=33,FILE='A4.DAT',STATUS='NEW')
 OPEN(UNIT=34,FILE='A5.DAT',STATUS='NEW')
 READ(21,*) NEQ,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,LRW,LIW,MF,
1Y(2),GG1,POLY1,RHOGAS(1),RHOGAS(2),RHOGAS(3),RHOGAS(4),
2RHOGAS(5),RHOGAS(6),RHOTEMP(1),RHOTEMP(2),RHOTEMP(3),
3RHOTEMP(4),RHOTEMP(5),RHOTEMP(6),RHOSTEAM(1),RHOSTEAM(2),
4RHOSTEAM(3),RHOSTEAM(4),RHOSTEAM(5),RHOSTEAM(6),KPOLY,
5T,TOUT,DT,TSTOP,GEN,Q1,R1,TSUM,M1,ATOL(1),ATOL(2),ATOL(3),
6ATOL(4), ATOL(5),ATOL(6),ATOL(7),ATOL(8),ATOL(9),ATOL(10),
7ATOL(11),ATOL(12),QF,NF,VGF,PRESS(1),PRESS(2),PRESS(3),
8PRESS(4),PRESS(5),PRESS(6),TBULK(1),TBULK(2),TBULK(3),
9TBULK(4),TBULK(5),TBULK(6)
```

```
 WRITE(6,*) NEQ,ITOL,RTOL,ATOL,ITASK,
1ISTATE,IOPT,LRW,LIW,JT,RHOGAS,GG1,POLY1,KPOLY,ALPHA,
2T,TOUT,DT,TSTOP,TSUM,GEN,PSUM,Y(2),RHOTEMP(1),RHOTEMP(2),
3RHOTEMP(3),RHOTEMP(4),RHOTEMP(5),RHOTEMP(6),R1,NF,VF,VGF,
4VAR1,VAR2,T1
 WRITE(30,*) NEQ,ITOL,RTOL,ATOL,ITASK,ISTATE,IOPT,LRW,LIW,
1JT,RHOGAS,GG1,POLY1,KPOLY,ALPHA,T,TOUT,DT,TSTOP,TSUM,GEN,
2Y(2),RHOTEMP(1),RHOTEMP(2),RHOTEMP(3),RHOTEMP(4),RHOTEMP(5),
3RHOTEMP(6),R1,NF,VF,VGF,VAR1,VAR2,T1
   NBOT=6
   AMDA(1)=.0127
   AMDA(2)=.0317
   AMDA(3)=.115
   AMDA(4)=.311
   AMDA(5)=1.4
   AMDA(6)=3.87
   B(1)=.000247
   B(2)=.0013845
   B(3)=.001222
   B(4)=.0026455
   B(5)=.000832
   B(6)=.000169
   BT=0.D+0
   DO I=1,6
         BT=BT+B(I)
   END DO
   DO I=1,NBOT
         RHO1(I)=288.38097
   END DO
   IWORK(6)=10000
   PI=3.14159
   G=9.80665
   DIAMCYL=.3
   THICKNESS=.003
   HEIGHT=.2664
```

```
      TAMB=20.0
      IFLG=0
      AREACYL=PI*DIAMCYL*HEIGHT
      AEDIT=0.09999
      BEDIT=0.10001
      F1(1)=.1111
      F1(2)=.2222
      F1(3)=.2222
      F1(4)=.1111
      F1(5)=.2222
      F1(6)=.1111
      AREACYL=PI*DIAMCYL*HEIGHT
      DO L=1,NBOT
            NUCF(L)=1.D-4
            IFLAG(L)=0
            MASS(L)=47.7
      END DO
*****************************************************************************
* ESTABLISH A DO LOOP WHICH CALCULATES PARAMETERS OF
* INTEREST
*****************************************************************************
      DOWHILE (TOUT .LE. TSTOP)
        WRITE(30,*) 'FRTEMP=',FRT
        WRITE(30,*) 'FRGAS=',FRG
        WRITE(30,100) TOUT,ISTATE,Y(1),Y(2),Y(9),Y(10),Y(11),Y(12),
     1Y(13),Y(14),MGAS(1),MGAS(2),MGAS(3),MGAS(4),MGAS(5),MGAS(6),
     2NUCLEATION,TOTALREAC,PRESS(1),PRESS(2),PRESS(3),PRESS(4),
     3PRESS(5),PRESS(6),TBULK(1),TBULK(2),TBULK(3),TBULK(4),
     4TBULK(5),TBULK(6)
        WRITE(30,*) '-----------------------------------'
        WRITE(6,100) TOUT,ISTATE,Y(1),Y(2),Y(9),Y(10),Y(11),Y(12),
     1Y(13),Y(14),MGAS(1),MGAS(2),MGAS(3),MGAS(4),MGAS(5),MGAS(6),
     2NUCLEATION,TOTALREAC,PRESS(1),PRESS(2),PRESS(3),PRESS(4),
     3PRESS(5),PRESS(6),TBULK(1),TBULK(2),TBULK(3),TBULK(4),
     4TBULK(5),TBULK(6)
```

```
      WRITE(6,*) 'FRTEMP=',FRT
      WRITE(6,*) 'FRGAS=',FRG
      WRITE(6,*) 'VOLGAS(1)=',VOLGAS(1),' VOLGAS(2)=',VOLGAS(2)
      WRITE(6,*) '-----------------------------------'
      WRITE(31,*) Y(2)
      WRITE(32,*) Y(1)
      WRITE(33,*) TOUT,',',Y(2)
      WRITE(34,*) TOUT,',',Y(1)
      ISTATE=1
*************** CALL ODE SOLVER (LSODE) ***************************
      CALL LSODE(F,NEQ,Y,T,TOUT,ITOL,RTOL,ATOL,ITASK,ISTATE,
     1IOPT,RWORK,LRW,IWORK,LIW,JEX,JT)
****** CALCULATE RADIOLYTIC GAS PRODUCTION AND RELEASE *****
      DO L=1,NBOT
          NUCLEATION=(MGAS(L)/MASS(L))
          IF (NUCLEATION .GE. NUCF(L)) THEN
           IF (PRESS(L) .GE. 0.345) THEN
               MOUT(L)=MGAS(L)
           ELSE
               MOUT(L)=0.0
           END IF
           IFLAG(L)=1
           MGAS(L)=GG1*Y(1)*F1(L)
           MASSH2(L)=MGAS(L)/9.0
           MASS1O2(L)=MGAS(L)*32.0/36.0
           MASSO2(L)=MASS1O2(L)
           WO2(L)=MASSO2(L)/DT
           WH2(L)=MASSH2(L)/DT
           EO2(L)=0.92*(TBULK(L)+273.0)*MASSO2(L)
           EH2(L)=14.3*(TBULK(L)+273.0)*MASSH2(L)
           VOLH2(L)=((MASSH2(L)*4124.289*(TBULK(L)+273.0))/
     1(PRESS(L)*1.D+6))
           VOLO2(L)=((MASSO2(L)*259.832*(TBULK(L)+273.0))/
     1(PRESS(L)*1.D+6))
           VOLGAS(L)=VOLH2(L)+VOLO2(L)-TEMP
```

```
            WRITE(6,*) 'ZZZ',(NUCLEATION-NUCF(L))
            WRITE(6,*) 'NUCLEATION=',NUCLEATION
            TEMP=VOLGAS(L)/VAR1
          ELSE
            MOUT(L)=0.0
            MGAS(L)=GG1*Y(1)*F1(L)
            MASSH2(L)=MGAS(L)/9.0
            MASS1O2(L)=MGAS(L)*32.0/36.0
            MASSO2(L)=MASS1O2(L)
            VOLH2(L)=((MASSH2(L)*4124.289*(TBULK(L)+273.0))/
   1(PRESS(L)*1.D+6))
            VOLO2(L)=((MASSO2(L)*259.832*(TBULK(L)+273.0))/
   1(PRESS(L)*1.D+6))
            VOLGAS(L)=VOLH2(L)+VOLO2(L)
            IF (IFLAG(L) .NE. 0) THEN
                WRITE(6,*) 'YYY',(NUCLEATION-NUCF(L))
                WRITE(6,*) 'NUCLEATION=',NUCLEATION
            END IF
            MOUT(L)=0.0
          END IF
          MASS(L)=MASS(L)-MOUT(L)
******** INCORPORATE STEAM TABLE CORRELATIONS ******************
          CALL STEAM(Y,L)
      END DO
      WRITE(6,*) ERRMSG
      TOUT=TOUT+DT
    END DO
    CLOSE(UNIT=21)
    CLOSE(UNIT=30)
    CLOSE(UNIT=31)
    CLOSE(UNIT=32)
    CLOSE(UNIT=33)
    CLOSE(UNIT=34)
100  FORMAT(X,'TOUT=',F7.3,X,'ISTATE=',I2,X,'Y(1)=',E11.3,
   1/,X,'Y(2)=',E11.3,X,'ENERGY #1=',E11.3,X,'#2=',E11.3,X,'#3=',E11.3,
```

```
  2/,X,'#4=',E11.3,X,'#5=',E11.3,X,'#6=',E11.3,X,'SOLN MASS #1=',E11.3,
  3/,X,'#2=',E11.3,X,'#3=',E11.3,X,'#4=',E11.3,X,'#5=',E11.3,
  4/,X,'#6=',E11.3,X,'NUCLEATION=',E11.3,X,'TOTAL REACTIVITY=',E11.3,
  5/,X,'PRESS #1=',E11.3,X,'#2=',E11.3,X,'#3=',E11.3,X,'#4=',E11.3,
  6/,X,'#5=',E11.3,X,'#6=',E11.3,X,'TBULK #1=',E11.3,X,'#2=',E11.3,
  7/,X,'#3=',E11.3,X,'#4=',E11.3,X,'#5=',E11.3,X,'#6=',E11.3)
      STOP
      END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      SUBROUTINE F(NEQ,T,Y,YDOT)
************************************************************************
* THIS SUBROUTINE REQUIRED BY LSODE. IT CONTAINS ALL                   *
* OF THE DIFFERENTIAL EQUATIONS SOLVED BY LSODE.                       *
************************************************************************
      IMPLICIT NONE
     REAL*8  TOUT,TSTOP,DT,TSUM,POLY1,TBULK(6),T,FRGAS(6),FRTEMP(6),
    1Y(26),YDOT(26),GEN,BT,HEIGHT,RHOTEMP(6),AREACYL,B(6),AMDA(6),
    2THICKNESS,RHOEXT,RHOGAS,KPOLY,GG1,TOTALREAC,PI,G,DIAMCYL,
    3P0,RHO1(6),EOUT(6),TEMP1(6),HBAR(6),TAMB,TWALL(6),PRESS(6),
    4ALPHA,SUM,YSUM,R1,Q1,VCYSK,ESTEAM(6),MOUT(6),MASSH2(6),
    5MASSO2(6),MASS1O2(6),MASSGAS(6),VOLH2(6),VOLF2(6),VOLGAS(6),
    6NUCLEATION,WSTEAM(6),QGEN(6),QHTRANS(6),VOLO2(6),WO2(6),
    7WH2(6),EO2(6),EH2(6),EF2(6),MASS(6),FRT,FRG,SUM1,SUM2,F1(6)
     INTEGERNEQ,ITOL,ITASK,ISTATE,IOPT,IFLG,CNTR,L,LRW,LIW,MF,JEX,
    1I,IWORK(82),IFL,J,JT,NBOT
     CHARACTER*70 ERRMSG
     COMMON/DAT1/DT,POLY1,KPOLY,GG1,RHOGAS,RHOTEMP,TOUT,
    1TOTALREAC,RHOEXT,B,AMDA,BT,GEN,PI,G,DIAMCYL,THICKNESS,
    2HEIGHT,TBULK,ALPHA,FRGAS,FRTEMP,TWALL,TSUM,RHO1,TEMP1,
    3EOUT,AREACYL,HBAR,TAMB,PRESS,Q1,R1,MASS,FRG,FRT,VOLGAS,F1
     COMMON/DAT2/NBOT
     COMMON/ERRORS/ERRMSG
********* SET INITIAL DIFF EQ CONDITIONS ****************************
    IF (T .EQ. 0.0) THEN
      Y(3)=B(1)*Y(2)/AMDA(1)/GEN
```

```
      Y(4)=B(2)*Y(2)/AMDA(2)/GEN
      Y(5)=B(3)*Y(2)/AMDA(3)/GEN
      Y(6)=B(4)*Y(2)/AMDA(4)/GEN
      Y(7)=B(5)*Y(2)/AMDA(5)/GEN
      Y(8)=B(6)*Y(2)/AMDA(6)/GEN
      DO L=1,NBOT
        Y(L+8)=83.93525*MASS(L)
      END DO
    END IF
************************** TOTAL FISSION POWER **********************
    YDOT(1)=Y(2)
***************************** FISSION POWER *************************
    YDOT(2)=((TOTALREAC-BT)*Y(2)/GEN)+SUM
    SUM=0.0D+0
************************ DELAYED NEUTRON PRECURSORS *****************
    YDOT(3)=(B(1)*Y(2)/GEN)-(AMDA(1)*Y(3))
    SUM=SUM+(AMDA(1)*Y(3))
    YDOT(4)=(B(2)*Y(2)/GEN)-(AMDA(2)*Y(4))
    SUM=SUM+(AMDA(2)*Y(4))
    YDOT(5)=(B(3)*Y(2)/GEN)-(AMDA(3)*Y(5))
    SUM=SUM+(AMDA(3)*Y(5))
    YDOT(6)=(B(4)*Y(2)/GEN)-(AMDA(4)*Y(6))
    SUM=SUM+(AMDA(4)*Y(6))
    YDOT(7)=(B(5)*Y(2)/GEN)-(AMDA(5)*Y(7))
    SUM=SUM+(AMDA(5)*Y(7))
    YDOT(8)=(B(6)*Y(2)/GEN)-(AMDA(6)*Y(8))
    SUM=SUM+(AMDA(6)*Y(8))
    QGEN(1)=Y(2)*POLY1*F1(1)
    QGEN(2)=Y(2)*POLY1*F1(2)
    QGEN(3)=Y(2)*POLY1*F1(3)
    QGEN(4)=Y(2)*POLY1*F1(4)
    QGEN(5)=Y(2)*POLY1*F1(5)
    QGEN(6)=Y(2)*POLY1*F1(6)
    SUM1=0.0
    SUM2=0.0
```

```
    DO L=1,NBOT
      HBAR(L)=10.0*(VCYSK(TBULK(L),TAMB,G,HEIGHT,DIAMCYL,
   1KPOLY,HEIGHT))
      QHTRANS(L)=HBAR(L)*(TBULK(L)-TAMB)
      TEMP1(L)=QGEN(L)-QHTRANS(L)
************************** ENERGY BALANCE ***************************
      YDOT(L+8)=TEMP1(L)-EOUT(L)
      IF(TBULK(L) .LT. 20.0) THEN
          TBULK(L)=20.0
      END IF
      MSTEAM(L)=Y(L+8)/LHV
      EOUT(L)=ESTEAM(L)+EO2(L)+EH2(L)+EF2(L)
      FRGAS(L)=VOLGAS(L)*RHOGAS(L)
      SUM1=SUM1+FRGAS(L)
      FRTEMP(L)=RHOTEMP(L)*(TBULK(L)-20.0)
      SUM2=SUM2+FRTEMP(L)
    END DO
    FRT=SUM2
    RHOEXT=R1*(T+TSUM)
    FRG=SUM1
*************************** TOTAL REACTIVITY **********************
    TOTALREAC=FRT+FRG+RHOEXT
    RETURN
    END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      SUBROUTINE STEAM(Y,L)
*****************************************************************
* THIS SUBROUTINE CALLS THE STEAM PROPERTIES PROGRAM WHICH   *
* CALCULATES PERTINENT PROPERTIES OF THE FLUID IN THE BOTTLES*
*****************************************************************
      IMPLICIT NONE
    REAL*8 DT,SPECH,ERRTOL,SFP,SGP,EFP,EGP,VOL,TOTM,TOTH,TOTS,
   1TOTE,X,VOID,RHO,SPECVOL,SPECS,HGP,SPECE,PS,TS,RHOG,VFP,VGP,
   2RHOF,HFP,P,TOUT,TSTOP,TSUM,AEDIT,BEDIT,POLY1,TBULK(6),PSUM,
   3RTOL,ATOL,T,FRGAS(6),FRTEMP(6),Y(26),YDOT(26),GEN,BT,HEIGHT,
```

```
4RHOTEMP(6),AREACYL,B(6),AMDA(6),THICKNESS,RHOEXT,RHOGAS,
5KPOLY,GG1,TOTALREAC,PI,G,DIAMCYL,P0,RHO1(6),EOUT(6),TEMP1(6),
6HBAR(6),TWALL(6),TAMB,PRESS(6),ALPHA,MASS(6),QGEN(6),
7QHTRANS(6),UNOW(6),BMASSGAS(6),TMASS(6),MASSH2(6),MASSO2(6),
8MASS1O2(6),MASS2O2(6),MASSF2(6),MASSGAS(6),VOLO2(6),VOLH2(6),
9VOLF2(6),VOLGAS(6),NUCLEATION,TOTMASS(6),WO2(6),WF2(6),WH2(6),
1MSTEAM(6),WSTEAM(6),EO2(6),EH2(6),EF2(6),TOTALVOL(6),VCYSK,
2ESTEAM(6),MOUT(6),U1,P1,TM1,T1,R1,Q1,FRG,FRT
 INTEGER ISAT,ITYPE,NMAX,J,L,NBOT,IFLAG
 CHARACTER*70 ERRMSG
 COMMON/DAT1/DT,POLY1,KPOLY,GG1,RHOGAS,RHOTEMP,TOUT,
1TOTALREAC,RHOEXT,B,AMDA,BT,GEN,PI,G,DIAMCYL,THICKNESS,
2HEIGHT,TBULK,ALPHA,FRGAS,FRTEMP,TWALL,TSUM,RHO1,TEMP1,
3EOUT,AREACYL,HBAR,TAMB,PRESS,Q1,R1,MASS,FRG,FRT,VOLGAS
 COMMON/DAT2/NBOT
 COMMON/ERRORS/ERRMSG
 COMMON/PROPERTY/VFP,VGP,RHOF,RHOG,HFP,HGP,SFP,SGP,EFP,EGP,
1VOL,TOTM,TOTH,TOTS,TOTE,X,VOID,RHO,SPECVOL,SPECH,SPECS,
2SPECE,PS,TS
 SPECH=Y(L+8)/MASS(L)
 TOTM=MASS(L)
 NMAX=10
 ERRTOL=0.1
 IF (P .LE. 0.345) THEN
     RHO=RHO1(L)
     IFLAG=1
     ISAT=3
     ITYPE=2
    CALL PROP(P,T,ISAT,ITYPE,IFLAG,NMAX,ERRTOL,ERRMSG,.5)
 ELSE
     IFLAG=1
     ISAT=6
    ITYPE=2
    CALL PROP(P,T,ISAT,ITYPE,IFLAG,NMAX,ERRTOL,ERRMSG,.5)
 END IF
```

```
      TBULK(L)=T
      PRESS(L)=P
      RETURN
      END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      FUNCTION VCYSK(TBULK,TCA,G,SL,DOUT1)
*************************************************************************
* THIS FUNCTION SUBROUTINE CALCULATES THE OVERALL HEAT          *
* TRANSFER COEFFICIENT USED IN THE CALCULATION OF THE HEAT      *
* TRANSFER TERM IN THE ENERGY BALANCE                           *
*************************************************************************
      IMPLICIT NONE
      REAL*8 TBULK,TCA,G,SL,DOUT1,VCYSK,TFILM,DENSA,CPA,
     1CKA,VISCA,COTEA,PR,RA,GR,FCTERM1,FCTERM2
      IF (TBULK.LE.TCA) THEN
        VCYSK=0.D+0
        RETURN
      END IF
      TFILM=((TBULK+TCA)/(2.D+0))
      CALL PRPA(TFILM,DENSA,CPA,CKA,VISCA,COTEA)
      GR=(((DENSA**2.D+0)*G*(SL**3.D+0)*COTEA*(TBULK-TCA))/
     1(VISCA**2.D+0))
      PR=((VISCA*CPA)/(CKA))
      RA=GR*PR
      IF (RA.LT.1.D+12) THEN
        FCTERM1=((4.D+0*CKA)/(3.D+0*SL))*(((7.D+0*GR*
     1(PR**2.D+0))/(5.D+0*(20.D+0+(21.D+0*PR))))**2.5D-1)
        FCTERM2=((4.D+0*(2.72D+2+(3.15D+2*PR))*CKA)/(3.5D+1*
     1(6.4D+1+(6.3D+1*PR))*DOUT1))
        VCYSK=(FCTERM1+FCTERM2)
      ELSE
        WRITE(6,1)
 1      FORMAT(1H0,' ERROR(VCYSK)....Flow is not laminar')
        STOP
      END IF
```

```
      RETURN
      END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
      SUBROUTINE PRPA(TMPE,DENSA,CPA,CKA,VISKA,COTEA)
************************************************************************
* THIS SUBROUTINE CALCULATES PERTINENT AIR PROPERTIES                  *
* USED IN THE EVALUATION OF THE OVERALL HEAT TRANSFER                  *
* COEFFICIENT                                                          *
************************************************************************
      IMPLICIT NONE
      REAL*8 TMPE,DENSA,CPA,CKA,VISKA,COTEA,TR
      IF (TMPE.LT.-2.3D+1) THEN
        WRITE(6,1)
 1      FORMAT(' ERROR(PRPA)....Temperature less than -23 C')
        STOP
      ELSEIF (TMPE.GT.1.027D+3) THEN
        TR=(1.027D+3)+(2.7315D+2)
        GO TO 3
      END IF
      TR=TMPE+2.7315D+2
 3    DENSA=((6.32611D-18*(TR**6.D+0))+(-3.35972D-14*(TR**5.D+0))+
     1 (7.35676D-11*(TR**4.D+0))+(-8.57601D-8*(TR**3.D+0))+
     2 (5.7247D-5*(TR**2.D+0))+(-2.1793D-2*TR)+(4.36348D+0))
      CPA=((2.40236D-13*(TR**4.D+0))+(-9.60387D-10*(TR**3.D+0))+
     1 (1.31534D-6*(TR**2.D+0))+(-5.19672D-4*TR)+(1.0656D+0))
      CKA=((-1.37853D-14*(TR**4.D+0))+(4.16364D-11*(TR**3.D+0))+
     1 (-5.9969D-8*(TR**2.D+0))+(9.83911D-5*TR)+(9.45229D-4))
      VISKA=(((-5.26671D-13*(TR**4.D+0))+(2.45986D-9*(TR**3.D+0))+
     1 (-4.8643D-6*(TR**2.D+0))+(6.97124D-3*TR)+(1.35554D-1))*1.D-5)
      COTEA=((7.71607D-15*(TR**4.D+0))+(-2.93729D-11*(TR**3.D+0))+
     1 (4.22333D-8*(TR**2.D+0))+(-2.84058D-5*TR)+(8.8277D-3))
      RETURN
      END
!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!!
```

Appendix E: Sample Input

The following is a sample input file. This input file is for the six bottle array using the COS model and the 1.0 $/sec ramp.

THE NUMBER OF EQUATIONS=14 ITOL=2 RTOL=1.0D-8
ITASK=1 ISTATE=1 IOPT=1 LRW=344 LIW=34 MF=22
INITIAL POWER=729.0 GG1=6.408D-21 POLY1=3.0D-11
RHOGAS(1)=-39.1 RHOGAS(2)=-34.5 RHOGAS(3)=-34.5 RHOGAS(4)=-39.1
RHOGAS(5)=-34.5 RHOGAS(6)=-39.1
RHOTEMP(1)=-3.0D-4 RHOTEMP(2)=-8.4D-5 RHOTEMP(3)=-8.4D-5
RHOTEMP(4)=-3.0D-4 RHOTEMP(5)=-8.4D-5 RHOTEMP(6)=-3.0D-4
RHOSTEAM(1)=-29.3 RHOSTEAM(2)=-25.0 RHOSTEAM(3)=-25.0
RHOSTEAM(4)=-29.3RHOSTEAM(5)=-25.0RHOSTEAM(6)=-29.3KPOLY=200.0
T=0.0 TOUT=0.05 DT=0.05 TSTOP=1000.0
GEN=3.7D-5 Q1=-2.62D-20 R1=7.0D-3 TSUM=0.0 M1=0.0
ATOL(01)=1.0D-08 ATOL(02)=1.0D-10 ATOL(03)=1.0D-08
ATOL(04)=1.0D-08 ATOL(05)=1.0D-08 ATOL(06)=1.0D-08
ATOL(07)=1.0D-08 ATOL(08)=1.0D-08 ATOL(09)=1.0D-08
ATOL(10)=1.0D-08 ATOL(11)=1.0D-08 ATOL(12)=1.0D-08
QF=1.00 NF=0.0 VAR1=1.0D-9
PRESS(01)=1.0D-08 PRESS(02)=1.0D-10 PRESS(03)=1.0D-08
PRESS(04)=1.0D-08 PRESS(05)=1.0D-08 PRESS(06)=1.0D-08
TBULK(07)=1.0D-08 TBULK(08)=1.0D-08 TBULK(09)=1.0D-08
TBULK(10)=1.0D-08 TBULK(11)=1.0D-08 TBULK(12)=1.0D-08

Appendix F: Sample Output

This is a sample output file. This output file is for the six bottle array and 1.0 $/sec ramp. The outputs include bottle temperature, bottle pressure, reactivity, total energy, and various other parameters.

```
 14          1 .0000000000000000E-07  1.0000000000000000E-08
 1           1           1          344          34          22
-37.10000000000000      6.4080000000000001E-20  3.2000000000000000E-11
 200.0000000000000      841800.0000000000       0.0000000000000000E+00
 9.9999999999999999E-04  9.9999999999999999E-04   20.00000000000000
 0.0000000000000000E+00  3.3000000000000000E-05   1.000000000000000
 300.0000000000000      -2.9000000000000000E-04 -1.0000000000000000E-04
 -1.0000000000000000E-04 -2.9000000000000000E-04
 -1.0000000000000000E-04  -2.9000000000000000E-04  0.2600000000000000
 1.000000000000000    9.0000000000000001E-05   30.00000000000000
 1.2000000000000000E-15 5.0000000000000000E-05  2.2000000000000000E-03
```

```
FRTEMP=  0.0000000000000000E+00
FRGAS=  0.0000000000000000E+00
TOUT=  0.100 ISTATE= 2 Y(1)=  0.470E+10
Y(2)=  0.265E+13 ENERGY #1=  0.400E+04 #2=  0.400E+04 #3=  0.400E+04
#4=  0.400E+04 #5=  0.400E+04 #6=  0.400E+04 GAS MASS #1=  0.334E-10
#2=  0.669E-10 #3=  0.669E-10 #4=  0.334E-10 #5=  0.669E-10
#6=  0.334E-10 NUCLEATION=  0.399E-12 TOTAL REACTIVITY =  0.257E-01
PRESS #1=  0.234E-02 #2=  0.234E-02 #3=  0.234E-02 #4=  0.234E-02
#5=  0.234E-02 #6=  0.234E-02 TBULK #1=  0.200E+02 #2=  0.200E+02
#3=  0.200E+02 #4=  0.200E+02 #5=  0.200E+02 #6=  0.200E+02
```

VITA

Roger Wayne Brewer was born at Fort Meade, Maryland on May 20, 1958. He attended elementary schools in Laurel, Maryland and Woodbridge, Virginia, and graduated from Woodbridge Senior High School in May 1976. In November 1978 he enlisted in the United States Navy and served on board the USS Ray SSN 653 as a Machinist Mate and Engineering Laboratory Technician and was honorably discharged in November 1984. In December 1984 he began work with the Tennessee Valley Authority as a Senior Health Physics Technician. In June 1985, while employed with TVA, he entered Roane State Community College. In August 1988 he transferred to the University of Tennessee-Knoxville. In May 1991 he received the degree of Bachelor of Science in Nuclear Engineering. In June 1991 he reentered the University of Tennessee-Knoxville in pursuit of the degree of Master of Science in Nuclear Engineering. He will receive the Master of Science Degree in either May or August of 1993. He has accepted a staff position with Los Alamos National Laboratory.