NUREG/CR-3913
SAND84-1522
R3
Printed February 1985

HECTR Version 1.0 User's Manual

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Prepared by
Sandia National Laboratories
Albuquerque, New Mexico 87185 and Livermore, California 94550
for the United States Department of Energy
under Contract DE-AC04-76DP00789

Prepared for
U. S. NUCLEAR REGULATORY COMMISSION

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U.S. Nuclear Regulatory Commission
Washington, D.C. 20555

and

National Technical Information Service
Springfield, Virginia 22161

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Operated by
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Prepared for
Division of Accident Evaluation
Office of Nuclear Regulatory Research
U.S. Nuclear Regulatory Commission
Washington, DC 20555
Under Memorandum of Understanding DOE 40-550-75
NRC FIN No. A1246

AUTHOR'S NOTE

Many calculations have been published in the past using pre-release versions of HECTR. In some cases, descriptions of various models were provided. This report supersedes all such publications, and users should be aware that many of the models have evolved significantly since those documents were prepared.

As HECTR Version 1.0 is the first version of HECTR to be formally released, it is likely that different users will encounter various shortcomings in the performance of the code. Because we plan to release updated versions of HECTR, we would appreciate suggestions for improvement or information concerning any errors that are encountered. Also, we ask anyone who changes the code to document the changes and to properly identify the version of the code in any publications. This will limit future confusion should several versions of HECTR be in use simultaneously. Please send questions or comments to the following address:

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ABSTRACT

This report describes the features and use of HECTR Version 1.0. HECTR is a relatively fast-running, lumped-volume containment analysis computer program that is most useful for performing parametric studies. The main purpose of HECTR is to analyze nuclear reactor accidents involving the transport and combustion of hydrogen, but HECTR can also function as an experiment analysis tool and can solve a limited set of other types of containment problems. HECTR Version 1.0 has been particularly tailored to analyze accidents in ice-condenser PWR and Mark III BWR containments. HECTR is designed for flexibility and provides for user control of many important parameters, particularly those related to hydrogen combustion. Built-in correlations and default values of key parameters are also provided.

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ACKNOWLEDGMENT

Many people contributed to this effort, and while it is not possible to discuss in detail the ways in which help was provided, the authors thank the following people for their assistance in model development and assessment:

Michael L. Corradini
Steven N. Kempka
Donald B. King
Joan F. Kotas
Peter G. Prassinos
Arthur C. Ratzel
Douglas J. Rzepecki
Martin P. Sherman
Robert A. Watson
Herman A. Watts
C. Channy Wong

We particularly acknowledge the advice provided by Randall K. Cole, Jr. during model development and code assessment, especially while developing our basic numerical solution scheme.

HECTR VERSION 1.0 USER'S MANUAL

1. INTRODUCTION

1.1 Background

Since the accident at Three Mile Island (TMI), there has been a great deal of interest regarding the problem of hydrogen production and combustion in light water reactors (LWRs). During the TMI accident, significant quantities of hydrogen were produced and released to containment. This hydrogen eventually ignited, causing a pressure rise of about 192 kPa within containment. While this event did not threaten the TMI containment, there is concern that other, weaker containments might be vulnerable to hydrogen combustion or that more severe pressure rises might be seen under other accident conditions. Concerns have also been raised regarding the survival of safety-related equipment in hydrogen burn environments.

Because of the concerns noted above, the Nuclear Regulatory Commission has sponsored a program at Sandia National Laboratories, Albuquerque (SNLA) to investigate hydrogen behavior in LWR containments. Part of the work under the Hydrogen Behavior Program has involved reviewing utility proposals for mitigation schemes to deal with potential hydrogen problems. In 1981 SNLA was asked to review and comment on the deliberate ignition system proposed for hydrogen control at Grand Gulf Unit 1, which has a boiling water reactor (BWR) Mark III containment. As part of that review, we attempted to estimate the pressure rises that might occur in the containment as a result of hydrogen deflagrations. At the time, the only analysis tool readily available to us was the MARCH computer code, which had severe limitations in its treatment of containment thermal-hydraulics and hydrogen burns. Therefore, in order to provide a more realistic analysis, we combined some recently developed containment heat-transfer models, a simple thermodynamics package, and a simple intercell gas flow model into a computer program called HECTR (Hydrogen Event: Containment Transient Response).

While the first version of HECTR served its intended purpose, it was very limited in capability and slow in execution. It was apparent that there would be additional need for analyses of hydrogen burns in containments, so an effort was undertaken to develop and expand the capabilities of HECTR to

analyze hydrogen burns in various types of containments. Our goal was to produce a flexible, user-friendly, and relatively fast-running code that would be useful for parametric analyses. HECTR Version 1.0 represents our first attempt at meeting that goal. Emphasis has been placed on providing capabilities important in the analysis of pressurized water reactor (PWR) ice-condenser and BWR Mark III containments, as those are the containments currently considered to have the greatest concerns with respect to hydrogen combustion.

1.2 Capabilities of HECTR Version 1.0

HECTR is a lumped parameter containment analysis code developed for calculating the containment atmosphere pressure-temperature response to hydrogen burns. As noted above, HECTR Version 1.0 has been developed primarily for analysis of ice-condenser PWR and Mark III BWR containments, although its use need not be restricted to these systems. References 1 and 2 present calculations for these containments using prerelease versions of HECTR. HECTR is also useful for modeling hydrogen transport and combustion experiments. Furthermore, HECTR is useful for analyzing experiments involving only the release of steam and liquid water. The reader should refer to References 3 and 4 for more examples of the capabilities of HECTR.

Four gases--steam, nitrogen, oxygen, and hydrogen--are modeled in HECTR along with sumps containing liquid water. To calculate the pressure, temperature, and composition of gases in a containment, the containment is divided into "compartments" with flow between compartments occurring through "junctions." As shown in Figure 1-1, each compartment is essentially a gas control volume. Flows between compartments are pressure and buoyancy driven with inertial and resistance terms included. Steam is treated as a real gas, and the other gases are treated as ideal. Gases in each compartment are instantaneously mixed, and source terms are user-specified. Simplified conservation equations are solved to determine compartment and junction conditions during the transient. The thermal response of surfaces and equipment in the containment can also be calculated in HECTR, using either one-dimensional finite difference slabs or lumped masses. Models are included to calculate hydrogen combustion, radiative and convective heat transfer, and steam condensation or evaporation. The engineered safety features (ESFs) modeled in HECTR are containment sprays, fans, ice condensers, sumps, suppression pools, and heat exchangers.

With the capabilities identified above, HECTR can model virtually all the containment systems of importance in ice-condenser and Mark III containments. The combination of combustion models that are based on recent experimental data, experimentally verified models for gas transport, and models

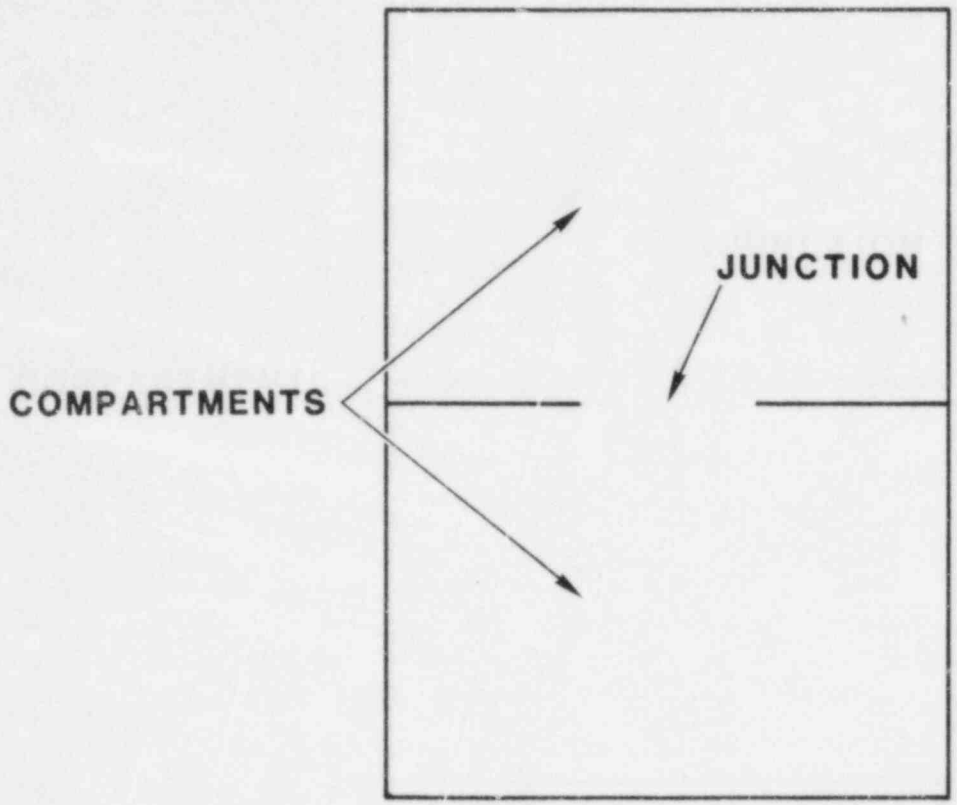


Figure 1-1. HECTR Compartment and Junction Arrangement

for containment systems and heat-transfer mechanisms makes HECTR an extremely valuable tool for evaluating many aspects of the containment response to a variety of accidents.

HECTR has been developed with emphasis on hydrogen combustion. It is not intended to model all possible phenomena that might occur during a severe accident. For example, steam explosions, core-concrete interactions, and aerosol transport are not modeled by HECTR. For many accidents, such as most degraded-core accidents, these phenomena may not be important. In other cases, HECTR results can still provide insights when combined with analyses that address the phenomena not modeled in HECTR. Currently, no code exists that can model all possible phenomena. However, there are efforts in progress at SNLA to develop and improve codes that will deal with a broader range of problems than HECTR. Both the CONTAIN and MELCOR codes eventually should treat many of the problems that HECTR can now treat in addition to a broader range of problems.

In the future, new models will be added to HECTR as needed to treat the phenomena that are important for accident scenarios involving combustion. In particular, the development of a model to treat diffusion flames is planned. Also, versions of HECTR now operational at SNLA include the treatment of

carbon monoxide and carbon dioxide, fan coolers, and continuous burning. Checkout and testing of these models are in progress. Additionally, with the support of the Severe Accident Sequence Analysis Program, containment leakage, core concrete, and reactor cavity models are being coupled to HECTR.

1.3 Description of This Manual

The remainder of this manual provides a description of HECTR, along with instructions for using the code. We caution the user that codes such as HECTR contain many subjective models, and the results that are produced must be carefully interpreted. Merely running the sample problems does not qualify one to perform analyses with HECTR. It is essential that the user acquire a general understanding both of the methods used and of the physics important to the events being analyzed.

Chapter 2 provides a general description of the code structure, solution techniques, and physical models in HECTR. Chapter 3 provides guidance in using the code and presents many of the insights that we have acquired during our experience using the code. Detailed input instructions, including instructions for interfacing HECTR to a primary system code such as MARCH, are found in Chapter 4; Chapter 5 describes the output that will be produced by HECTR. Chapter 6 presents three example problems: a simple two-compartment problem, an ice-condenser PWR containment problem, and a Mark III BWR containment problem.

For serious users of HECTR, three appendices are provided. Appendix A contains details of the models in HECTR that were summarized in Chapter 2. Appendix B provides a detailed breakdown of the code structure. The control language necessary to run HECTR on various SNLA computer systems is described in Appendix C.

To get started, we recommend reading Chapters 2 and 3 to obtain a general understanding of the physical models and numerical methods used in HECTR. This should be followed by setting up and running one or more of the sample problems, referring to Chapters 4 and 5 as necessary. Before running additional problems with HECTR, we recommend reading Appendix A, which contains a detailed description of the models in the code. Also, frequent referral to Chapter 3 is useful when setting up a new problem. Those desiring to make changes to HECTR will find Appendix B useful, although changes should be attempted only when a thorough understanding of and familiarity with the code are achieved.

2. DESCRIPTION OF MODELS

In this chapter, the methods used in HECTR are briefly described. A more detailed description (including the equations used in the models) is provided in Appendix A. The code structure and governing equations are discussed first, followed by descriptions of the physical models that provide terms for the governing equations.

2.1 General Code Structure

2.1.1 Multicompartment Mass, Energy, and Momentum Equations and the Equation of State

The multicompartment gas-transport model is a system of ordinary differential equations expressing conservation of mass, energy, and momentum. The mass conservation equations are formulated for each of four gas species (water vapor, nitrogen, oxygen, and hydrogen) in each compartment on a molar basis. The conservation of energy equation is formulated for the total mixture in each compartment. These equations include terms for hydrogen combustion, heat transfer to surfaces, evaporation/condensation on surfaces, external sources, and the effects of ESFs. Gas flow rates between compartments are determined by using a simplified momentum equation at each flow junction. A transient momentum equation is used that includes gravitational and frictional forces, but neglects momentum flux terms. Within each compartment the gases are perfectly mixed. Steam is treated as a real gas, while the other gases are assumed to be ideal. The mass, energy, and momentum equations are solved simultaneously to obtain the compartment thermodynamic conditions and junction flow rates throughout a transient. External sources can be treated by HECTR in a variety of ways. Any of the four species can be injected into any compartment or sump. Tabular source input can be provided by the user, or procedures can be used to interface HECTR to source files produced by primary reactor system codes such as MARCH.

2.1.2 Method of Sclution

The conservation equations in HECTR are solved using a linearized implicit formulation (backward Euler method). The linear system of equations that results from this formulation is solved by a standard LU decomposition followed by back substitution (see Section A.1.2 for more details).

2.1.3 Timestep Control

There are two major kinds of timesteps in HECTR: heat-transfer timesteps and flow timesteps. Normally, heat-transfer rates are relatively constant over a longer time

scale than that required to solve the conservation (flow) equations. Therefore, we decoupled the heat-transfer calculations from the flow equations in HECTR. To accomplish this, heat-transfer rates from radiation, convection, condensation, and sprays are computed at the beginning of a heat-transfer timestep. These rates are then held constant while the flow calculations are performed (the conservation equations are solved). When compartment conditions change sufficiently to significantly affect the heat-transfer rates, HECTR recalculates these rates. The time between heat-transfer updates is termed the heat-transfer timestep, and the timestep used when solving the conservation equations is termed the flow timestep. Note that each heat-transfer timestep can contain one or more flow timesteps.

HECTR automatically controls the size of the heat-transfer and flow timesteps. The flow timestep is controlled by changes in compartment pressure and by the total volumetric flow leaving each compartment. The heat-transfer timestep is controlled by changes in compartment pressures and temperatures. Both types of timesteps are further constrained to fall within minimum and maximum limits, and the rate of growth of each timestep is also controlled.

2.2 Physical Models

2.2.1 Flow Junctions

The standard type of flow junction in HECTR allows for flow in either direction, with the flow rate determined from the momentum equation. Two other types of flow junctions are available to calculate flow that predominantly occurs in only one direction. These two types of flow junctions model check valves and variable area doors. To model check valves, the momentum equation for two-way junctions is used, but flow is allowed to occur only in one direction. The variable area doors are modeled by allowing the flow area of the junction to vary with the differential pressure across it. A fourth type of junction is used to model drains between the upper and lower compartments of an ice-condenser containment. This junction is treated as a standard two-way junction, except that it is blocked under certain conditions. (See Section A.2.1.)

2.2.2 Intercompartment Fans

The HECTR fan model can treat flow between any two compartments. A head flow curve can be used to calculate the fan flow rate, or a constant volumetric flow rate can be specified. The fans can be either actuated at the beginning of a calculation or set to come on automatically based on pressure or temperature setpoints.

2.2.3 Hydrogen Combustion

The hydrogen combustion model in HECTR treats both ignition of hydrogen in a compartment and propagation of burns between compartments. The burns are assumed to behave like ordinary deflagrations; flame acceleration and detonations are not treated in HECTR. The hydrogen in a compartment is ignited if the concentrations of hydrogen, oxygen, and steam in the compartment satisfy specified ignition limits. This burn can propagate into adjacent compartments if the hydrogen, oxygen, and steam concentrations in these compartments satisfy specified propagation limits, which can be different from the ignition limits. To define the ignition and propagation limits, minimum concentrations are specified for hydrogen and oxygen, and maximum concentrations are specified for steam. The propagation limits can be different for upward, horizontal, and downward propagation. The user car specify values for these parameters or use the default values included in HECTR.

HECTR does not model combustion as a flame front; instead, it calculates a rate at which the hydrogen and oxygen in a compartment are combined to form steam and assumes the reaction occurs uniformly throughout the compartment. Thus, during a burn, a compartment will contain a homogeneous mixture of burned and unburned gases. The duration of the burn (the burn time) and the final mole fraction of hydrogen are calculated at the start of a burn. A burning rate is then calculated such that the burn finishes at the predetermined time with the correct final mole fraction of hydrogen. The burning rate is adjusted at each timestep during the burn to account for changes in the hydrogen concentration from flows out of the compartment or from injection of sources. A burn will terminate if all the oxygen in the compartment is consumed.

The burn time can be a user-specified constant, or it can be calculated as the ratio of a user-specified flame propagation length (travel distance) to the flame speed. The flame speed can be calculated from a default correlation that varies with hydrogen and steam concentration, or it can be specified as a constant by the user. The final mole fraction of hydrogen that will remain at the end of the burn can also be calculated from a correlation built into HECTR, or it can be specified as a constant by the user. The default combustion completeness and flame speed correlations were derived from a variety of experiments that were performed in the Variable Geometry Experimental System (VGES) and Fully Instrumented Test Series (FITS) experimental facilities at SNLA [5,6].

2.2.4 Radiative Heat Transfer

The radiative heat-transfer model in HECTR includes radiation from the steam in the compartments to the surfaces as well as

radiative exchange between the surfaces. The gas and the surfaces are both assumed to be gray. The emittance of steam is calculated using the Cess-Lian model [7]. Surface emissivities, and view factors and characteristic beam lengths between surfaces, are provided by the user. A network for radiative heat transfer among the surfaces is then constructed, and the resulting linear system of equations is solved to give the net heat flux to each surface. In HECTR Version 1.0 radiative exchange is allowed only between surfaces in the same compartment or in adjacent compartments.

2.2.5 Convective Heat Transfer

The convective heat-transfer package in HECTR contains models for sensible heat transfer, latent heat transfer (evaporation and condensation), and liquid films. Three basic types of surfaces are treated: walls, sumps, and ice-condenser surfaces. The sensible heat transfer to each surface is determined using correlations for the Nusselt number. For walls and sumps, both free and forced convection solutions are calculated, then the larger heat flux is used. Only forced convection is modeled for ice-condenser surfaces.

Two types of latent heat-transfer models are included in HECTR: air-steam diffusion models and pure steam models. Both evaporation and condensation are treated in HECTR. The air-steam diffusion model is used whenever a significant amount of air is present and is based on a heat-transfer/mass-transfer analogy relating the Sherwood number to the Nusselt number that was calculated for sensible heat transfer. Steam partial pressure differences between the gas and the surface provide the driving force for mass transfer (either evaporation or condensation).

Different pure-steam latent heat-transfer models are used for the different types of surfaces. A modified Nusselt film model is used for condensation on wall and ice-condenser surfaces. Condensation on sump surfaces is based on a heat-transfer boundary layer at the top of the sump surface.

Liquid films are allowed to build up on wall surfaces only. The films can build up to a specified maximum film thickness. Any additional condensate will be added to a specified sump. Changes in film thickness are based on the calculated evaporation or condensation rate. If the film becomes superheated relative to the gas, a portion of the film will boil or flash in order to bring the film back to saturation.

2.2.6 Surface Conduction

The surfaces in HECTR are treated either as one-dimensional slabs or as lumped masses. For both cases, the heat transfer to the front side of the surface is calculated from the models for radiative and convective heat transfer described in Sections 2.2.4 and 2.2.5.

For lumped-mass surfaces, the temperature and all of the material properties are assumed to be constant throughout the surface. Therefore, a simple energy balance using the net heat-transfer rate to the surface can be integrated to give the transient surface temperature.

One-dimensional conduction is modeled for slab surfaces. The slab surfaces can consist of multiple layers of different materials. Three types of boundary conditions can be specified for the back sides of slabs: insulated, constant temperature, or constant heat-transfer coefficient. The slab is nodalized by HECTR, and a finite difference formulation is used to calculate the temperatures in the slab.

2.2.7 Containment Sprays

Sprays can be injected into any specified compartment. The drops from containment sprays are assumed to be isothermal, spherical, and traveling at the terminal velocity corresponding to their instantaneous size and mass. Ordinary differential equations are formulated, which express the rates of change of the mass and temperature of a drop with respect to the distance it has fallen. These equations are integrated for drops from each drop size in a user-specified droplet distribution as they fall through a compartment. The contribution of the sprays to the heat- and mass-transfer rates for the compartment are determined by the final temperature and masses of the drops. The gas is assumed to be homogeneous with constant properties during the fall time of the drops. Therefore, the solutions represent a quasi-steady-state model. A user-specified fraction of the drops that have reached the bottom of a compartment is allowed to fall into lower compartments. Water not falling into other compartments can be transferred to a specified sump.

Like the fans, the sprays can be either actuated at the start of a calculation or set to come on automatically whenever specified pressure or temperature setpoints are exceeded. Logic in HECTR allows operation of the sprays in either the injection mode or the recirculation mode. In the injection mode, sprays are introduced from a constant-temperature external source. After a specified time in the injection mode, the sprays automatically switch to the recirculation mode. In the recirculation mode, spray water is drawn from a specified sump and, if desired, passed through a heat

exchanger before being introduced into the desired compartments. Only one spray heat exchanger is allowed. Thus, if sprays are injected into several compartments while in the recirculation mode, HECTR assumes that the entire spray flow for all of the compartments is drawn from a single sump, then passed through a single heat exchanger. Thereafter, the flow can be split to allow spray injection into several compartments.

2.2.8 Ice-Condenser Model

To model an ice condenser, HECTR subdivides the ice-bed region into a specified number of compartments (the default number is 4) and uses two more compartments for the lower and upper plenums. This relatively large number of compartments is necessary because the steam concentration can vary significantly across the ice condenser. The metal in the ice condenser and the ice are modeled as separate surfaces. The metal surfaces are treated as lumped masses. The ice surfaces are treated as having a constant temperature with variable mass and surface area to account for the ice melting. Heat transfer to the surfaces is calculated by the convective and radiative heat-transfer models discussed previously. Liquid formed in the ice regions by melting ice and steam condensation falls down through the ice condenser to a sump on the floor of the lower plenum. While falling through the lower plenum, this water is assumed to heat up to a user-specified temperature because of steam condensation on the water.

2.2.9 Containment Sumps

An arbitrary number of sumps can be specified in each compartment. Water and energy can be added to or removed from each sump by several processes that are listed in the following paragraphs. The temperature and mass of each sump are calculated by performing mass and energy balances that include all of these processes. Each sump can be either subcooled or saturated at the pressure of the compartment containing the sump. If a sump becomes superheated, enough water is removed from the sump during each timestep and added as steam to the associated compartment to keep the pool at saturation.

Water can be added to the sumps by several processes: runoff of condensate that collects on heat-transfer surfaces, water that condenses from the atmosphere if the gas becomes supersaturated, and water that drains out of the lower plenum of an ice condenser. Any spray droplets that reach the bottom of a compartment and which will not be carried over into lower compartments are also added to a sump. If an external source of water is injected into a compartment and flashes to a mixture of liquid and steam in the compartment, the liquid portion is added to a sump. External sources of liquid water or any of the four gases modeled in HECTR can also be injected

directly into a sump. Any steam injected into a sump is assumed to condense in the sump, and any other gases are assumed to be cooled to the sump temperature before escaping into the associated compartment. The energy removed from the gases by condensation and cooling is added to the sump.

Water can be drawn from a sump for emergency core cooling or containment sprays. Water can also overflow from one sump to another.

Sumps can be cooled by heat exchangers, using the model described in Section 2.2.11. Convective heat transfer, condensation/evaporation, and radiative heat transfer are calculated for the surface of each sump.

2.2.10 Suppression Pool Model

The suppression pool model includes all of the effects described previously for the sumps, as well as models for phenomena that are unique to BWR Mark III containments. These additional models calculate the motion of the suppression pool, gas flow rates between the drywell and wetwell (in either direction) if the suppression pool vents are uncovered, draining of water from the upper pool into the suppression pool, flow of water over the weir wall onto the drywell floor, and flow of water back into the suppression pool if the water level in the drywell rises above the weir wall. Pool level swell due to voiding associated with gas flow is not treated.

The water levels in the drywell region (between the weir wall and the drywell wall) and the wetwell region of the suppression pool determine whether or not a vent is cleared such that gas can flow between the drywell and the wetwell. The volumes of the drywell and wetwell compartments are increased or decreased to reflect pool level changes. To calculate the pool motion, the suppression pool is divided into nine compartments: a vertical stack of three compartments on the drywell side of the pool, an array of three rows of vents, and a vertical stack of three compartments on the wetwell side of the pool (see Figure 2-1). The water in the suppression pool is assumed to be incompressible. To calculate the motion of the suppression pool, mass and momentum balances are written for each of the nine control volumes. These equations are then integrated over time using Euler's method to give pool velocities and levels. The timestep size used to calculate the pool motion can be smaller than the flow timestep.

The gas flow rates through suppression pool vents that have cleared are calculated using a form of the momentum equation that is similar to that used for the flow junctions in

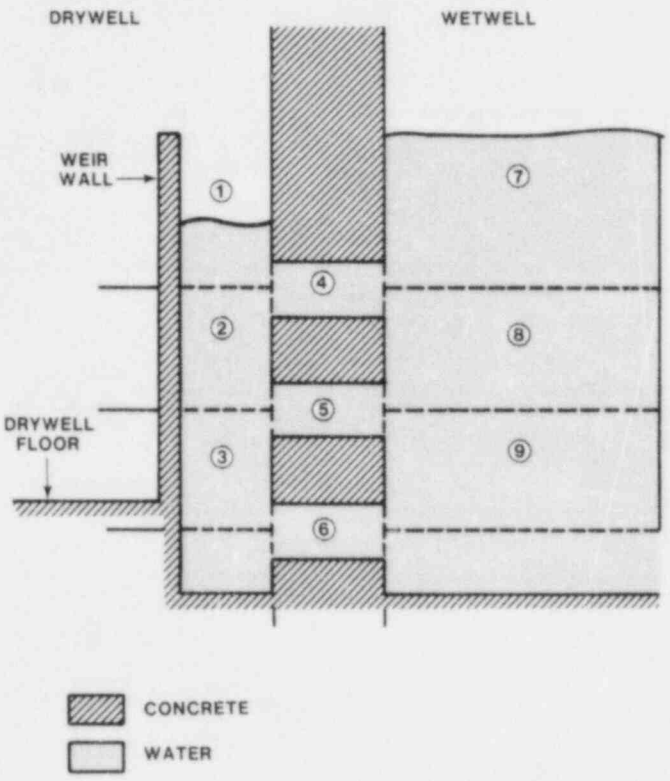


Figure 2-1. Suppression Pool Compartmentalization

HECTR. The equation used for the junctions is modified to include the pressure head of water that is above the vent centerline in the suppression pool downstream of the vent.

The upper-pool dump that occurs in Mark III containments is also modeled in HECTR. At a user-specified time, the valves on the drain lines are assumed to open such that water is transferred from the upper pool to the suppression pool at a user-specified rate. The upper pool is not allowed to drain past a user-specified minimum volume. However, the drain valves are assumed to remain open for the duration of the calculation such that any water added to the upper pool that increases its level above the minimum (e.g., by sprays) will drain into the suppression pool.

2.2.11 Heat Exchanger Model

The heat exchanger model in HECTR is used for cooling sumps or suppression pools, or for cooling containment sprays when they are in the recirculation mode and are drawing water from the sump. The heat exchanger model in HECTR is for a once-through counter-current flow heat exchanger. An iterative model is used that matches the heat-transfer rates to the changes in outlet flow temperature. A separate heat exchanger can be specified for each sump, but only one heat exchanger can be used for cooling containment sprays.

3. INPUT GUIDELINES AND CODE SENSITIVITIES

3.1 Introduction

In this chapter we provide some general guidance for using HECTR and indicate the relative sensitivity of the results to changes in various parameters. The information presented reflects the experience that we have had applying HECTR to various problems. However, the guidance presented reflects only our opinions. Users are encouraged to try different approaches, with recognition that proper analysis of a reactor accident will generally require several runs, varying parameters so that an understanding of the important phenomena can be achieved.

In the sections that follow, the models presented in Chapter 2 (and Appendix A) are reexamined in terms of recommended input values and sensitivity to those values. It is very important to understand that there are many threshold effects in the HECTR analysis of a reactor accident (e.g., start of a hydrogen burn, initiation of containment sprays, etc.). Changing a parameter that is expected to cause only a few percent difference in the results may cause a certain threshold to be exceeded (or not exceeded) and so produce dramatically different results. Therefore, the user must examine the results in detail and not look just at the final result in determining the effects of changing various parameters. For additional insight into using HECTR, the reader should examine the sample problems presented in Chapter 6.

3.2 Compartmentalization

One of the major decisions when performing containment analyses is determining how to compartmentalize the containment. Very often the arrangement of compartments will control the gas transport and, thus, the course of the accident. In this section we provide some guidance, but because no cookbook approaches are available, users will be required to exercise some judgment in each specific case.

First, one should examine a containment and locate large, physically separated compartments. Individual rooms are certainly candidates to be computational compartments. Individual rooms can be further subdivided, depending on their size and the mixing mechanisms that may be present in the room. If a room is expected to be well mixed due to forced convection, then a single compartment should be adequate. Generally, we recommend that the subdividing of individual rooms be minimized, both because it increases the run time and because the radiative heat-transfer model is of limited validity for multicompartment situations, as discussed in Section 3.7 and in Appendix A.

Numerical problems can arise if the compartmentalization is done improperly. For example, problems can arise if two different compartments have volumes that are different by many orders of magnitude. Occasionally, a user may wish to simulate venting to the atmosphere by adding a very large compartment to simulate the atmosphere. If a volume on the order of 10^{30} or 10^{40} m^3 is specified, and the other compartments have volumes on the order of 10^3 m^3, the solver may produce incorrect results. Generally, specifying an atmosphere volume of 10^9 or 10^{10} m^3 will prove adequate.

Specifying volumes that are very small may excessively slow down the calculation. One of the limits on the flow timestep is related to the fraction of a volume that may leave a compartment during a timestep. HECTR limits the flow timestep so that no more than 95% of the compartment volume may leave during a timestep. For flow out of a compartment through a single junction, the maximum timestep size would be

$$\Delta t \leq 0.95 \frac{V}{Av} \qquad (3\text{-}1)$$

where V is the volume, A is the flow area, and v is the gas velocity. Thus, it is apparent that, apart from the other timestep controls, the maximum step size will be reduced for a given flow velocity as the volume is decreased.

Once obvious compartments are identified, the user should look at the containment as a whole and examine the potential for gas transport and mixing. If all of the computational compartments are connected in series with only one junction connecting the compartments, then convective mixing will be suppressed. Parallel flow paths are required for convective mixing loops to form. For example, consider the Mark III BWR containment shown in Figure 3-1. Figures 3-2 and 3-3 show two different compartmentalizations of the outer containment. Figures 3-4 and 3-5 show the hydrogen concentration as a function of time in the dome and wetwell regions for the two different arrangements, using the same input and source term assumptions (no combustion was allowed in these cases). With only serial flow paths (Figures 3-2 and 3-4), mixing is significantly suppressed. If the flows are forced-convection dominated as in many ice-condenser problems, then serial connections may be appropriate. Note that HECTR sets up an ice condenser as a group of serially connected compartments. If natural convection is the dominant mixing mode, such as in the Mark III BWR problem presented here, then parallel flow paths should be included in the input model. Appropriate compartmentalizations for ice-condenser PWR and Mark III BWR containments are presented in Chapter 6. We feel that this level of compartmentalization represents the minimum number of compartments necessary to adequately treat the type of mixing that will be present in these containments.

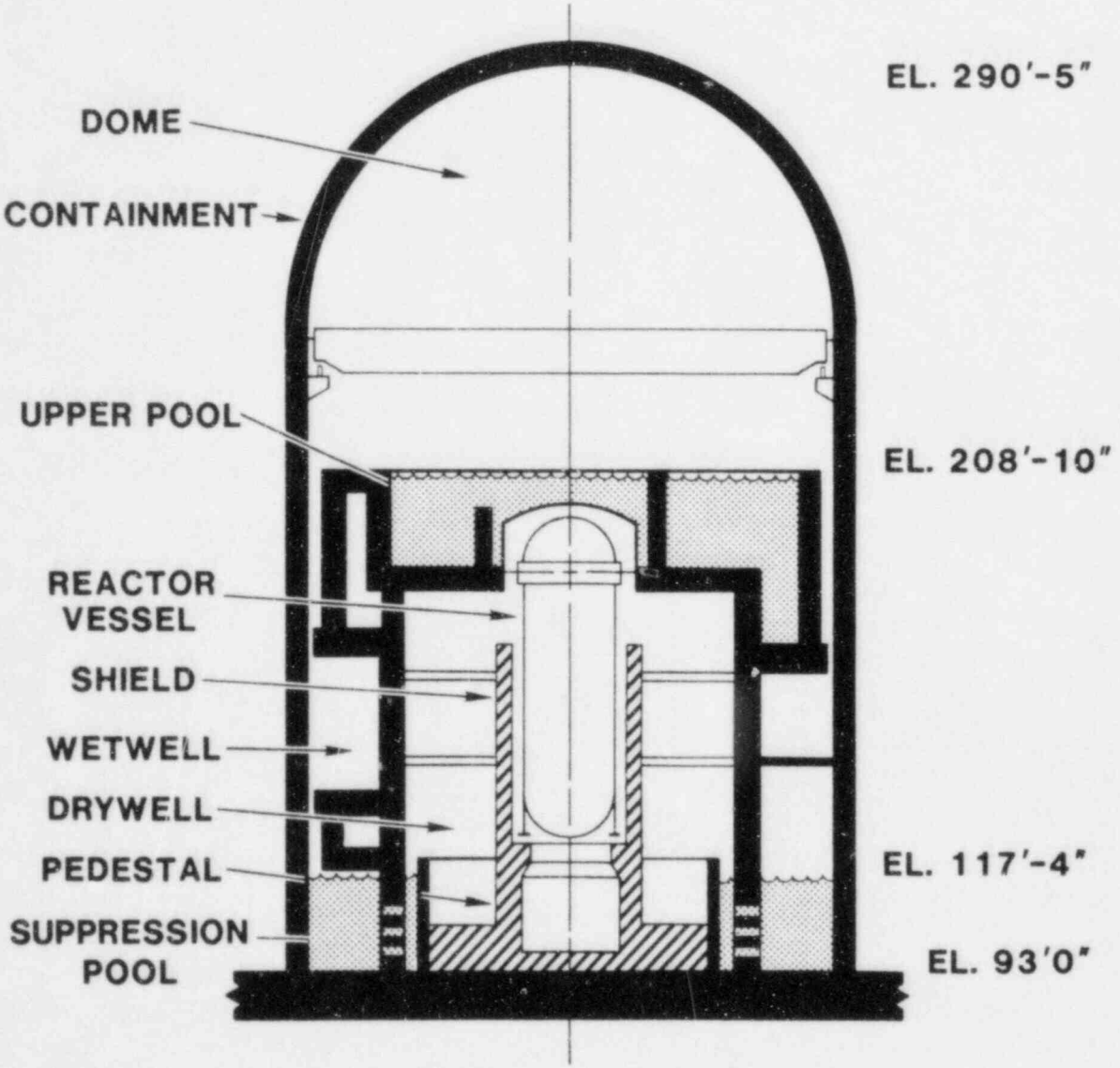
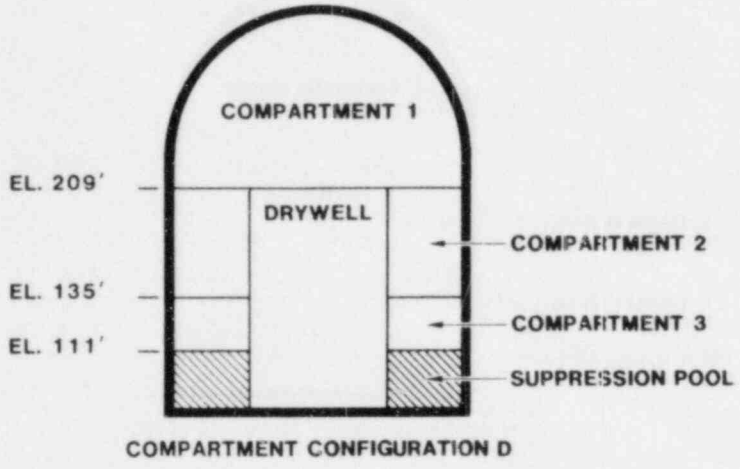


Figure 3-1. Mark III BWR Containment



Figures 3-2. Three-Volume Compartmentalization of Outer Containment

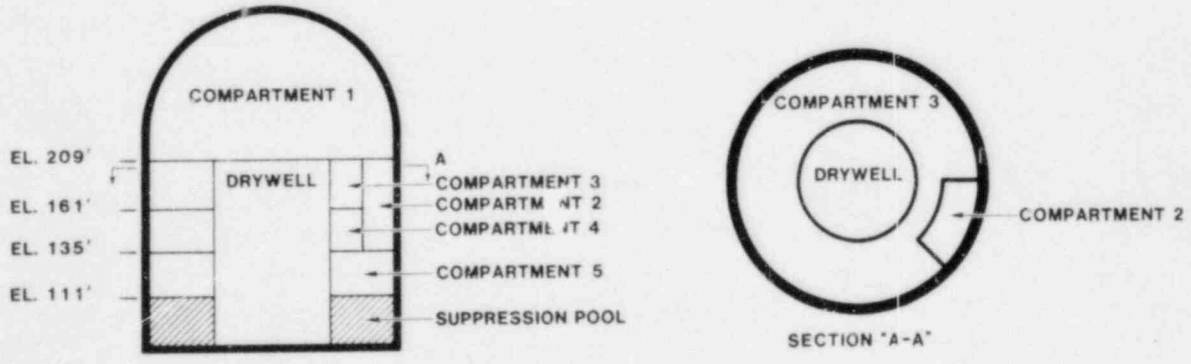


Figure 3-3. Five-Volume Compartmentalization of Outer Containment

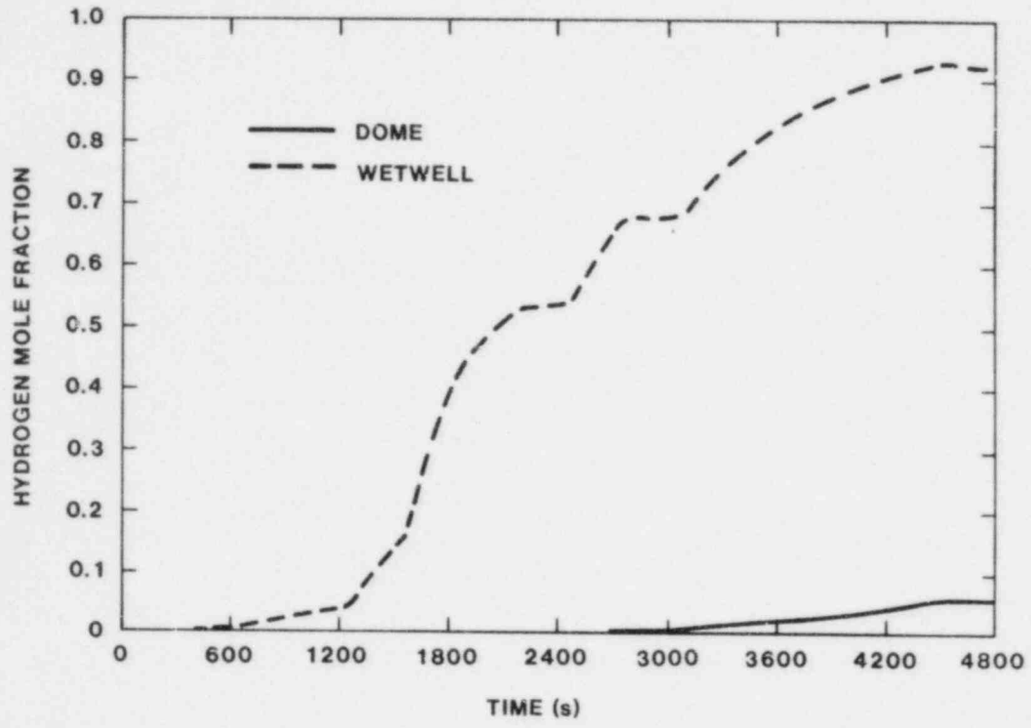


Figure 3-4. Hydrogen Concentration in Dome and Wetwell for 3-Volume Compartmentalization

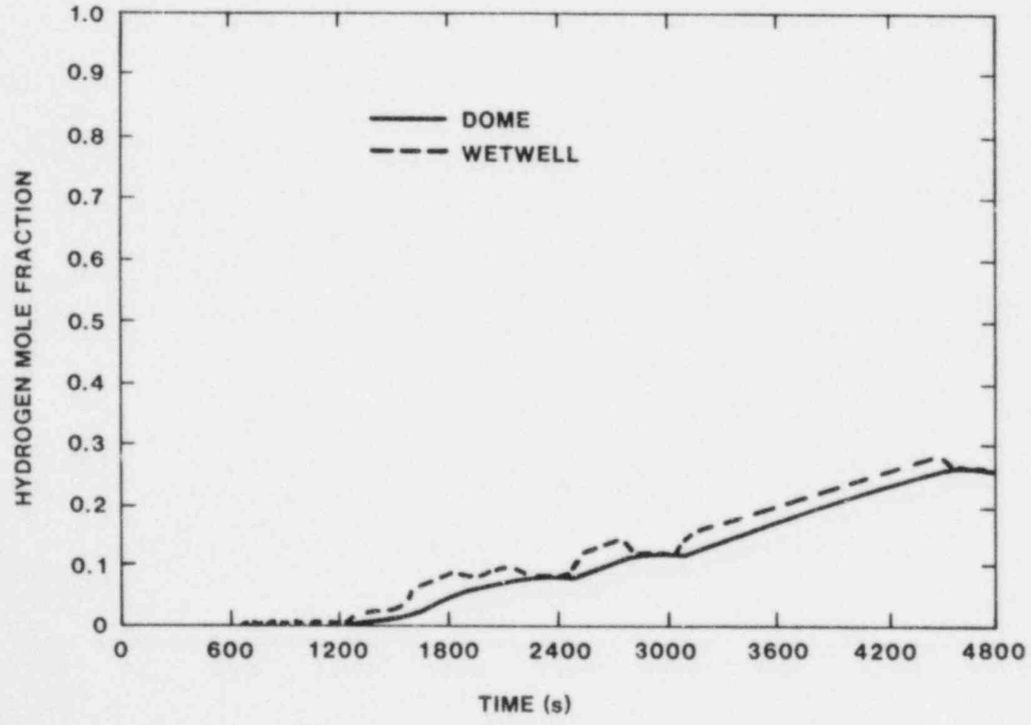


Figure 3-5. Hydrogen Concentration in Dome and Wetwell for 5-Volume Compartmentalization

Once an input deck for HECTR has been developed, it is fairly simple to alter the deck to combine smaller compartments into larger ones. However, increasing the number of compartments may be more difficult, because surfaces may need to be subdivided to correspond to the larger number of compartments, requiring the user to revise the radiative heat-transfer input. Thus, we recommend starting with a compartmentalization that is as detailed as you are likely to need.

When setting up any new problem, the user should experiment with various compartmentalizations until the behavior of the code in various situations is understood. Then, the minimum number of compartments that adequately model the containment should be used in order to minimize the execution time.

3.3 Timestep Control

Timestep control is an important part of the HECTR numerical package. The main purpose of the controls is to maintain numerical stability, accuracy, and physical validity of the solutions produced by integrating the conservation equations. These controls limit in various ways the lengths of the two major kinds of timesteps found in HECTR: heat-transfer timesteps and flow timesteps (see Section A.1.3). In the following discussion, remember that a heat-transfer timestep can contain one or more flow timesteps.

In general, we discourage increasing the maximum allowable timestep beyond the default value of two seconds. With timesteps larger than two seconds, the wall conduction model may become unstable. If cases are run in which there are long periods with little change in the conditions within the system, larger timesteps may be tried. However, the user should examine the results carefully and check for signs of instability or inaccuracy, since HECTR has not been tested extensively using longer timesteps. The key variables to check are gas temperatures, gas pressures, and surface temperatures.

If a calculation appears to be taking an excessive computation time, the user may wish to relax one or more of the timestep constraints. As noted in Section 5.1.3, HECTR prints information at the end of a run indicating which factors are controlling the timesteps. This information can be used to determine which NAMELIST variables described in Section 4.2.3 should be changed to increase the computation speed. However, the results should be examined carefully any time that the timestep controls are relaxed.

The minimum allowable timestep (either heat-transfer or flow) may need to be decreased when a faster-than-normal transient occurs or when smaller-than-normal volumes are being treated. In either of the above situations, the calculation may terminate with a message indicating that the code is taking an

excessive number of timesteps smaller than the minimum. There are two possible solutions. The first is to increase the amount that the controlling variables are allowed to change during a timestep. The second is to reduce the minimum allowable timestep. The first method will result in shorter execution times, but may result in inaccurate solutions. The second method will maintain accuracy, but will have a longer execution time. Problems with the minimum timestep are particularly likely to occur when modeling combustion experiments where the vessels are small and the hydrogen concentrations are high. For these cases, the duration of the experiment is usually short, so that the total execution time is relatively small. Thus, we recommend reducing the minimum timestep in order to preserve accuracy.

When using very short timesteps in multicompartment situations, some oscillatory behavior may be noted. This behavior results from the code attempting to follow the acoustic modes in the solution to the flow equations. These modes are usually not important for containment calculations. The acoustic modes can be damped out either by increasing the timestep size or by decreasing significantly the ratio of inertial length to flow area (L/A) in the equations (see Section 3.4). It should be emphasized that HECTR is not intended to model acoustic or other wave phenomena, and if these phenomena significantly affect the results, then HECTR is not the appropriate code to use.

3.4 Flow Junctions

Inputs to the flow junction model include the interconnection or orifice area, the ratio of inertial length to flow area (L/A), and the flow loss coefficient. These input values combine to determine the flow patterns within containment and the rate of pressure relief during pressure transients. Source terms and fans also have an important influence on the flow patterns, serving as forcing functions that impose a directionality on the overall flow.

The orifice area is based on the geometry. The L/A term can be explained in terms of simple flow through a pipe that is divided into segments, each of which represents a compartment. For that case, L is the cell-center-to-cell-center distance, and A is the cross-sectional area of the pipe. Unfortunately, the problem of a reactor containment is not so simple; a reactor containment is very complex with irregular geometries. The user must exercise engineering judgment in selecting the value of L, while A is usually the orifice area determined earlier. For compartments connected by large open areas, L/A is usually much less than one. We have found that the results are usually very insensitive to the L/A values when varied over many orders of magnitude. This will be true whenever the inertial terms in the flow junction equations

are unimportant relative to the steady state terms, as is usually the case. The main purpose of including the L/A terms in the junction equations is to assist the code numerics, rather than to improve the physics. However, each new case should be evaluated thoroughly, as cases may arise where the terms become more important.

The flow loss coefficients are important for determining the flow velocity through a junction and also the direction of flow for geometries with parallel flow paths (i.e., the flow will take the path of least resistance). The steady-state flow velocity is proportional to $(1/K)^{1/2}$, where K is the loss coefficient. Usually, these coefficients are of order one. Values for standard geometries can be found in engineering handbooks [8]. For large flow areas (many square meters), pressure equilibration occurs rapidly, and the results are insensitive to order of magnitude changes in the coefficients. The relative values of the loss coefficients rather than their absolute magnitudes are most important for cases with parallel flow paths. For example, consider the geometry of Figure 3-6. If a hot hydrogen source is introduced into the bottom compartment (5), the flow loss coefficients indicated in the figure will produce the flow pattern shown by the arrows. The hydrogen will preferentially rise up through Compartment 2, while the cooler air in the dome (Compartment 1) will sink down through Compartments 3 and 4 forming a natural convective mixing loop. A second loop between Compartments 2, 3, and 4, may also form. In general, the user must examine the geometry and make some judgments as to which paths appear to be the most restricted. Sensitivity studies should be performed for cases with parallel flow paths, and users should exercise appropriate caution when examining the gas transport results. For more insight into gas transport calculations, see Reference 3.

In ice-condenser containments, drains may be present that connect the upper and lower compartments. These drains allow spray water to drain into the lower compartment sump. The configuration of these drains may vary from plant to plant. HECTR assumes that gas flow through drains is blocked if the sprays are on or if the lower compartment sump has filled sufficiently to cover the bottoms of the drains. In practice, the junctions are sufficiently small that their influence on the results will be minimal.

Values for the variable area door parameters can usually be found in FSARs or other material supplied by the reactor vendor. The user should remember that the model used is really an empirical model rather than a physical one and may not be entirely correct for cases other than those for which it was developed [9]. Also, the model does not consider possible failure of the doors in cases with high differential pressures.

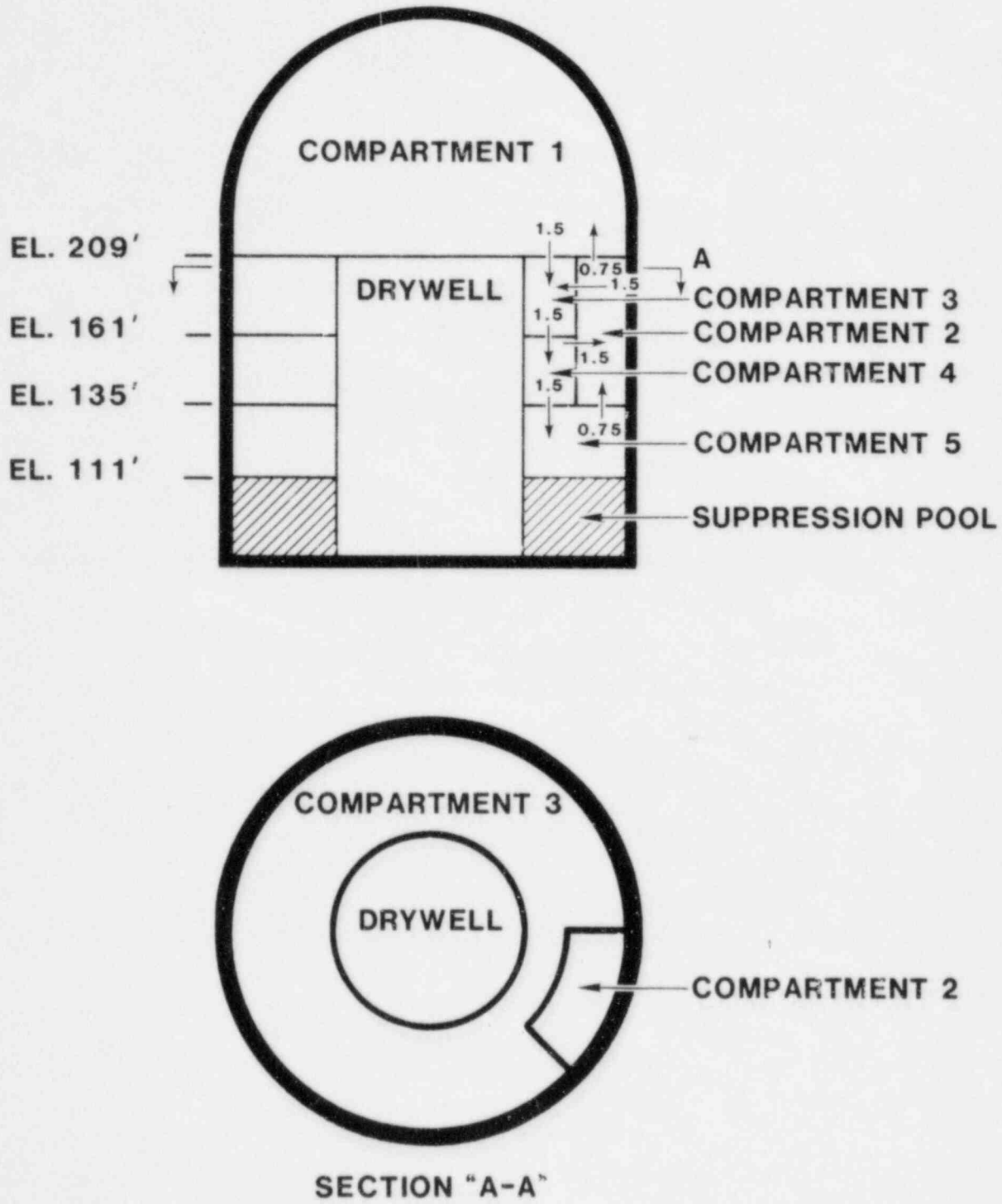


Figure 3-6. Flow Loss Coefficients and Flow Pattern in 5-Volume Compartmentalization

As discussed in Section A.1.1, the flow junction equations neglect the momentum flux or convective acceleration terms. These terms tend to become more important as the flow becomes more compressible (i.e., higher velocities). HECTR limits the maximum gas velocity to the speed of sound and will continue to run for cases with very high pressure differentials between compartments. However, the user should recognize the limitations of the code for high velocity flows and interpret the results accordingly.

3.5 Intercompartment Fans

The containment geometry and flow junction configuration will affect the flow rates predicted for intercompartment fans when calculated from head-flow curves. For example, in an ice-condenser containment the fans recirculate air from the upper compartment or dome region into the lower compartment. This fan flow and the injection of hydrogen and steam from the reactor primary system into the lower compartment cause the pressure in the lower compartment to be higher than in the upper compartment. The calculated pressure difference depends on the flow coefficients specified for the flow paths through the ice condenser (i.e., the flow path connecting the upper and lower compartments). If the flow resistances are high enough, the fan flow based on the head curve will be significantly reduced or even stopped. Thus, when specifying flow junction parameters, their influence on the fans should be considered.

3.6 Hydrogen Combustion Model

Default values or correlations are included in HECTR for all combustion parameters (see Chapter 4). As discussed in Chapter 4, the parameters can be changed in the NAMELIST-type input. The parameters of interest are ignition limits, propagation limits, flame speed or burn time, postburn hydrogen concentration, and the time for a burn to propagate from one compartment to another.

The default values for ignition and propagation limits are presented in Table 3-1. For containments with deliberate ignition systems operating, we recommend that the hydrogen concentration necessary for ignition be set in the range of 5 to 8% for compartments containing igniters. It has been experimentally demonstrated that, for relatively dry hydrogen/air mixtures, ignition will probably occur below 8% hydrogen.[10] This value could be higher for steam and/or oxygen concentrations near the limiting values. If igniters are not present, then ignition will be more or less random, depending on available ignition sources, and the problem should be treated parametrically. The propagation limits shown are for quiescent mixtures. The propagation limits may be lower if there is significant convective gas flow in the direction of the propagation.

Table 3-1

Default Hydrogen Ignition and Propagation Limits

Parameter	Mole Fraction		
	H_2	O_2	H_2O
Ignition Limits	$\geq$ 0.08	$\geq$ 0.05	$\leq$ 0.55
Upward Propagation	$\geq$ 0.041	$\geq$ 0.05	$\leq$ 0.55
Horizontal Propagation	$\geq$ 0.06	$\geq$ 0.05	$\leq$ 0.55
Downward Propagation	$\geq$ 0.09	$\geq$ 0.05	$\leq$ 0.55

Higher hydrogen concentrations at the time of ignition produce correspondingly higher pressures and temperatures, with fewer burns that are spaced farther apart in time. Burn spacing can affect the calculated results. Generally, for burns that are more than a few tens of seconds apart, pressure rises do not tend to be cumulative. However, the gas temperature rises can show some cumulative effects, and surface temperatures for some types of surfaces can reflect virtually direct addition of temperature rises during closely spaced burns.

The flame speed correlations are presented in Section A.2.3. The user has the option of overriding these correlations with either a constant flame speed or a constant burn time. The correlations are based on intermediate-scale experiments in relatively turbulent (fans on) environments. The effects of steam are included, but not the effects of depleted oxygen. These correlations should not be treated as conservative in terms of producing the highest possible completeness and pressure rise values, because the large-scale containment environments will generally be turbulent due to sprays, fans, jet flow from a break, etc. For moderately rich mixtures, flame acceleration could produce values many times the values produced by the correlations. However, the flow junction equations in HECTR are valid only for low Mach number (incompressible) flows, and the code is not well suited for examining phenomena such as flame acceleration.

The flame speed affects both the combustion pressure and temperature, because it controls the time available for heat transfer during the burn and for venting into other compartments. Burns that are less than a few seconds in duration become nearly adiabatic, so that further increases in the flame speed have little effect on the HECTR heat-transfer

calculations (although venting times may still be important). For slow burns, heat transfer becomes important, particularly if containment sprays are present. Figure 3-7 shows the effect of varying the flame speed predicted by HECTR for a single-volume analysis of a Mark III BWR containment (excluding the drywell), assuming ignition at 10% hydrogen. This figure shows the nearly adiabatic response to burns that are a few seconds or less in duration and the effect of sprays on very slow burns.

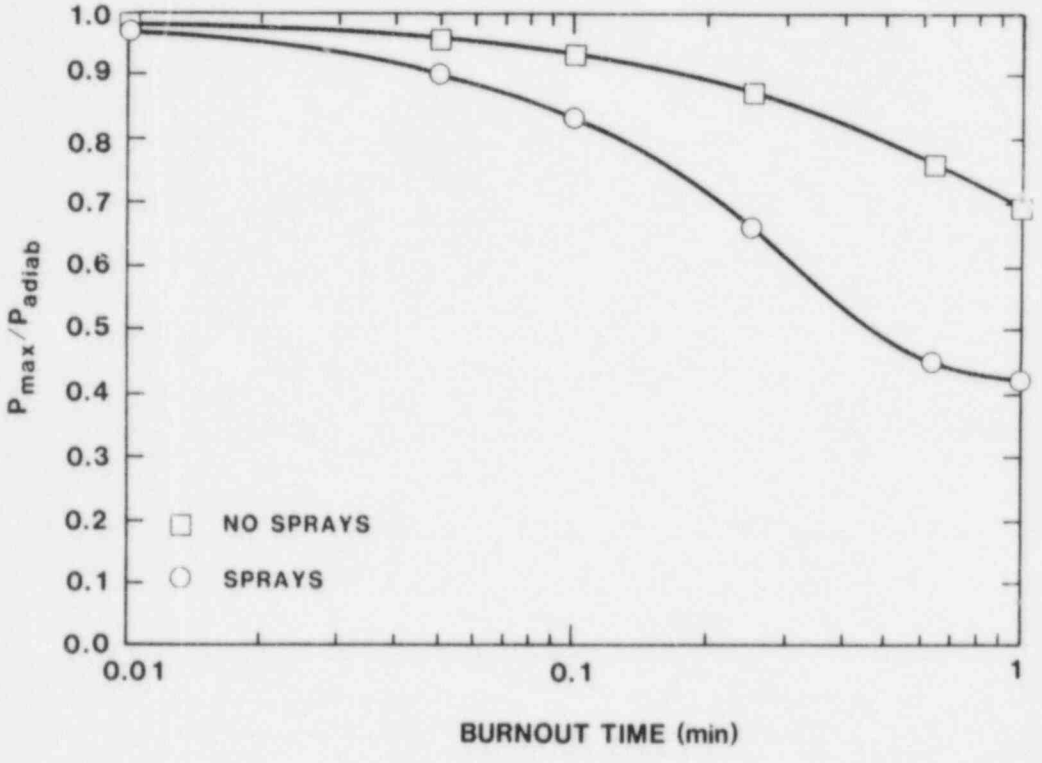


Figure 3-7. Effects of Burnout Time on Peak Pressure

The combustion completeness model presented in Section A.2.3 is a function of initial hydrogen concentration only. Burns would probably be less complete for high steam or low oxygen concentrations. The model presented would be somewhat conservative with respect to pressure rises based on small-scale experimental results.[5 6] However, large-scale combustion may tend to be more complete, due to the large convection loops and associated turbulence. Thus, the model may not be conservative for dry hydrogen-air mixtures, particularly in turbulent environments. The user has the option of specifying a constant postburn hydrogen concentration or using the default correlations.

When the default combustion completeness correlation is used, HECTR will normally limit the postburn hydrogen concentrations to values slightly greater than zero (even for initial

hydrogen concentrations that are greater than 8%). This is done to account for the outflow of gases from a compartment that occurs concurrently with the burn. The user can specify a zero postburn hydrogen concentration, but HECTR may occasionally calculate a negative number of moles of hydrogen at the end of a burn, causing the program to terminate (see the description of the first error message listed under CONTRL in Section 5.1.1). In this case, it will be necessary to rerun the problem using a small but nonzero value for this parameter.

HECTR is sensitive to combustion completeness in virtually the same way that it is sensitive to ignition criteria. Incomplete combustion produces lower pressure rises and more burns that are spaced closer together in time.

The final combustion parameter of importance is the time that must elapse before a burn can propagate from one compartment to another (the propagation factor). This time is specified as a fraction of the burn time in the compartment in which the burn originates and can vary from zero to one. (Note that if the propagation time is set to zero, then propagation will not actually occur until the next timestep after burn initiation.) Some care is required in selecting the propagation factor, as it may control whether propagation actually occurs and will affect the total time for a particular burn sequence. HECTR determines whether a burn can propagate into an adjacent compartment at the time corresponding to the propagation factor, not at the time the burn initiates in the first compartment. If propagation does not begin at that time, HECTR will continue to test for propagation each timestep until the burn in the first compartment is completed. After a burn starts in a compartment, a mixture of burned and unburned gases is pushed from the burning compartment into the adjacent compartments. If the propagation time from the burning compartment is too large, the mixture in adjacent compartments may no longer be flammable at the time the propagation should begin. This is particularly true for propagation from a large compartment into a small one. The user should examine the location of known ignition sources and the compartment geometry when specifying the propagation factor.

3.7 Radiative Heat Transfer

The radiative heat-transfer model requires input consisting of the surface emissivities and the view factors and beam lengths defining surface-to-surface radiant exchange. Gas emissivities and transmissivities are calculated internally in HECTR, as discussed in Section A.2.4. Methods for determining the necessary input values can be found in any of a number of textbooks on radiative heat transfer (e.g., Reference 11. Determining the view factors and beam lengths can be a very time-consuming process. The user should exercise

judgment when deciding how precise these values need to be and should use approximate values based on standard geometries whenever possible.

It is important to remember when computing view factors that the elements in the view factor matrix must satisfy two major conditions. Each off-diagonal element needs to satisfy a reciprocity relationship with its transpose element (see the discussion of VF(i,j) in Section 4.2.2.9). HECTR enforces this condition by allowing the user to specify only the upper right half of the view factor matrix and then calculating the values in the lower left half from reciprocity. The second condition specifies that the sum of the elements in each row of the view factor matrix (both user-specified elements and those calculated by HECTR from reciprocity) must equal 1. This is a requirement for conservation of energy. HECTR will warn the user if the sum of any row deviates from 1 by more than 0.001.

Normally, varying the radiative parameters has only a modest effect on the gas pressure-temperature response. However, the effect on surface temperatures can be quite significant, with some surfaces heating up at the expense of others. Whenever liquid layers are present on surfaces, HECTR changes the emissivity for that surface to 0.94.

When specifying the view factors, the user should prohibit radiative exchange between surfaces located in nonadjacent compartments. This is due to a limitation in the current model. The code will accept and calculate radiative exchange between surfaces in different compartments; however, the gas emissivity calculations may not be correct. HECTR will perform the calculations based on the volume-averaged gas conditions present in the compartments in which the surfaces reside. Therefore, the gas emissivities will not be correctly calculated for surfaces residing in compartments that are separated by intervening compartments. The method should be considered only a rough approximation even for surfaces in adjacent compartments.

3.8 Convective Heat Transfer

Convective and condensing heat transfer are significant sources of uncertainty in reactor accident analyses. The user-adjustable parameters in HECTR are forced-convection velocity, surface length scale, and maximum liquid film thickness.

The effects of the forced-convection velocity and the surface length scale are somewhat coupled. HECTR chooses between forced and natural convection solutions, taking the one with the higher heat-transfer coefficient. High forced-convection velocities increase the forced convection coefficient, while large length scales decrease this coefficient. The natural

convection coefficients are independent of both velocity and length scale for vertical surfaces, with a small dependence on length scale for sump surfaces. Normally, heat transfer to surfaces that are many meters in length will occur by natural convection, unless containment systems are operating to induce high forced convection velocities.

Typically, we input values for the forced convection velocity in the range of 0.3 to 1.0 m/s. In an ice condenser, actual calculated velocities are used. During hydrogen burns, HECTR sets the forced convection velocity equal to the flame speed. It may be possible to provide more accurate estimates by examining containment flow patterns in detail and calculating the flows induced by fans, steam jets, sprays, etc. However, before expending that effort, the user should parametrically examine the velocity to determine its importance. It is obviously not worthwhile for cases where the problem is dominated by natural convection. We have found that large changes in the value (factors of 2 to 10) are necessary to produce significant differences in the results. Thus, we recommend using engineering judgment to determine likely velocities and performing a limited number of sensitivity calculations to determine whether further analysis is warranted.

There are no fixed rules for specifying the convective length scale. For vertical surfaces, we generally use the height of a surface. If the surface is oriented horizontally, we use the width of the surface. The results are relatively insensitive to the length scale, as forced convection varies with the length scale to the -0.2 power. Natural convection for vertical surfaces is independent of the length scale, and natural convection for horizontal surfaces varies as the length scale to the -1/4 power (in HECTR, pools have horizontal surfaces, and all other surface types are assumed to have vertical surfaces). The correlations in HECTR were not developed for application in reactor containments, and all such correlations may be inaccurate when used at the very large scales present in containments.

The default liquid film thickness in HECTR is 1 mm. The liquid layer adds another heat-transfer resistance between the gas and the wall. However, for most cases this resistance is very small relative to the resistance in the gas boundary layer. The liquid layer resistance can be important for cases with high steam concentrations (>50%). The liquid layers also allow HECTR to keep track of the water inventory in containment and allow evaporation of condensed water from surfaces during and after hydrogen burns. As with the other convective heat-transfer parameters, the effects of changing the film thickness should be examined. In most cases the effects on the gas pressure-temperature response will be small, but the temperature response of individual surfaces may be significant.

3.9 Surface Conduction

All surfaces specified by the user will be either a water surface, a multilayered slab, or a lumped mass. Typically, a surface composed of a single material with a high thermal diffusivity and thermal conductivity (e.g., steel) is modeled well as a lumped mass. For such a surface, thermal equilibrium occurs rapidly throughout the material. Multilayered surfaces and single-layered surfaces composed of materials with low thermal diffusivities and thermal conductivities are best treated as slabs.

Generally, it is best to use the HECTR default noding for slabs. However, if a nodalization is specified, then care should be taken to avoid numerical inaccuracy and instability. Choosing too few elements can result in a stable but inaccurate solution. Choosing too many elements can cause global instability if element widths become too small (see the discussion of Eq. A-65). The element distribution exponent will determine how the elements will be distributed in the slab. This number should be chosen to be between zero and one so that the elements will be increasing in length as the back side of the slab is approached. This will result in increased resolution at the front surface, where it is most needed to handle the incoming heat transfer from the atmosphere, and less resolution in the back portion of the slab.

The HECTR conduction model is used primarily to calculate surface temperatures. Although HECTR calculates the temperatures at each node within the slab, internal temperatures at desired specified points are not readily available. This is due to the method used to nodalize layered slabs, i.e., the scaling of the thickness according to the thermal diffusivity (see Section A.2.6).

Occasionally, oscillations or "noisy behavior" may occur in the surface temperatures. This behavior usually results from repeated changes from condensing to evaporating modes in the mass-transfer models, sometimes accompanied by the repeated appearance and disappearance of liquid films on the surfaces. Precautions have been taken to minimize this problem; however, if encountered, the most straightforward solution is to reduce the heat-transfer timestep.

3.10 Containment Sprays

The adjustable parameters in the spray model are the inlet temperature and the drop size distribution. If the sprays are in the recirculation mode and water is being drawn from the sump, then the spray temperature is calculated in HECTR. The spray temperature determines the long-term equilibrium temperature of the containment. The drop size distribution influences the transient response of the containment atmosphere to short-term events, such as hydrogen burns.

Generally, the spray temperature will not vary by more than a few tens of kelvins and will be below about 373 K (usually well below). The effect of changing the spray temperature on the equilibrium containment pressure can be determined by examining the corresponding change in saturation vapor pressure (usually much less than one atmosphere). The effects of spray temperature on hydrogen combustion are more important. The spray temperature controls the preburn pressure and steam concentration. It is generally valid to assume that for a given gas composition, the ratio of postburn pressure to preburn pressure is constant. Thus, relatively small changes in preburn pressure can translate into significant changes in the postburn pressure. Additionally, as discussed in Appendix A, the steam concentration significantly affects many of the combustion parameters.

The drop size distribution is important during rapid transients, such as hydrogen burns. During portions of a hydrogen burn, the smaller drops evaporate completely but the larger ones do not. Thus, the drop size distribution can determine the total evaporation rate. We have found that using a single mass-averaged drop size can result in overpredicting the heat- and mass-transfer rates during portions of a hydrogen burn. The mass-averaged drops can all evaporate while, if a distribution of drop sizes is used, some of the larger drops may not completely evaporate. A small number of very large drops in the distribution can carry relatively large quantities of water and significantly reduce the total evaporation rate. We have found that using distributions with two to four drop sizes is generally sufficient. We usually specify the distribution such that each drop size has approximately the same volumetric flow rate; however, this approach is arbitrary, and other methods could be used. The user should minimize the number of drop sizes, as the spray calculations generally represent a significant fraction of the total run time. It may be possible to define a more appropriate average drop size and eliminate the need for a distribution. Also, note that different drop size information appears in the literature for the same nozzles (Spraco 1713A), and all such information should be treated with caution.

The spray model has been tailored to deal with the types of containment problems that we have encountered to date. Other types of problems may not be properly treated. For example, the spray model is a diffusion model, based on the diffusion of steam through air. For high mole fractions of steam, this model becomes invalid. As now configured, HECTR will print a message and terminate the calculation if the sprays are on and the mole fraction of steam exceeds 0.99. Problems can arise in the Runge-Kutta solver if very small drop sizes are used and the gas temperature is very different from the drop inlet temperature. The problems arise because of the large values of the droplet mass and temperature derivatives calculated by the solver. By the nature of the Runge-Kutta solver,

large values of the derivatives can lead to internal extrapolations that result in nonphysical values for various parameters, particularly the droplet temperature. We have not encountered any problems during containment calculations when the drop sizes were above about 200 μm.

Some general comments are in order regarding the HECTR spray model: The user should always remember that the model is based on a quasi-steady-state formulation (see Section A.2.7). This assumes that conditions do not change much during the time it takes for a drop to fall to the bottom of a compartment (usually a few seconds). During rapid transients, this assumption is less valid. To improve the accuracy, the user could divide each compartment through which spray passes, vertically, into several shorter compartments with complete spray carryover between each of the vertically connected segments. However, this is usually not a practical solution because of the expense of calculating spray heat and mass transfer in additional compartments.

Finally, the user should be aware that when HECTR is run on machines with different computer word lengths, the spray model can be responsible for noticeable changes in the progression of a scenario. Given the same conditions, the actual results from the spray model may change only slightly. However, because of the typically large spray flow rates used in containments, small changes in single drop evaporation rates can lead to large changes in overall spray heat and mass transfer rates. This will result in differences in the compartment conditions (input to the spray model) throughout the containment, establishing a feedback loop. Therefore, the initial small differences can cause noticeable cumulative changes. It should be noted that the same qualitative trends probably will still be apparent. However, it is possible that these differences may result in a threshold effect occurring on one machine and not the other, which can then result in major qualitative and quantitative differences in the progression of the scenario. The user should be concerned about this problem when the computer word length is about 32 bits or less.

3.11 Ice-Condenser Model

Input to the ice-condenser model includes a geometrical description of the ice condenser, the ice temperature, and the drain temperature. The geometrical information can be found in plant-specific FSARs. The ice temperature is usually specified in the operating specifications for the plant. Changing the ice temperature affects the thermal mass of the ice and the associated melting rate. The heat-transfer rate to the ice surfaces is calculated using the maximum of the ice temperature and 273.15 K. Specifying an ice temperature below 273.15 K essentially has the effect of increasing the heat of fusion of the ice.

The drain temperature determines the amount of condensation on the water that is falling down through the lower plenum (melted ice plus condensate). Higher drain temperatures correspond to increased condensation and less steam entering the ice regions. Thus, the ice will last longer, and less steam will reach the upper compartment. Information regarding appropriate values for the drain temperature is scarce. Some data exist from experiments performed to examine large-break loss-of-coolant accident (LOCA) events, but the data are limited and not generally applicable to small-break flow regimes. However, we have found the results to be only moderately sensitive to the drain temperature. For example, consider the results of calculations performed for an S_1HF accident sequence in the Sequoyah plant.[12] An S_1HF sequence is a 0.15-m (6-in) diameter LOCA with loss of emergency core cooling and sprays in the recirculation mode. Figures 3-8 through 3-13 show the upper compartment pressure response and the fraction of ice remaining versus time for three calculations in which the drain temperatures were 290, 310, and 330 K, respectively. The results are only moderately affected by the drain temperature changes.

The heat-transfer coefficient for the ice-condenser surfaces is particularly uncertain, because of the complex geometry, rough surfaces, and variety of possible flow regimes. The only experimental data that we have available are for large-break LOCA simulations, and these data are not generally applicable to other scenarios. We have examined the effect of the heat-transfer coefficient in a parametric manner. Figures 3-14 through 3-17 illustrate the effects on the pressure and ice inventory of increasing and decreasing the heat-transfer coefficient by a factor of five during the S_1HF accident sequence described above for the Sequoyah plant.[12] High heat-transfer coefficients result in more steam removal and lower pressures early in the accident; however, the ice melts faster and is not available at later times, leading to higher pressures as the accident proceeds.

HECTR nodalizes the ice-region compartments internally. These compartments are set up as a vertical stack. Asymmetric flow and convection loops within the ice condenser are not currently treated by HECTR.

3.12 Containment Sumps

The sump model in HECTR allows the code to track the inventory of water in containment and to determine the effects of the sumps on the containment atmosphere. The important input parameters for the sumps (besides those described previously for heat-transfer surfaces) are the initial mass, initial temperature, and capacity.

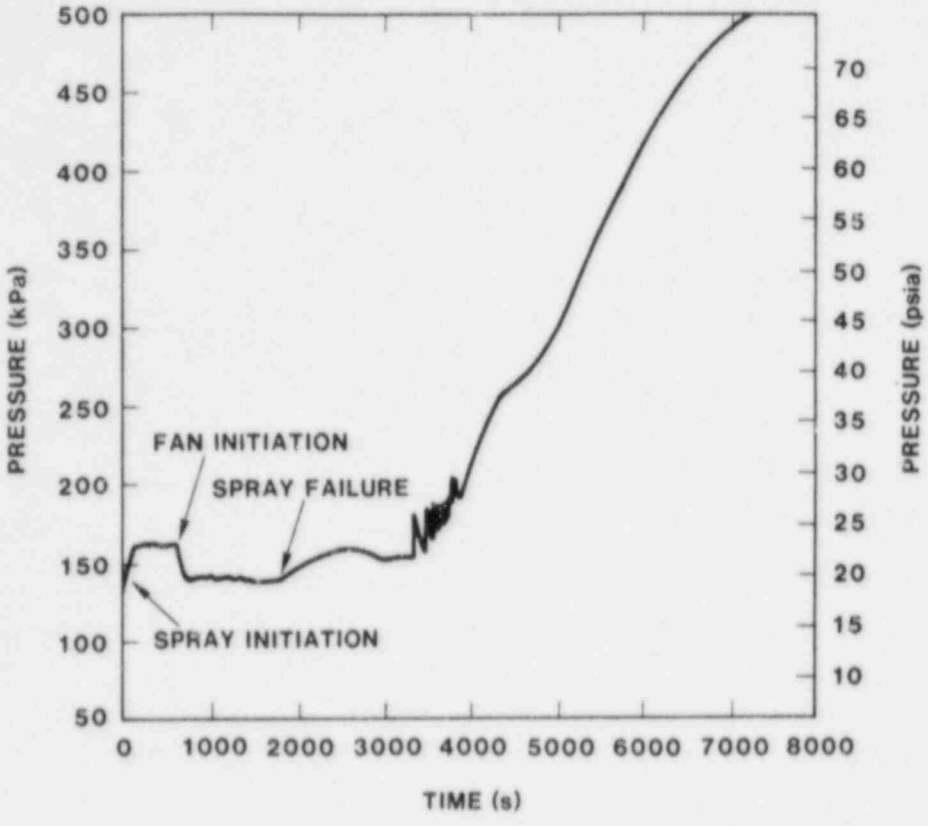


Figure 3-8. Dome Pressure Response (Drain Temperature = 290 K)

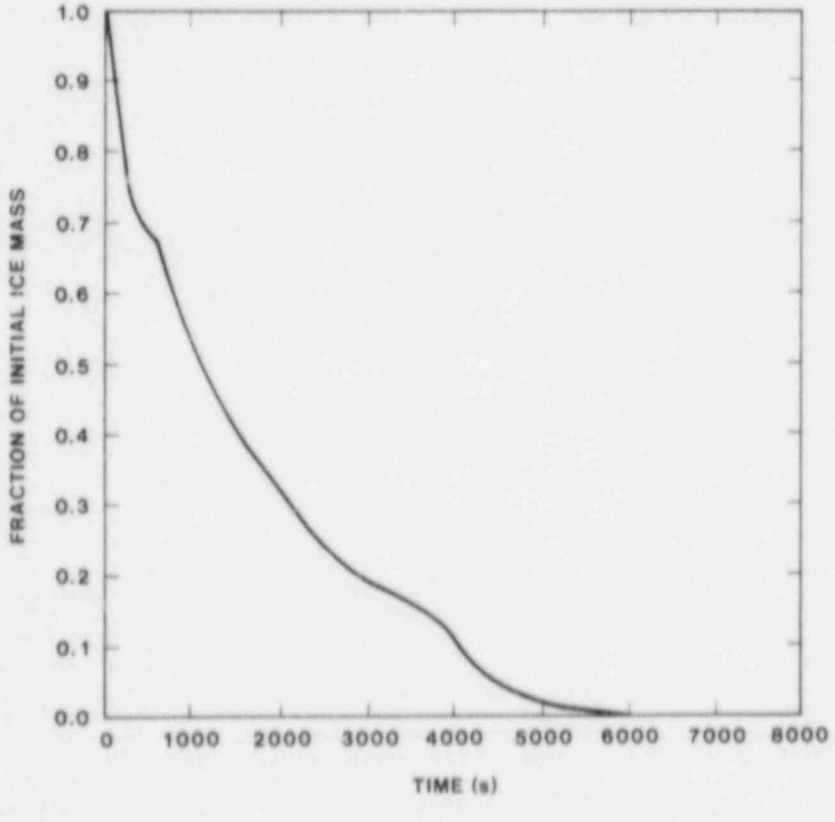


Figure 3-9. Ice-Inventory History (Drain Temperature = 290 K)

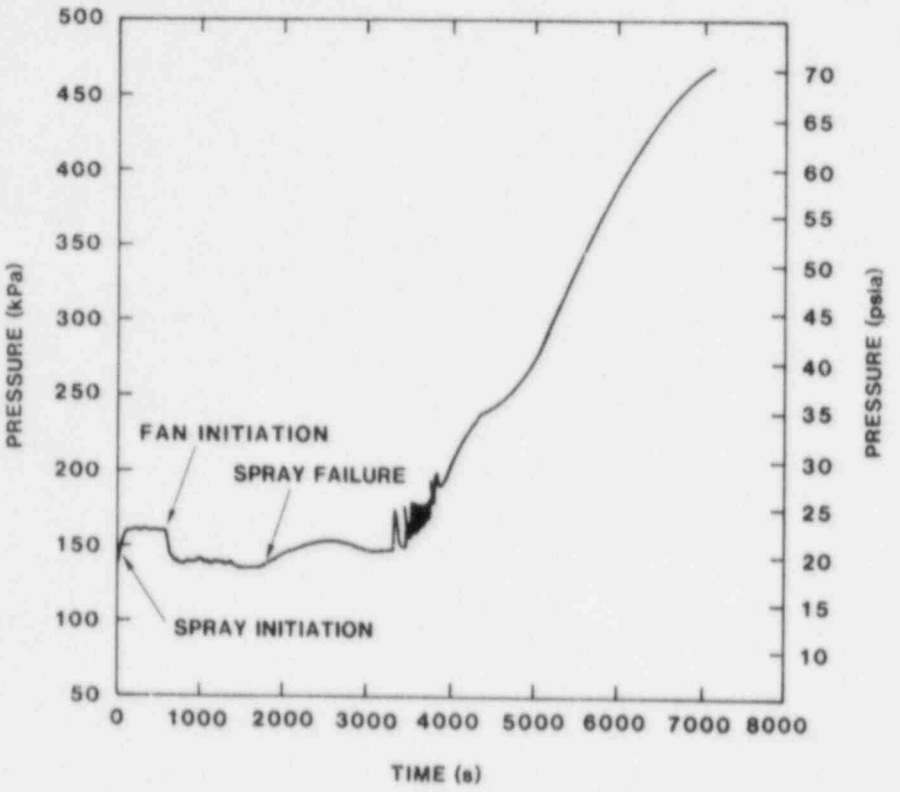


Figure 3-10. Dome Pressure Response (Drain Temperature = 310 K)

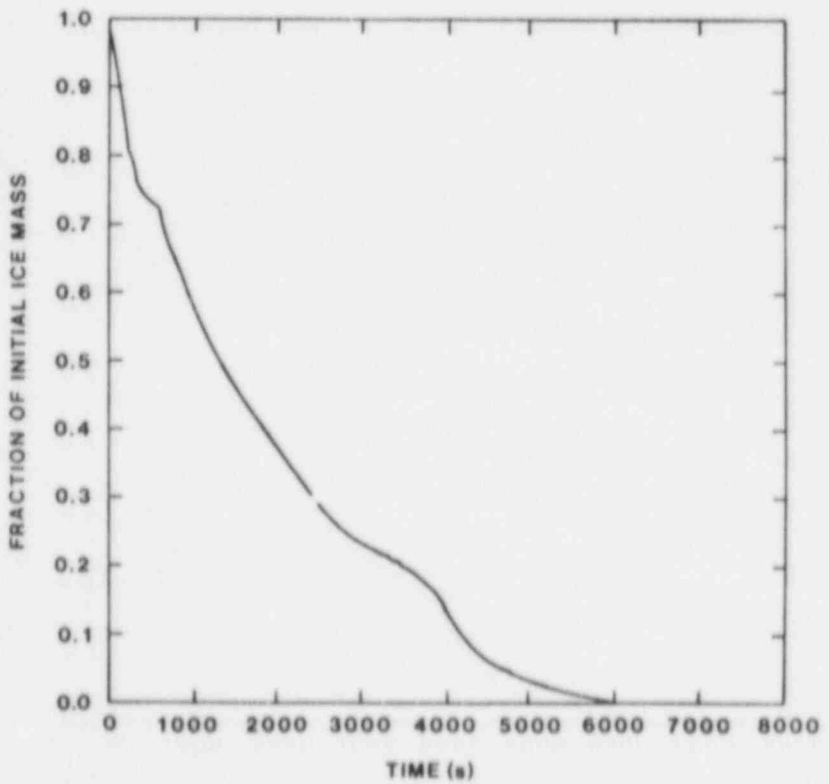


Figure 3-11. Ice-Inventory History (Drain Temperature = 310 K)

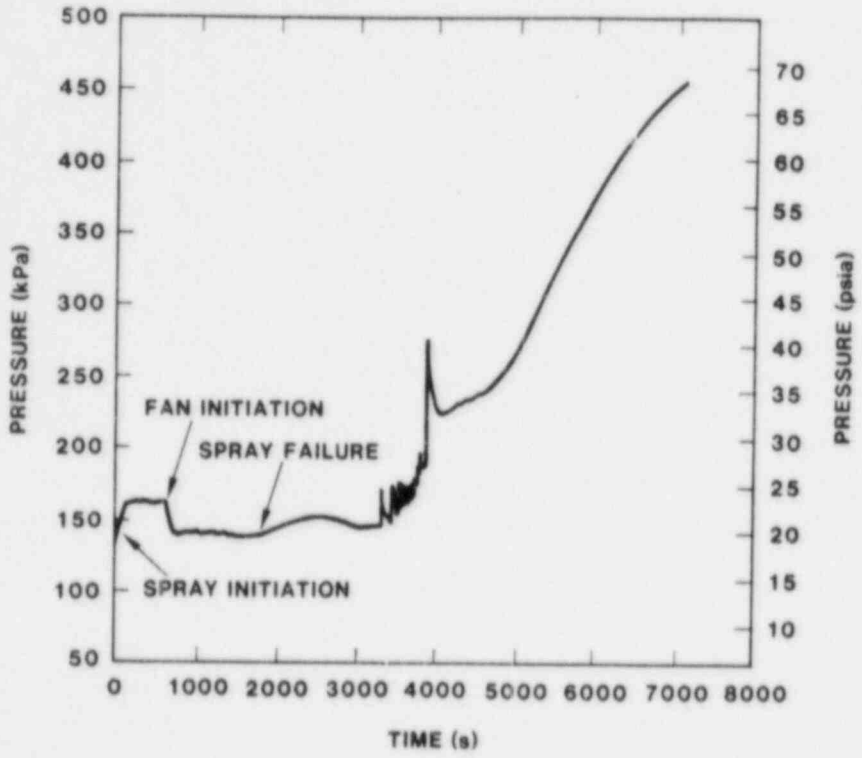


Figure 3-12. Dome Pressure Response (Drain Temperature = 330 K)

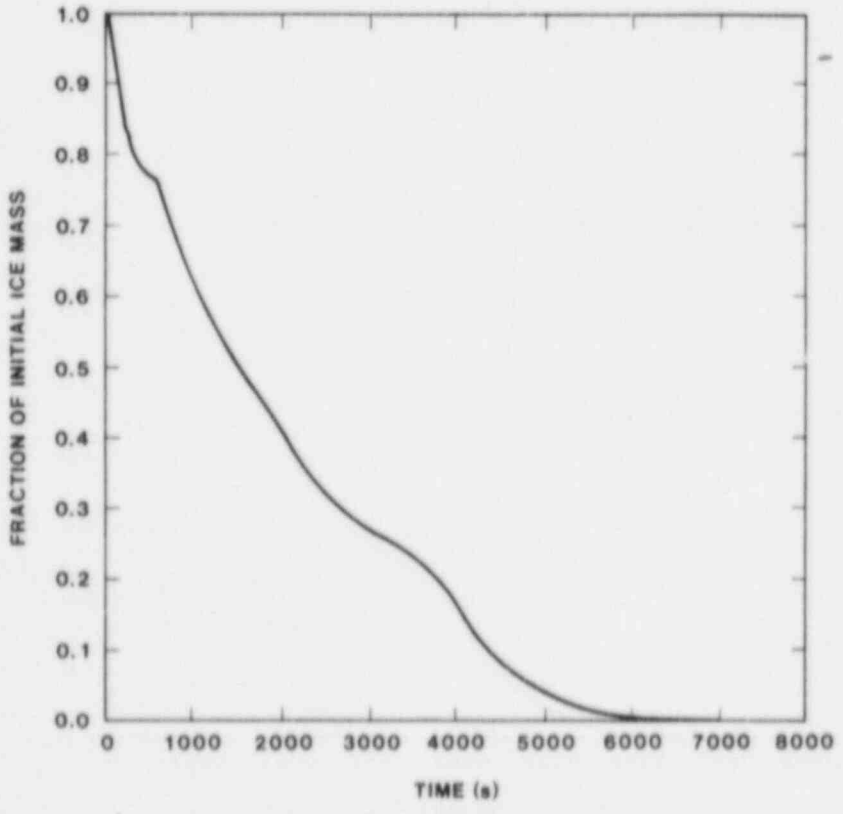


Figure 3-13. Ice-Inventory Response (Drain Temperature = 330 K)

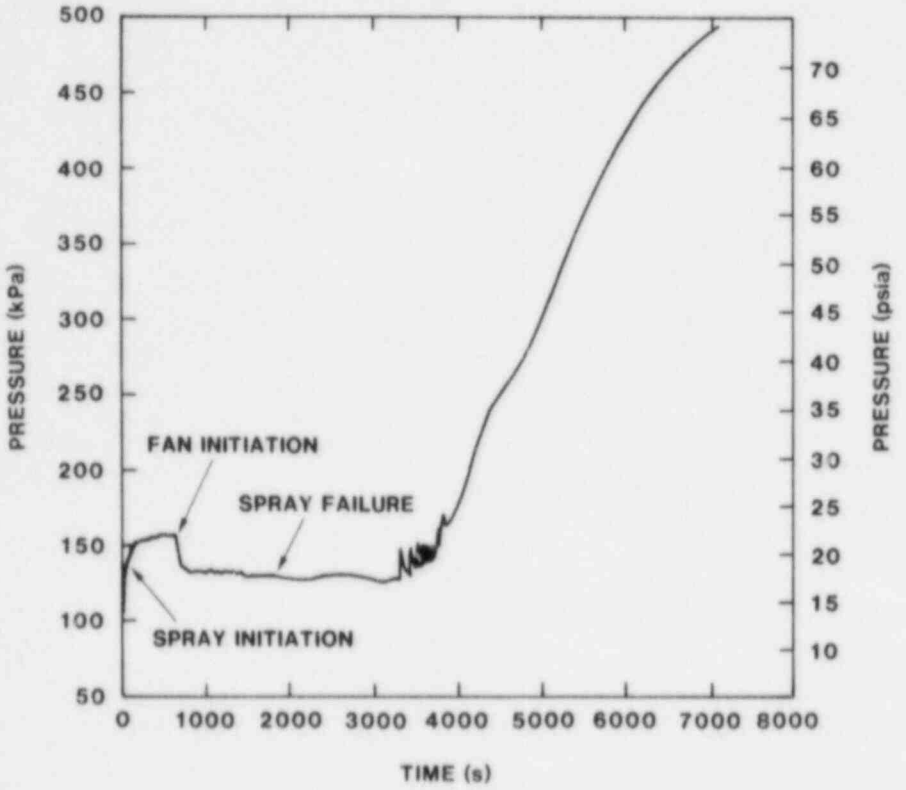


Figure 3-14. Dome Pressure Response (Ice-Condenser Heat-Transfer Coefficient Increased by Factor of 5)

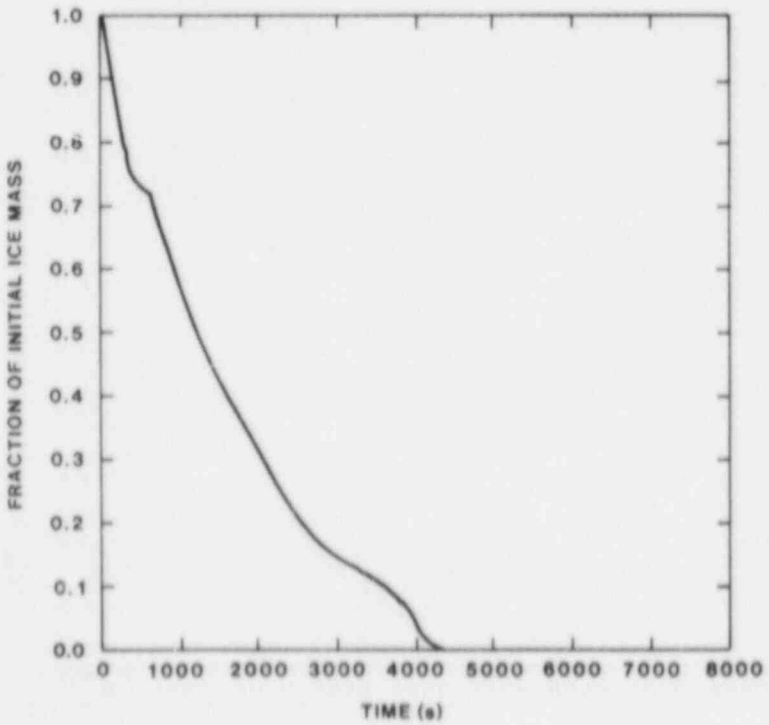


Figure 3-15. Ice-Inventory History (Ice-Condenser Heat-Transfer Coefficient Increased by Factor of 5)

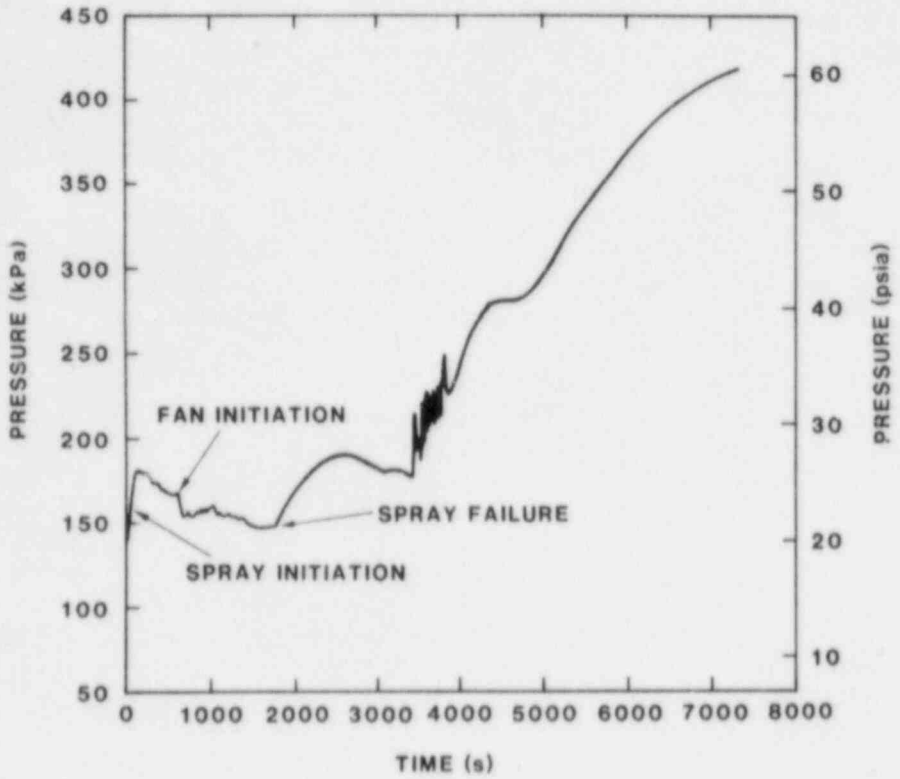


Figure 3-16. Dome Pressure Response (Ice-Condenser Heat-Transfer Coefficient Decreased by Factor of 5

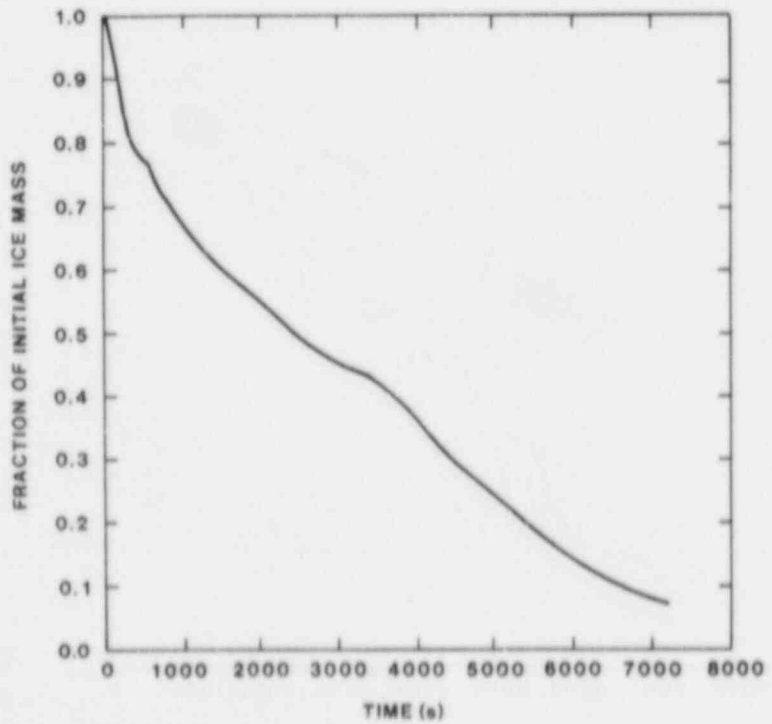


Figure 3-17. Ice-Inventory History (Ice-Condenser Heat-Transfer Coefficient Decreased by Factor of 5)

The initial temperature is important for cases where the initial sump mass is significant. Otherwise, the sump temperature will be determined by water that is added later. The sump temperature determines whether a sump will be heating or cooling the connected compartment. It also determines the rate of condensation or evaporation on the sump surface and determines whether the sump is subcooled or saturated. If a sump is saturated, steam will be added to the connected compartment at the rate that water boils from the sump. These processes will affect the pressure, temperature, and composition of gases in the compartment connected to the sump. As with the other surfaces in the containment, it takes a relatively long time for the compartment atmosphere to reach equilibrium with a sump. Thus, changes in sump temperatures do not affect compartment conditions as rapidly as do changes in some of the other HECTR models (e.g., sprays).

Gases that are injected into a sump are cooled to the sump temperature before flowing into the connected compartment. Thus, a hotter sump will result in more energy being added to the compartment. Also, the temperature of water drawn from a sump for sprays while in the recirculation mode will be affected by the sump temperature.

Figures 3-18 through 3-21 show examples of four different HECTR sump configurations that can be modeled using various sump overflow specifications. The sump specifications for the four cases are described in the following paragraphs.

To model a single sump that is not expected to overflow into a second sump, the configuration shown in Figure 3-18 could be used. In this figure, the sump capacity has been specified to be larger than the maximum expected sump volume and, since no overflow is expected, the sump would be specified to overflow to Sump 0 (i.e., any water added to the sump beyond its capacity will disappear from the system).

Figure 3-19 shows an example of overflow between two sumps. In this example, Sump 1 is specified to overflow into Sump 2 and vice versa. At the time depicted in the figure, the capacity of Sump 1 has been exceeded, such that Sump 1 is overflowing into Sump 2. Eventually, Sump 2 will also fill to its capacity, and thereafter both sumps will fill up together. Note that specifying the capacity of both sumps as 0 would cause the two sumps to fill up together during the entire calculation. Also note that only two sumps can be specified to fill together in HECTR.

A possible sump configuration for an ice-condenser containment is shown in Figure 3-20. In this example, Sumps 1 and 2 represent small sumps in the lower plenum of the ice condenser and the refueling canal, respectively. Both sumps are specified to overflow into a sump in the lower compartment (Sump 3). The lower compartment sump is in turn specified to

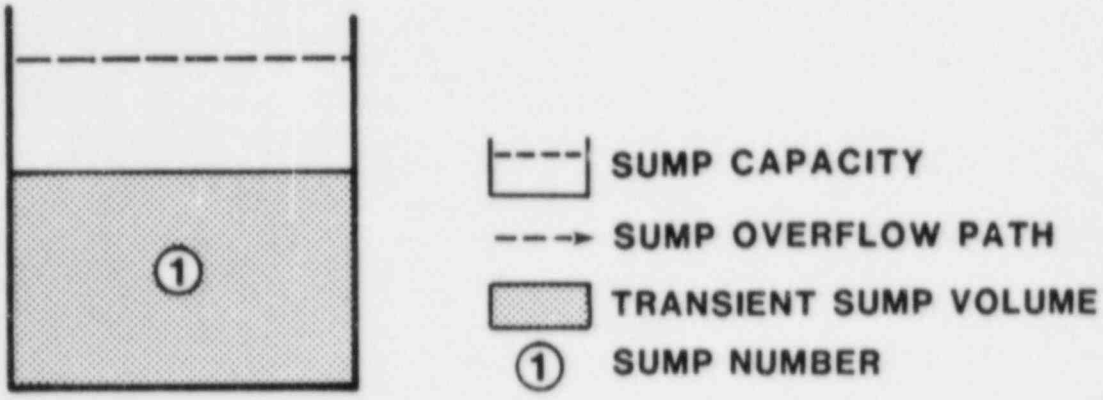


Figure 3-18. Configuration for Single Sump

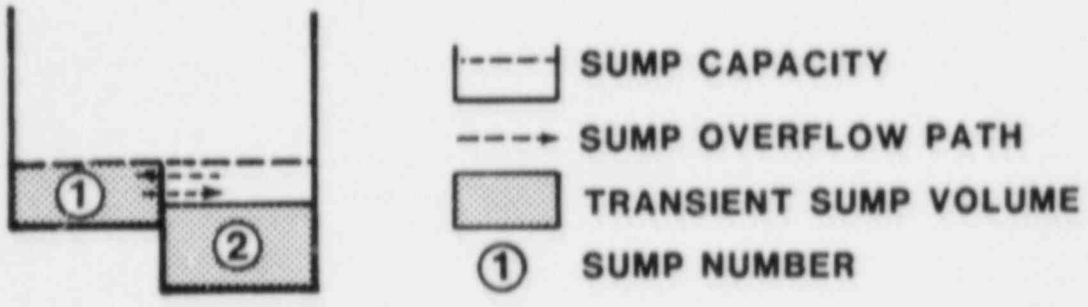


Figure 3-19. Configuration for Overflow between Two Sumps

overflow into Sump 4, which represents the reactor cavity. Sump 4 is specified to overflow back into Sump 3. The figure depicts a point in the transient where both Sumps 1 and 2 have filled to their capacities and are overflowing into Sump 3, and Sump 3 is overflowing into Sump 4. If Sump 4 continues to fill, it will eventually fill to its capacity. Thereafter, Sumps 3 and 4 will fill together.

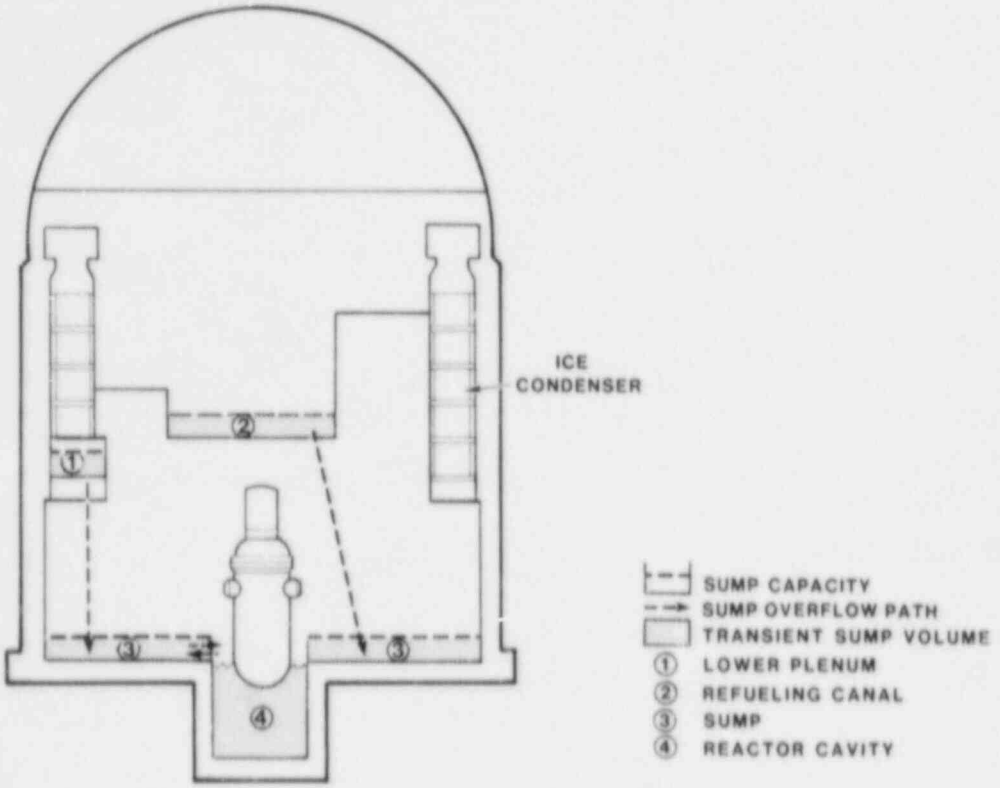


Figure 3-20. Sump Configuration for Ice-Condenser Containment

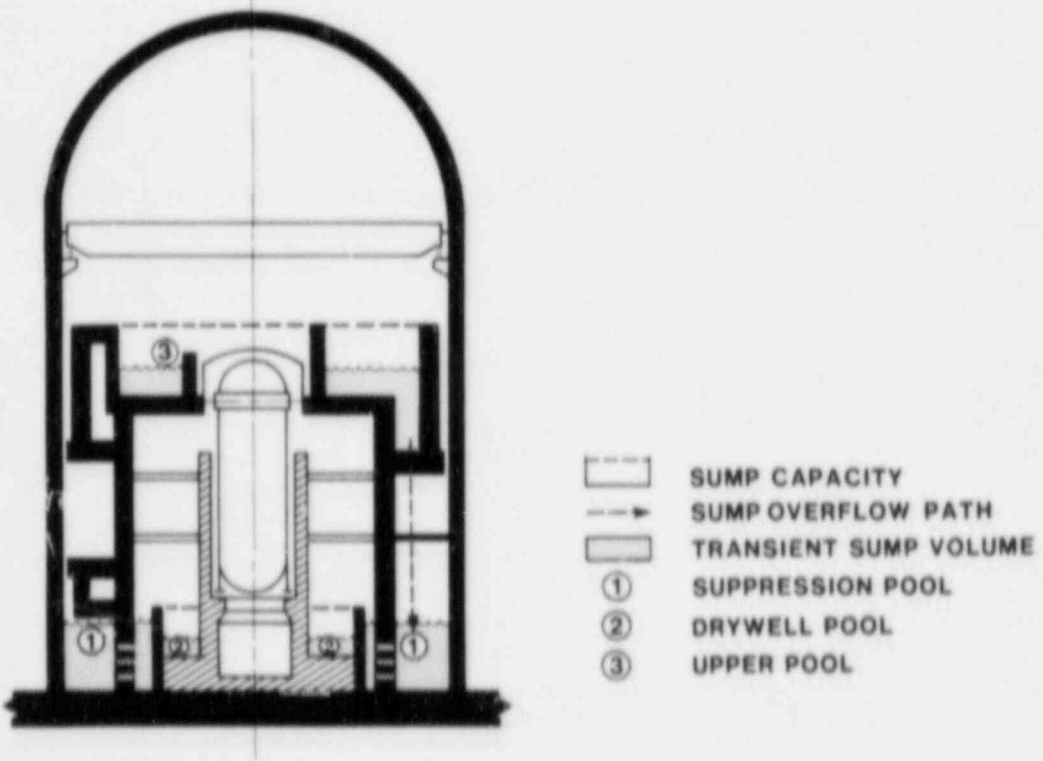


Figure 3-21. Sump Configuration for BWR Mark III Containment

The fourth possible sump configuration shown in Figure 3-21 is for a BWR Mark III containment. Sumps 1, 2, and 3 represent the suppression pool, drywell pool, and upper pool, respectively. The upper pool is specified to overflow into Sump 1; this overflow is separate from the upper pool dump. The sump overflow paths specified in the HECTR input for the suppression pool and drywell pool are not used because HECTR forces the overflow between these sumps to follow the paths described in Sections 2.2.10 and A.2.10. Thus, the user can simply input 0 for the overflow sumps for the suppression and drywell pools. The capacity of the drywell pool is used to determine the amount of water that will remain in the drywell pool (i.e., the amount that will not flow back into the suppression pool). The capacity of the suppression pool is not used in HECTR. Thus, the user can specify 0 for the capacity of the sump corresponding to the suppression pool.

Increases in sump volume are reflected as decreases in the connected compartment volume. Thus, the user should not allow a sump volume (or the sum of all the sump volumes in a compartment) to increase beyond the volume of the connected compartment. If this occurs, the calculation will terminate. It should also be noted that these compartment volume changes can affect the distribution of gases throughout the containment.

3.13 Suppression Pool Model

Input to the suppression pool model includes a geometrical description of the suppression pool, the initial water level, and the specifications for the upper pool dump. For the vent clearing calculations, flow loss coefficients must be specified at both ends of the vents, and an equivalent length must be specified to account for the deceleration of water flowing from the vents into the suppression pool. An additional loss coefficient must be specified for gas flow through the vents following vent clearing. Except for these flow loss parameters, the necessary suppression pool input can be found in plant-specific FSARs and operating specifications.

There are not many experimental data available in the open literature to aid in selecting flow loss parameters for the vent clearing calculations. Experiments have been performed to analyze the response of Mark III suppression pools, but most of the results are proprietary. Thus, depending on the scenario being examined, the suppression pool input may need to be varied parametrically to analyze the problem. The water flow loss coefficients and the equivalent length used in the calculation will affect the clearing time for the vents. This may be important for some scenarios, while in others it will have little effect. For example, the vent clearing time will usually have little effect on the pressure rise resulting from burns in the wetwell, because the vents do not generally clear quickly enough to provide significant

pressure relief. However, if the burns occur in the drywell, the vents will clear faster, allowing more pressure relief during a burn. Thus, for drywell burns, the vent clearing time may affect the pressure rise.

The water level in the suppression pool will also affect the vent clearing time. Higher water levels will produce longer vent clearing times. The water level will be determined by the initial level, the amount of water added from the reactor coolant system, the amount of water removed for ECC or sprays, the amount of water added by an upper pool dump, and the amount of water removed because of spillover onto the drywell floor. As discussed above, the importance of the vent clearing time will depend on the scenario being examined.

The gas flow rates through the vents after they have cleared will be affected by the vent loss coefficient. Since experimental data are not available to determine appropriate values, it may be desirable to vary the loss coefficient to determine the effect on the results. Generally, the loss coefficients will not significantly affect the results. Throughout most of a calculation, the flow through the suppression pool vents will be controlled by the rate of steam injection into the drywell and the flow rate of the purge compressors. During these times, lower vent loss coefficients will result in the vents opening and closing more often with higher gas flow rates while open, but the net integrated flow will be the same as with higher vent loss coefficients. Vent loss coefficients for gas flow will not usually affect the pressure rise caused by burns in the wetwell because the vents do not usually clear during the burn. However, burns in the drywell are more likely to result in vent clearing and subsequent gas flow through the vents and thus may be affected by the loss coefficient used for the gas flow.

3.14 Heat Exchanger Model

The heat exchanger model was taken from the MARCH computer code.[13] The model is for counter-current flow heat exchangers. The input parameters needed can usually be found in FSARs or manufacturer's specifications. The heat exchanger model is important in determining the spray inlet temperature when the sprays are in recirculation mode and in determining pool temperatures in sumps that are cooled by heat exchangers. The importance of spray temperature was discussed in Section 3.10. The pool temperatures are usually somewhat less important than the spray temperature, as discussed in Section 3.12. One of the more significant heat exchanger parameters is the secondary side inlet temperature. Both the spray and the pool temperatures will tend toward this value.

3.15 Output Control

The controls for the output are used to limit the amount of data (which can be excessive for long runs) written by HECTR into files that will be processed by ACHILES. Values of important variables (such as pressures, temperatures, flow junction velocities, and heat fluxes) are written out whenever certain parameters change more than a specified amount. The user should recognize the potential for losing information as the controls are loosened. HECTR will write out data values at each timestep during a burn, produce messages at the start and end of a burn, and keep track of the peak values produced for pressure and temperature during a run. Thus, global peaks should not be lost during normal runs. If the output files are too large, the plotting routine in ACHILES may discard data to make the plot data fit into memory on the computer, and information may be lost from the plots. Therefore, we recommend that global maximum values be taken directly from the HECTR output. If this is not possible, then the ACHILES tabular output and initial summary information can be examined. For a general discussion of the output produced by both HECTR and ACHILES and how this output is controlled, see Chapter 5.

4. INPUT DESCRIPTION

4.1 Introduction

Input is required for both the main program, HECTR, and the program that processes the output, ACHILES. Input to HECTR can be provided in a single file or in two files: one describing the problem geometry and one describing the initial conditions and accident scenario. These files are combined with another file to control ACHILES, as described in Appendix C.

Real, integer, and alphanumeric data are included in the input. These data types are identified below by the symbols [R], [I], and [A], respectively. A fourth type, symbolized by [L] (for logical), can have only the alphanumeric values TRUE or FALSE. All real and integer values are read in free format. This means that the values can be separated by blanks or commas with blanks interspersed freely (note that no other character, such as a tab, is a valid separator). Also, the values may have replication factors such that 3*2.7 (equivalent to 2.7 2.7 2.7) is a valid input.

In the input description provided below, three angle brackets (>>>) are used as delimiters to indicate the beginning of a new data record. Variables listed between two sets of these delimiters may be placed either all on one line or on as many separate lines as desired (all of these variables will correspond to a single read). The names of the variables are those actually used by HECTR or ACHILES.

A dollar sign ($) in column 1 signifies the end of a table input section when appropriate--the rest of the line may be used as a comment. The beginning of a table input section is indicated in the variable description below by the notation "while column 1 not = '$'". The variables listed below this statement (indented in the text), and before the matching "end while", form the table entries. A table can have an indefinite number of entries (including no entries). To create an empty table, it is necessary only to enter a single line containing a dollar sign in column 1. The notation, "for i=1, Number of Entries", indicates a loop on i over the indented variables following this statement and preceding the matching "end for". If the "Number of Entries" is zero, then the loop and the variables within it should be ignored (i.e., do not input any values). The notation "if condition then" indicates that the indented variables listed after this statement and above the matching "end if" will be read if the condition is true. Any text following an exclamation mark (!) (except within a line of alphanumeric input) is treated as a comment and thus ignored. Any lower case letters found in the input will be converted to upper case. The only exception is lower case letters in comments, which

will be echoed unchanged. Three sample problems are presented in Chapter 6 that should help clarify the input description that follows.

4.1.1 NAMELIST-Type Input

Some input to HECTR is in a pseudo-NAMELIST-type format. Default values are provided for all such variables. The variables that can be changed using NAMELIST-type input are listed in Sections 4.2.1, 4.2.3, and 4.3.1. Variables are assigned new values (one per line of input) using the following format:

varble = <value>

where the variable name is 6 characters or less in length. Blanks can be interspersed fairly freely throughout the entry. <value> can be either a number (real or integer) or a character string, depending on the variable type. Variable types with alphanumeric values include status variables (such as whether the sprays are on, off, or automatic), specification variables (e.g., the type of computer being employed), and logical variables (which can only have character string values of either "TRUE" or "FALSE"). If the variable in the above expression is an array, then all elements in the array will be set equal to <value>. To assign a value to a single array element, use the following format instead of the format shown above:

varble(i)=<value>

where the i is an integer subscript. The NAMELIST-type input is terminated with a dollar sign ($) placed in column 1. Lines that begin with an exclamation mark are always treated as comments as is any text following an exclamation mark located elsewhere in an entry line. For example, a typical set of input might look like

```
! Namlst input
XHMNIG=.1          ! Set the ignition limit in all
                   ! compartments to 10% hydrogen
BURNT(2) = 1.      ! Set the burn time in Compartment 2 to 1
                   ! second
FANS =ON
$ END OF NAMLST INPUT
```

4.1.2 Special Notes on Sump Input

Each sump in a containment must be identified by a unique number (specified in the Sump Data section) that lies between one and the total number of sumps being modeled, inclusive. A heat-transfer surface for each sump must be

listed in the Surface Data section. The initial mass of water in each sump is also specified in the Surface Data section. Each compartment can contain an arbitrary number of sumps (including no sumps). The relationship between compartment volume (specified in the Compartment Data section), sump capacity (specified in the Sump Data section), and the initial mass of water in the sump (specified in the Surface Data section) for the simple case of a single sump in a compartment is illustrated in Figure 4-1. The variable names shown in parentheses are those that appear later in Section 4.2.2, except for the density, ρ, which is calculated internally. The user should be careful to specify these values such that a compartment volume is not reduced to 0 because of sumps filling excessively.

4.1.3 Special Notes on Ice-Condenser Input (See also Section 6.2)

HECTR automatically generates compartments, surfaces, and junctions for the ice-bed region based on information input in the Ice-Condenser Data section. However, the lower and upper plenums must be entered as regular compartments. The flow junctions entering and exiting the ice-bed region must also be entered by the user. All references to the number of compartments (NCOMPS) or surfaces (NSURFS) in the HECTR input sections refer to the total number of compartments or surfaces directly input by the user; the compartments and surfaces generated internally by HECTR should not be included when calculating NCOMPS or NSURFS. Note that, in the ACHILES input section, asking for all compartments, flow junctions, or surfaces WILL include the HECTR generated compartments, flow junctions, and surfaces.

4.1.4 Special Notes on Mark III BWR Input (See also Section 6.3)

The suppression pool, upper pool, and drywell pool of a Mark III BWR must be entered in the Sump Data section. Information describing the surfaces of these pools is input in the Surface Data section. The surface of the suppression pool should be specified to be in the wetwell compartment. The drywell must be represented as a single compartment. Further input for the suppression pool must be entered in the Suppression Pool Data section.

4.2 Input File(s) for HECTR

The HECTR input file consists of three major sections. These are the initial NAMELIST-type input in which the computing environment is defined, a description of the problem geometry, and a description of the initial conditions and the accident scenario.

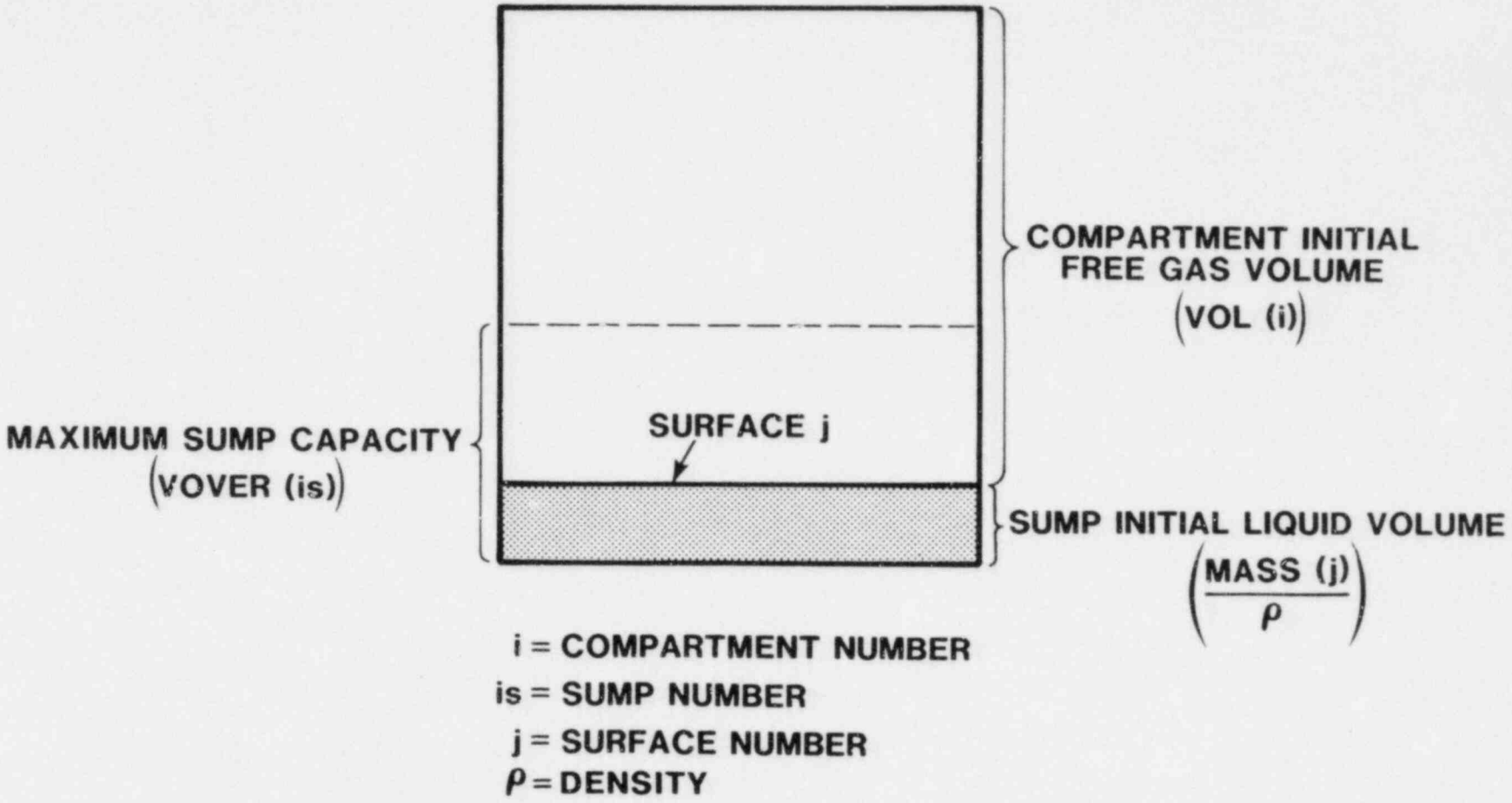


Figure 4-1. Relationship between Compartment Volume, Sump Capacity, and Sump Liquid Mass in HECTR

4.2.1 Initial NAMELIST-Type Input

The form of this input was described previously. This data is read from Unit 5. Default values are provided for all of the variables in this section (as shown by the quantities within the angle brackets), and new values need be assigned only for those variables that the user wishes to change. This section of input is terminated with a dollar sign ($) placed in column 1. Normally, this first pseudo-NAMELIST input is used to define the HECTR input/output units and to set the input echoing flag. These variables can be set individually; however, a shortcut is sometimes possible. A variable exists (CMPUTR) that defines the type of computer on which HECTR is running and, depending on the computer type, causes certain default actions to be taken. Basically, input is echoed, and the input units are set to 5, if HECTR is being run in a noninteractive mode (as often will be the case on a CDC [CYBER] or CRAY computer). Input is not echoed and the input units are set differently on a VAX where HECTR will typically be run interactively. It is very important to note that while these actions are desirable in the computing environment available at SNLA, they may not be optimal at other installations. If these actions are not desirable, the CMPUTR variable should be ignored, and the units and flags should be set individually to the values desired by the user. If setting CMPUTR produces the appropriate results, this section of input can be considerably simplified. For example, when running on a VAX, this section of input will consist simply of a dollar sign in column 1 (since the VAX is the default computer type); on a CRAY this input will be

```
CMPUTR=CRAY
$
```

>>>

4.2.1.1 Input Control Variables

BATCH [L] - <Default = FALSE>
If TRUE, then all input will be echoed. This will normally be desirable when running HECTR in batch (noninteractive) mode and undesirable when running HECTR interactively. See also CMPUTR.

CMPUTR [A] - <Default = VAX>
Type of computer on which HECTR is running. The effects of the possible values of this variable are

	CDC	sets BATCH to TRUE and sets URD and UIC to 5
	CYBER	same as for CDC
	CRAY	same as for CDC
	VAX	sets BATCH to FALSE and sets URD and UIC to 4

These actions are desirable in the computing environment available at SNLA, but they may not be optimal at other installations.

INPCHK [L] - <Default = FALSE>
In a future version of HECTR, this will cause (if TRUE) the validity of HECTR input to be checked.

UMI [I] - <Default = 1>
The unit from which external (MARCH) input is read.

URD [I] - <Default = 4>
The unit from which the reactor data (Section 4.2.2) is read. See also CMPUTR.

UIC [I] - <Default = 4>
The unit from which the initial conditions and the accident scenario (Section 4.2.3) are read. See also CMPUTR.

4.2.1.2 Output Control Variables

See Section 5.2.3.1 for a general discussion of the output units described below.

UOM [I] - <Default = 6>
The unit to which output messages produced by HECTR are written.

UOH [I] - <Default = 7>
The unit to which the output of major variables defined on heat-transfer timesteps is written (in unformatted WRITEs). ACHILES processes the data written to this unit to produce tables and graphs. The ACHILES input unit corresponding to UOH is UHD (which defaults to 7). If UOH is set to zero, then no timestep information of any kind will be written by HECTR (UOF and UOA will also be set to zero).

UOF [I] - <Default = 8>
The unit to which the output of major variables defined on flow timesteps is written (in unformatted WRITEs). ACHILES processes the data written to this unit to produce tables and graphs. The ACHILES input unit corresponding to UOF is UHF (which defaults to 8). If UOF is set to zero, then no flow timestep information will be written by HECTR.

UOA [I] - <Default = 0>
The unit to which the output of additional variables defined on heat-transfer timesteps is written (in unformatted WRITEs). ACHILES processes the data written to this unit to produce tables and graphs. The ACHILES input unit corresponding to UOA is UHA (which defaults to 9). If UOA is set to zero, then no additional heat-transfer timestep information will be written by HECTR. The information written with this unit is typically used for debugging or for other special interest purposes.

4.2.1.3 Miscellaneous Variables

NICEC [I] - <Default = 4>
The number of compartments automatically generated by HECTR for the ice-bed region of an ice condenser. This number must be less than or equal to the value of the symbolic constant NICE set in PARAMETER statements in HECTR (see Section B.2.7). See Section A.2.8 for further information.

Remember to enter a $ in column 1 at the end of the NAMELIST type input!

4.2.2 Problem Geometry

This data is read from unit URD (URD is defined in Section 4.2.1.1: Input Control Variables).

4.2.2.1 General

>>>
LTITLE [A] - A title of 37 characters or less used as a header for output. The last non-blank character must be a dollar sign ($).

for i=1,9
>>>
Any of the following lines of text may be blank, but all nine lines must be included. If the first nonblank character is a !, then that line will be considered a comment rather than one of the nine text line inputs.

TEXT(i) [A] - A line of 80 characters or less used for descriptive comments.

end for
>>>
PFAIL [R] - (pascals)
Containment failure pressure. If this number is positive, then a message will be written if this pressure is exceeded in any compartment during a run.

>>>
NCOMPS [I] - Number of compartments. For an ice-condenser geometry, this number includes the lower and upper plenums of the ice condenser but does not include the compartments in the ice-bed region.

4.2.2.2 Compartment Data

for i=1,"Number of Compartments" (see Section 4.1.3)
>>>
COMPID(i) [A] - A 72-character or less compartment descriptor.

>>>
VOL(i) [R] - (cubic meters)
Initial free gas volume of compartment i.

Z(i) [R] - (meters)
Compartment elevation. Normally, this is the elevation of the middle of the compartment. All compartments are referenced to the same baseline elevation.

CHRLEN(i) [R] - (meters)
Characteristic length for flame propagation. The burn time is calculated by dividing the characteristic length by the flame speed. See Section 3.6 for further information.

NSURFC(i) [I] - Number of heat-transfer surfaces in compartment i. This number may be zero.

ISV(i) [I] - The number of the sump where water condensed from the atmosphere of compartment i due to subcooling (supersaturation) is placed. If this number is zero, then the water produced from subcooling in this compartment will disappear from the system, and hence, mass will not be conserved.

ISSP(i) [I] - The number of the sump where unevaporated spray drops that reach the floor of compartment i and are not carried over into lower compartments are placed. If this number is zero, then the unevaporated drops will disappear from the system.

end for

4.2.2.3 Sump Data

If this simulation does not include sumps, then enter a $ in column 1 and skip the rest of this section of input.

while column 1 not = '$' (see Section 4.1.2)
>>>
is [I] - The number identifying the sump.

VOVER(is) [R] - (cubic meters)
Capacity of the sump. When modeling Mark III suppression pools, this quantity indicates the holdup volume for the sump representing the drywell pool (corresponding to H_{DP} in Section A.2.10). For the sump representing the suppression pool, this quantity must be entered, but will not be used by the code.

DUMPTO(is) [I] - The number of the sump into which any overflow from the current sump (is) is dumped. Overflow will occur if the sump volume exceeds the capacity (defined above). If this number is zero, then any water that overflows from this sump will disappear from the system. If the sump is specified to overflow into a second sump and the second sump is specified to overflow back into the first sump, then whenever the capacities of both sumps are exceeded, the two sumps will both fill up beyond their capacities, and the excess water will be divided between them by the ratio of the surface areas of the two sumps. Overflow between the suppression pool and drywell pool is accounted for internally by HECTR. Thus, this quantity will be ignored for sumps specified to be either the drywell pool or the suppression pool.

end while

4.2.2.4 Surface Data

Because the surfaces will be automatically numbered in the order that they are entered, the order of entry for individual surfaces is important. The radiative heat-transfer input (see Section 4.2.2.9) must be consistent with the surface-data numbering.

Also, the surfaces entered in this section will be placed in compartments in the order in which they are entered, i.e., using the values for NSURFC(i) entered previously in Section 4.2.2.2, the first NSURFC(1) surfaces will be placed in Compartment 1, the next NSURFC(2) surfaces will be placed in Compartment 2, etc. However, the sumps need not be entered in any particular order. The value of ISS(i) will indicate the proper sump number, i.e., for each sump, is, defined in Section 4.2.2.3 there must be exactly one surface, i, entered below with STYPE(i) = 3 and ISS(i) = is.

The notation "Number of Surfaces" in this and all following "for" statements refers to the total number of surfaces in the containment excluding surfaces in the ice-bed region.

for i=1,"Number of Surfaces" (see Section 4.1.3)

>>>

SURFID(i) [A] - A 72-character or less surface descriptor.

>>>

STYPE(i) [I] - Describes the type of surface. Enter

1 if the surface is a multi-layered slab
2 if the surface is a lumped mass
3 if the surface is a pool (a sump)

Surface types 4 and 5 define ice surfaces and ice-condenser walls, respectively. These two types are set up internally by HECTR.

MASS(i) [R] - (kilograms)
Mass of lumped mass or sump surface. If surface i is the surface of a sump, then MASS(i) will be the initial liquid mass in the sump. This quantity must be entered but will be ignored if the surface is a slab (see above description of STYPE).

AREA(i) [R] - (square meters)
Surface area used for heat transfer.

L(i) [R] - (meters)
Characteristic length for convective heat transfer. See Section 3.8 for further information.

CP(i) [R] - (joules per kilogram per kelvin)
Specific heat of the surface. This quantity must be entered but will be ignored if the surface is not a lumped mass (STYPE = 2).

EMIS(i) [R] - Radiative emissivity of the surface.

ISS(i) [I] - If surface i is the surface of a sump, then ISS(i) will be the number of that sump. For all other types of surfaces, this value is the number of the sump where condensate that drains off the surface is placed. If this number is zero, then condensate runoff will disappear from the system.

if STYPE(i) = 1 then (the surface is a multilayered slab)
>>>
NUMLAY(i) [I] - Number of layers in the slab.

for j=1,NUMLAY(i)
>>>
LAYTHK(j,i) [R] - (meters)
Thickness of the jth layer. The layers are counted starting from

the front side of the slab (layer number 1 receives the heat transfer directly from the compartment atmosphere).

LAYA(j,i) [R] - (square meters per second) Thermal diffusivity of the layer.

LAYK(j,i) [R] - (watts per meter per kelvin) Thermal conductivity of the layer.

end for

>>>

NUMEL(i) [I] - Number of elements in the slab heat-conduction model. The number of elements must lie between 0 and 100 inclusive. If this value is zero, then the number of elements will be chosen automatically by HECTR. See Section 3.9 for further information.

ELEXP(i) [R] - Element distribution exponent. Choosing a positive number less than 1 will result in a distribution of elements increasing in length as the back side of the slab is approached (where less resolution is normally needed than at the front surface in the heat-conduction model). If this number is zero, then HECTR will automatically choose an appropriate value. See Section 3.9 for further information.

HCONV(i) [R] - (watts per square meter per kelvin) Convective heat-transfer coefficient for the back side of the slab. Set this value to 0 if the back side of the slab is to be insulated or to -1. if it is to have a constant temperature boundary condition.

TENV(i) [R] - (kelvins) Temperature of the environment on the back side of the slab. If the back side is to be insulated, then set this quantity to 0.

end if

end for

4.2.2.5 Flow Junction Data

If this simulation does not include flow junctions, then enter a $ in column 1 and skip the rest of this section of input.

while column 1 not = '$'
>>>
Enter data associated with the nth flow junction (assuming the direction of positive flow is from compartment i into compartment j).

i [I] - Source compartment. If this number is zero, then the source compartment will be assumed to be in the ice-bed region of an ice condenser, and the receiving compartment should be the upper plenum.

j [I] - Receiving compartment. If this number is zero, then the receiving compartment will be assumed to be in the ice-bed region of an ice condenser, and the source compartment should be the lower plenum.

JTYPE(n) [I] - Junction type. Enter

1 for 2-way flow
2 for check valve type of 1-way flow
3 for inertial valve type of 1-way flow (variable area door)
4 for a drain between the upper and lower compartments in an ice-condenser containment.

AI(n) [R] - (square meters)
Interconnection area. For valve-type flow junctions (JTYPE = 2 or 3), this is the fully open door area.

FLOCO(n) [R] - Loss coefficient for flow between compartments i and j.

LA(n) [R] - (1/meters)
The flow length through the junction divided by an effective flow area. See Section 3.4 for further information.

RELATJ(n) [I] - Describes the spatial relationship of compartment i to compartment j for burn propagation. Enter

```
                              -1   if i is above j
                               0   if i is beside j
                               1   if i is below j

  ZJUN(n)          [R] - (meters)
                         Junction elevation.  This elevation is
                         referenced to the same baseline as the
                         compartment elevations (see Z(i) in
                         the Compartment Data section).

  if JTYPE(n) = 3 then     (junction allows inertial valve
                           type of 1-way flow)
>>>
     In the following, "ii" is the number of the inertial
     valve (door) corresponding to flow junction n.  "ii" is
     an internal HECTR index.

     DAMIN(ii)    [R] - (square meters)
                        Minimum door area.  The door has this
                        area for differential pressures across
                        the door that are less than DPMIN(ii).

     DPMIN(ii)    [R] - (pascals)
                        Minimum differential pressure needed
                        to begin opening the door.

     DPMAX(ii)    [R] - (pascals)
                        Differential pressure necessary to
                        hold the door fully open.

     THETMX(ii)   [R] - (radians)
                        Fully open door angle.  This number
                        must lie between 0 and π/2, inclu-
                        sive.

  end if

  if JTYPE(n) = 4 then   (junction is a drain)
>>>
     In the following, "ij" is the number of the drain corre-
     sponding to flow junction n.  "ij" is an internal HECTR
     index.

     ISUMPD(ij)   [I] - Number of the lower-compartment sump
                        which the drain feeds into.

     VSMPDR(ij)   [R] - (cubic meters)
                        Volume of water in the above sump
                        ( ISUMPD(ij) ) needed to cover the
                        drain opening and block gas flow.
  end if

end while
```

4.2.2.6 Ice-Condenser Data

>>>
If this simulation does not include an ice condenser, then enter a $ in column 1 and skip the rest of this section of input. This section of input deals primarily with the ice-bed region. The lower and upper plenums should already have been entered as regular compartments.

LPCOM [I] - Compartment number of the lower plenum.

UPCOM [I] - Compartment number of the upper plenum.

ISICE [I] - Number of the sump that water in the lower plenum, produced from ice melting and steam condensation in the ice-condenser compartments, drains into.

>>>
MICET [R] - (kilograms)
Total mass of the ice initially present in the ice condenser.

AICET [R] - (square meters)
Total heat-transfer area of the ice initially present. Normally, this is the sum of the surface areas of the full ice baskets, treating each as a smooth right circular cylinder, i.e., do not attempt to differentiate between the ice and the baskets.

TICE [R] - (kelvins)
Initial temperature of the ice.

LICET [R] - (meters)
Total (vertical) length of the ice initially present.

EMISIC [R] - Radiative emissivity of the ice.

VICET [R] - (cubic meters)
Total volume of the ice initially present.

>>>
MSTRCT [R] - (kilograms)
Total mass of heat-transfer structures, excluding baskets, in the ice region.

ASTRCT [R] - (square meters)
Total heat-transfer area of the structures, excluding baskets, present in the ice region.

CSTRUC [R] - (joules per kilogram per kelvin) Specific heat of the heat-transfer structures in the ice region.

EMISTR [R] - Radiative emissivity of the heat-transfer structures in the ice region.

>>>
MBASKT [R] - (kilograms) Total metal mass of the ice baskets in the ice condenser.

ABASKT [R] - (square meters) Total heat-transfer area of the ice baskets after all the ice has melted.

TMELTF [R] - (kelvins) Final temperature of water, produced from melting ice and steam condensation on the ice, after it falls through the lower plenum.

>>>
ZBOT [R] - (meters) Elevation of the bottom of the ice region in the ice condenser.

AFICE [R] - (square meters) Flow area for flow junctions in the ice region. This is the open cross-sectional area of the ice region.

LOSCO [R] - Loss coefficient to be applied at each flow junction within the ice region.

VOLICE [R] - (cubic meters) Initial free gas volume in the ice region.

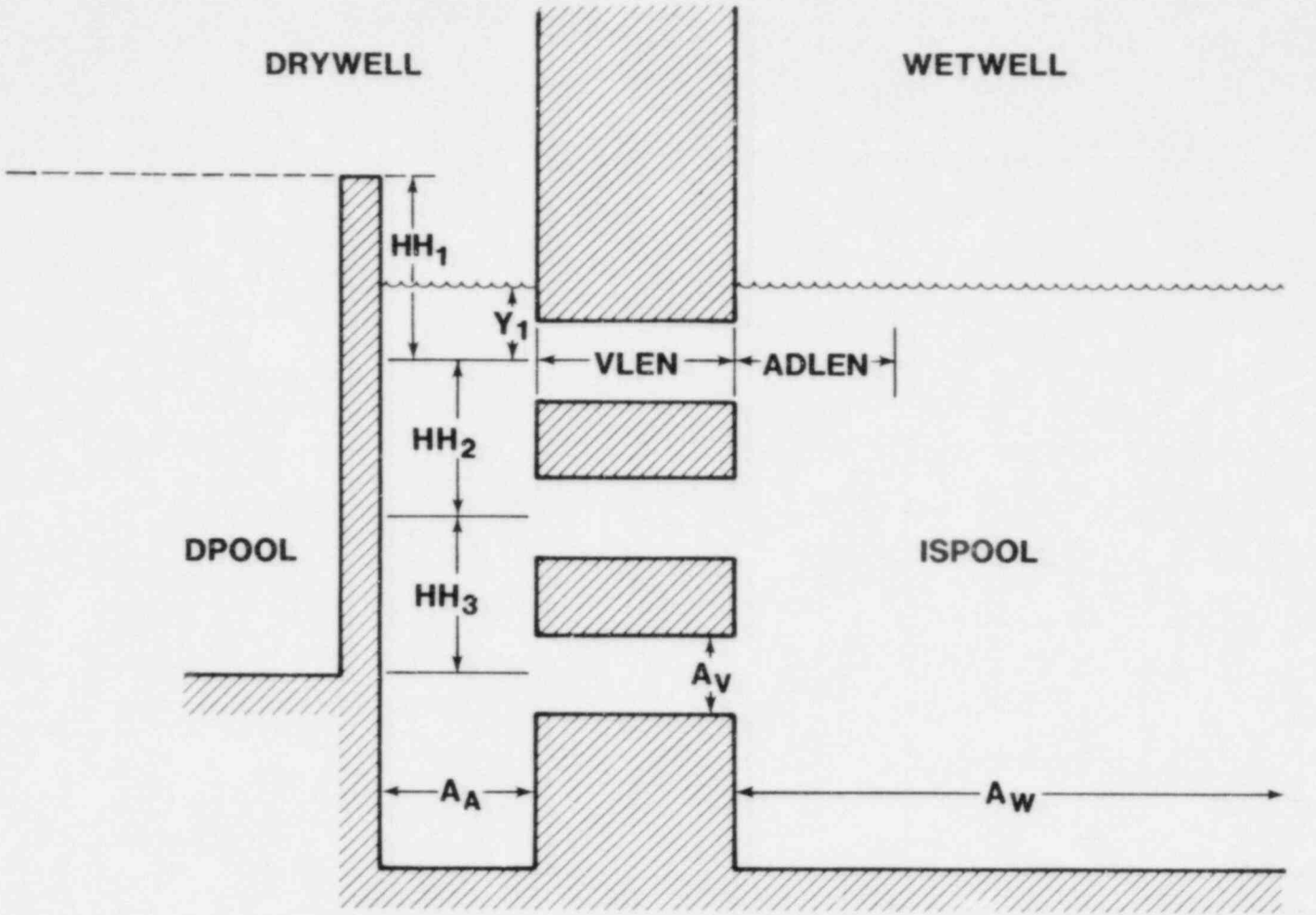
4.2.2.7 Suppression Pool Data

>>>
If this simulation does not include a suppression pool, then enter a $ in column 1 and skip the rest of this section of input. Figure 4-2 shows several of the suppression pool input variables. See Sections A.2.10 and 3.13 for discussions of these variables.

DW [I] - Drywell compartment number.

WW [I] - Wetwell compartment number.

ISPOOL [I] - Number of the sump that is the suppression pool.



A_A = SURFACE AREA OF DRYWELL SIDE OF SUPPRESSION POOL

A_V = CROSS-SECTIONAL AREA OF 1 ROW OF VENTS

A_W = SURFACE AREA OF WETWELL SIDE OF SUPPRESSION POOL

Figure 4-2. Suppression Pool Input Variables

UPOOL [I] - Number of the upper pool sump.

DPOOL [I] - Number of the drywell sump.

>>>

HH(1) [R] - (meters)
Distance from the top of the weir wall to the center of the top vent.

HH(2) [R] - (meters)
Distance between the centers of the top and middle vents.

HH(3) [R] - (meters)
Distance between the centers of the middle and bottom vents.

VLEN [R] - (meters)
Vent length. This is the thickness of the drywell wall (wall between the drywell and wetwell).

Y(1) [R] - (meters)
Initial distance from the surface of the suppression pool to the center of the top vent. The drywell and wetwell sides are assumed to be at the same level initially (Y(7) = (Y(1)).

>>>

AA [R] - (square meters)
Area of the drywell portion of the suppression pool surface.

AV [R] - (square meters)
Total cross-sectional area of one horizontal row of suppression pool vents.

AW [R] - (square meters)
Area of the wetwell portion of the suppression pool surface.

KIN [R] - Loss coefficient for water flowing through the vent opening on the drywell side (same value used for flow in either direction).

KOUT [R] - Loss coefficient for water flowing through the vent opening on the wetwell side (same value used for flow in either direction).

KVENT [R] - Loss coefficient for gas flowing through one horizontal row of vents.

ADLEN [R] - (meters)
Equivalent additional vent length used in vent clearing calculations.

>>>

WDRNUP [R] - (kilograms per second)
Draining rate of the upper pool into the suppression pool for upper pool dump.

TDRNUP [R] - (seconds)
Absolute time when the upper pool begins to drain into the suppression pool (see also the discussion of TIMZER in Section 4.2.3.6.4).

MMINUP [R] - (kilograms)
Residual mass of water left in the upper pool after upper pool dump has occurred.

4.2.2.8 Fan Data

>>>

If this simulation does not include fans, then enter a $ in column 1 and skip the rest of this section of input.

TSETF [R] - (kelvins)
Temperature set point for automatic activation of the fans. This quantity is used when the fans are in AUTO mode (described later), otherwise this value is ignored.

PSETF [R] - (pascals)
Pressure set point for automatic activation of the fans. This quantity is used when the fans are in AUTO mode (described later), otherwise this value is ignored.

DELAYF [R] - (seconds)
Time delay for fan activation in AUTO mode. The fans are turned on at a time DELAYF after either TSETF or PSETF is exceeded anywhere in the containment (excluding the drywell if a suppression pool is modeled).

TFRUN [R] - (seconds)
Length of time that the fans will remain on once they have been turned on. If the fans should continue to operate indefinitely, then enter a

large number. This time applies to all modes of fan operation (see FANS in Section 4.2.3.6.4).

```
while column 1 not = '$'
>>>
```

Enter data associated with the nth fan path (assuming the direction of flow is from compartment i into compartment j).

i	[I] -	Source compartment.
j	[I] -	Receiving compartment.
FANVFR(n)	[R] -	(cubic meters per second) Volumetric flow rate of the fan. Enter +X if the fan is blowing at a constant flow rate of X or -X if the fan is blowing at a maximum flow rate of X, with the actual flow rate determined from a head curve.
DPFMAX(n)	[R] -	(pascals) Maximum pressure difference under which the fan can operate when using a head curve (shut-off head).
ETA(n)	[R] -	Fan efficiency. This number is equal to 1. for an ideal fan.
RELATF(n)	[I] -	Describes the spatial relationship of compartment i to compartment j for burn propagation through the fans. Enter -1 if i is above j 0 if i is beside j 1 if i is below j

```
end while
```

Enter a head curve for the fans. This curve will be used for all fans that are using a head curve to determine their volumetric flow rate. If the default head curve is desired, enter a $ in column 1 and skip the rest of this section of input.

```
while column 1 not = '$'
>>>
```

Enter the head curve table. "if" is an internal HECTR index that starts counting from 1. The maximum number of table entries is 11.

```
  PHEAD(if)        [R] - Normalized value of the differential
                         pressure across the fan (P(j)-P(i))/
                         DPFMAX).

  FRHEAD(if)       [R] - Normalized value of the fan volumetric
                         flow rate (flow rate/FANVFR).
end while
```

4.2.2.9 Radiative Heat-Transfer Data

```
for i=1,"Number of Surfaces"      (see Section 4.1.3)
>>>
  for j=i,"Number of Surfaces"

     BEAM(i,j)     [R] - (meters)
                         Beam length between surfaces i and j.
                         BEAM(j,i) is automatically set equal
                         to BEAM(i,j) so that only half of the
                         array must be specified.
  end for

end for

for i=1,"Number of Surfaces"      (see Section 4.1.3)
>>>
  for j=i,"Number of Surfaces"

     VF(i,j)       [R] - View (shape) factor for surface i
                         looking at surface j.  VF(j,i) is cal-
                         culated automatically using the reci-
                         procity relation for view factors
                         ( AREA(I)*VF(I,J) = AREA(J)*VF(J,I) ).
                         See Section 3.7 for further informa-
                         tion.
  end for

end for
```

4.2.2.10 Spray Data

```
>>>
INCWSP           [I] - Number of compartments with spray
                       sources.  This should include only
                       compartments in which spray is ini-
                       tially injected, not compartments that
                       are receiving spray carryover from
                       compartments above them.  If this num-
                       ber is zero, then skip the rest of
                       this section of input.
```

```
for i=1,INCWSP
>>>
  INITSC(i)        [I] - Compartment that sprays are injected
                         into.  Only one spray source should be
                         specified for a compartment.

  TDO(i,           [R] - (kelvins)
                         Spray inlet temperature when in
                         injection mode.  This value must be
                         less than 477 K.

  SPFLO(i)         [R] - (cubic meters per second)
                         Spray inlet flow rate.

  INDS(i)          [I] - Number of drop sizes to be modeled in
                         the spray.

  for j=1,INDS(i)
>>>
     FREQ(i,j)     [R] - Fraction of drops that are of the jth
                         drop size.

     DIAM(i,j)     [R] - (micrometers)
                         Diameter of drops of the jth drop size.

  end for

end for

while column 1 not = '$'
>>>
  Enter data associated with spray carryover.  Note that
  information needs to be entered only for paths for which
  there is actually spray carryover.  If no spray carryover
  is allowed, then enter a $ in column 1 and skip to the end
  of this table input section.

  i                [I] - Source compartment for spray carryover.

  j                [I] - Compartment receiving spray carryover.

  FRDRP(i,j)       [R] - Fraction of the drops that reach the
                         bottom of compartment i that are
                         allowed to carry over into compartment
                         j.

end while

while column 1 not = '$'
>>>
  Enter spray fall heights.  Note that these values need to
  be entered only for compartments through which spray drops
  can actually fall (i.e., spray injection and carryover com-
  partments).
```

i [I] - Compartment.

ZTOT(i) [R] - (meters)
Spray fall height for compartment i.

end while

>>>

TSET [R] - (kelvins)
Temperature set point for automatic activation of the sprays. This quantity is used when the sprays are in AUTO mode (described later), otherwise this value is ignored.

PSET [R] - (pascals)
Pressure set point for automatic activation of the sprays. This quantity is used when the sprays are in AUTO mode (described later), otherwise this value is ignored.

DELAY [R] - (seconds)
Time delay for spray activation in AUTO mode. The sprays are turned on at a time DELAY after either TSET or PSET is exceeded anywhere in the containment (excluding the drywell if a suppression pool is modeled).

TSPRUN [R] - (seconds)
Length of time that the sprays will remain on once they have been turned on. If the sprays should continue to operate indefinitely, then enter a large number. This time applies to all modes of spray operation (see SPRAYS in Section 4.2.3.6.4).

>>>

Enter data associated with sprays in recirculation mode. If this data is not relevant to the simulation, then enter a $ in column 1 and skip the rest of this section of input. Note that all sprays will be switched to the recirculation mode when TINJ has been exceeded. Also, all spray water will come from a single sump and pass through a single heat exchanger. Thus, if sprays are injected into more than one compartment, the total flow necessary to supply the sprays will be drawn from a single sump and passed through a single heat exchanger with splits occurring downstream of the spray heat exchanger. Therefore, the spray heat exchanger parameters should be based on total spray flow rates.

TINJ [R] - (seconds)
Time that the sprays spend in injection mode before switchover to the recirculation mode.

SPFLOR [R] - (kilograms per second)
Rated spray heat exchanger mass-flow rate.

HAEFFR [R] - (watts per kelvin)
Rated spray heat exchanger effective heat-removal rate.

TS1 [R] - (kelvins)
Spray heat exchanger secondary side inlet temperature.

WSR [R] - (kilograms per second)
Spray heat exchanger secondary side mass-flow rate.

SPRSRC [I] - Number of the sump from which the sprays draw water when in recirculation mode. This is also the sump from which water is drawn for recirculation into the emergency core cooling system (see Section 4.4.2) when using an external (MARCH) source.

4.2.2.11 Sump Heat Exchanger Data

If this simulation does not include sump heat exchangers, then enter a $ in column 1 and skip the rest of this section of input. Unlike the spray heat exchanger, multiple heat exchangers can be specified for sump cooling. When modeling plants where heat exchangers are shared between the sprays and sump cooling, it is necessary to provide input for two heat exchangers. The input for sump cooling is provided in this section, and the input for spray cooling is provided in the Spray Data input section.

while column 1 not = '$' then
>>>
i [I] - The number of the sump to be cooled by a heat exchanger.

MODEHE [I] - Enter

1 if the heat exchanger is turned off when the sprays come on
0 if the heat exchanger is not affected by sprays

FLOHER(i) [R] - (kilograms per second)
Rated mass flow rate.

EFFHE(i) [R] - (watts per kelvins)
Rated effective heat removal rate.

TSECHE(i) [R] - (kelvins)
Secondary side inlet temperature.

WSECHE(i) [R] - (kilograms per second)
Secondary side mass flow rate.

FLOWHE(i) [R] - (kilograms per second)
Actual primary side mass flow rate that passes through the heat exchanger.

>>>

TSETH(i) [R] - (kelvins)
Temperature set point for automatic activation of the heat exchanger. This quantity is used when the heat exchanger is in AUTO mode (described later), otherwise this value is ignored.

PSETH(i) [R] - (pascals)
Pressure set point for automatic activation of the heat exchanger. This quantity is used when the heat exchanger is in AUTO mode (described later), otherwise this value is ignored.

DELAYH(i) [R] - (seconds)
Time delay for heat exchanger activation in AUTO mode. The heat exchanger is turned on at a time DELAYH(i) after either TSETH(i) or PSETH(i) is exceeded anywhere in the containment, excluding the drywell if a suppression pool is modeled.

THERUN(i) [R] - (seconds)
Length of time that the heat exchanger will remain on once it has been turned on. This time applies to all modes of heat exchanger operation (see HTEXCH(i) in Section 4.2.3.6.4).

end while

4.2.3 Initial Conditions and Accident Scenario

This data is read from unit UIC (UIC is defined in Section 4.2.1).

4.2.3.1 General

>>>
TRUN [R] - (seconds)
Simulation time.

4.2.3.2 Compartment Data

for i=1,"Number of Compartments" (see Section 4.1.3)
>>>
TBULK(i) [R] - (kelvins)
Initial gas temperature in compartment i.

for j=1,"Number of Gases (= 4)"

PP(i,j) [R] - (pascals)
Initial partial pressure of gas species j in compartment i where j equal to

1	indicates steam	(H_2O)
2	indicates nitrogen	(N_2)
3	indicates oxygen	(O_2)
4	indicates hydrogen	(H_2)

end for

UX(i) [R] - (meters per second)
Convective gas velocity for forced convection in compartment i. During a burn, HECTR uses the flame speed as the convective gas velocity instead of this value. See Section 3.8 for further information.

end for

if LPCOM not = 0 then (this simulation includes an ice condenser)
>>>
TBICE [R] - (kelvins)
Initial gas temperature in the ice region of the ice condenser.

for j=1,"Number of Gases (= 4)"

PPICE(j) [R] - (pascals)
Initial partial pressure of gas species j (see PP(i,j) above for the

definition of the gas species) in the ice region of the ice condenser.

end for

end if

4.2.3.3 Source Data

Enter the source terms. Sources can be injected into either compartments or sumps. For each gas, if there are no sources, then enter a $ in column 1; otherwise read the location i in which there is a source, MODE and TORH. Next, the source term is specified in tabular fashion. The form of this input is TIME, the release RATE at this TIME and, if MODE was positive, the source temperature or enthalpy at this TIME. The actual source values used in HECTR at times intermediate to those specified are obtained from linear interpolation of the data. For times greater than the last TIME specified in the table, the source values at this last TIME will be used. Terminate the source table with a $ in column 1. Additional sources of this gas can then be specified in other locations in the same manner. Do not enter more than one source of the same gas in the same compartment. Terminate the current source gas input (which may include several tables) with a $ in column 1 (so that the last entry in the last table is followed by two dollar signs). Proceed then to the next source gas.

for j=1,"Number of Gases (= 4)"

while column 1 not = '$'

>>>

i [I] - Location in which there is a source of gas species j where j equal to

1	indicates water (liquid or vapor)	(H_2O)
2	indicates nitrogen	(N_2)
3	indicates oxygen	(O_2)
4	indicates hydrogen	(H_2)

If i is positive, then the source is injected into compartment i. If i is negative then the source is injected into the sump numbered -i.

MODE [I] - Indicates whether the source temperature or enthalpy will be specified. For the absolute value of MODE equal to

1 source temperature (kelvins) is specified

2 source enthalpy (joules per kilogram) using Janaf table base point is specified

3 source enthalpy (joules per kilogram) using steam table base point (i.e., the enthalpy is zero at 273.15 K or 0°C) is specified.

If MODE is negative, then TORH will specify the constant temperature or enthalpy of the source. Otherwise, for positive MODE, TORH will be ignored (but must still be entered), and the source temperature or enthalpy will be read in as a function of time along with the release rates.

TORH [R] - (kelvins OR joules per kilogram) Constant temperature or enthalpy of the source. This has meaning only if MODE (see above) is negative, but a value must always be entered.

```
while column 1 not = '$'
>>>
```

TIME [R] - (seconds) The absolute time at which the release rate (specified next) occurs (see also the discussion of TIMZER in Miscellaneous Variables below).

RATE [R] - (kilograms per second) Release rate of the source into location i at the given TIME.

```
if MODE > 0 then
```

TORH [R] - (kelvins OR joules per kilogram) Source temperature or enthalpy at the given TIME (see mode above).

```
end if
end while
end while
end for
```

4.2.3.4 Sump Water Removal Rates

Enter tables of sump water removal rates. These tables can be used to simulate emergency core cooling (ECC) recirculation. If there are no such tables, then enter a $ in column 1 and skip the rest of this section of input. Otherwise, read the number of the sump (isump) for which a leakage table will be specified. Next, enter the table. The form of this input is the time (TLEAKE) and the leakage rate at this time (WLEAKE). The actual leakage values used in HECTR at times intermediate to those specified are obtained from linear interpolation of the data. For times greater than the last time specified in the table, the leakage values at this last time will be used. Terminate the leakage table with a $ in column 1. Additional leakage tables can now be specified for other sumps in the same manner. Terminate this section of input (which may include several tables) with a $ in column 1 (so that the last entry in the last table is followed by two dollar signs).

```
while column 1 not = '$'
>>>
  isump          [I] - The number of the sump from which water
                       is to be removed during the run.

  while column 1 not = '$'
>>>
     TLEAKE      [R] - (seconds)
                       The absolute time at which the leakage
                       rate (specified next) occurs (see also
                       the the discussion of TIMZER in
                       Section 4.2.3.6.4).

     WLEAKE      [R] - (kilograms per second)
                       Leakage rate of water from sump isump
                       at the given time (TLEAKE).

  end while

end while
```

4.2.3.5 Surface Temperatures

```
>>>
for i=1,"Number of Surfaces"     (see Section 4.1.3)

  TW(i)          [R] - (kelvins)
                       Initial temperature of the ith
                       surface. For slab surfaces all nodes
                       will be set to this temperature.

end for
```

4.2.3.6 NAMELIST Input

This information is provided only when default values are to be overridden. The quantities within angle brackets indicate the default values for the variable. An (i) following the variable name indicates that this variable is an array.

>>>

4.2.3.6.1 Burn Model Parameters

BURNT(i) [R] - (seconds) <Defaults to an internal calculation>
Burn time for a burn occurring in compartment i. If this quantity is not specified, then the burn time will be calculated by dividing the compartment characteristic length by the flame speed.

FLAMEV(i) [R] - (meters per second) <Defaults to an internal calculation>
Flame speed for a burn occurring in compartment i. If this quantity is not specified, then an internal correlation based on the gas composition present at the start of the burn will be used. Do not enter both BURNT and FLAMEV for the same compartment.

FNLFH2(i) [R] - <Defaults to an internal calculation>
Final fraction of the initial concentration of hydrogen to be left at the end of a burn in compartment i. This quantity is 1 minus the combustion completeness (specified as a fraction). For example, enter 0 or a small number for complete combustion. If this quantity is not specified, then an internal correlation based on the gas composition present at the start of the burn will be used.

FDAMPR(i) [L] - <Default = TRUE>
If TRUE, then fan path i is assumed to have a nonreturn damper (or check valve) in it. This will prevent a burn from propagating upstream through the fan under any circumstances or downstream through the fan when the fan volumetric flow rate is zero. If FALSE, then propagation downstream through a fan can occur for any flow rate, and propagation upstream can

occur if the flow rate is zero or if the flow rate is nonzero and PRBKFN is TRUE.

KPROPF(i) [R] - <Default = .5>
Fraction of the burn time in either compartment connected by fan path i that must elapse before a burn can propagate into the other compartment through the fan path. This number must lie between 0 and 1 inclusive.

KPROPJ(i) [R] - <Default = .5>
Fraction of the burn time in either compartment connected by flow junction i that must elapse before a burn can propagate into the other compartment through the flow junction. This number must lie between 0 and 1 inclusive.

PRBKFN(i) [L] - <Default = FALSE>
If TRUE, then a burn can propagate upstream through fan path i when the flow rate is nonzero and FDAMPR is FALSE. For zero flow rates, propagation through a fan is controlled by FDAMPR.

PRJUCL(i) [L] - <Default = FALSE if JTYPE(i) = 2 and
TRUE if JTYPE(i) = 3
If TRUE, then a burn can propagate through flow junction i even if it is closed. Thus, by default, a burn will not propagate through a 1-way check valve (JTYPE(i) = 2) if it is closed, but a burn will propagate through a 1-way inertial valve (JTYPE(i) = 3) even if the door area has been reduced to zero. This flag applies only to these two types of flow junctions. For ice-condenser drains (JTYPE(i) = 4) that are closed, burns cannot propagate through the drains under any circumstances.

XHMNIG(i) [R] - <Default = .08>
Minimum hydrogen mole fraction needed for ignition in compartment i.

XHMNPD(i) [R] - <Default = .09>
Minimum hydrogen mole fraction needed for downward propagation into compartment i.

XHMNPS(i) [R] - <Default = .06>
Minimum hydrogen mole fraction needed for horizontal propagation into compartment i.

XHMNPU(i) [R] - <Default = .041>
Minimum hydrogen mole fraction needed for upward propagation into compartment i.

XOMNIG(i) [R] - <Default = .05>
Minimum oxygen mole fraction needed for ignition in compartment i.

XOMNPD(i) [R] - <Default = .05>
Minimum oxygen mole fraction needed for downward propagation into compartment i.

XOMNPS(i) [R] - <Default = .05>
Minimum oxygen mole fraction needed for horizontal propagation into compartment i.

XOMNPU(i) [R] - <Default = .05>
Minimum oxygen mole fraction needed for upward propagation into compartment i.

XSMXIG(i) [R] - <Default = .55>
Maximum steam mole fraction that will permit ignition in compartment i.

XSMXPD(i) [R] - <Default = .55>
Maximum steam mole fraction that will permit downward propagation into compartment i.

XSMXPS(i) [R] - <Default = .55>
Maximum steam mole fraction that will permit horizontal propagation into compartment i.

XSMXPU(i) [R] - <Default = .55>
Maximum steam mole fraction that will permit upward propagation into compartment i.

4.2.3.6.2 Output Control Variables

See Section 5.1.5 for a general discussion of the usage of the output control variables described below.

DELPA [R] - (pascals) <Default = 0.>
Minimum absolute change in any compartment pressure that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. Values will be written for all compartments. If this quantity is zero, then the pressure check will be a pure relative test.

DELPR [R] - <Default = .03>
Minimum relative change in any compartment pressure that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. Values will be written for all compartments. If this quantity is zero, then the pressure check will be a pure absolute test.

DELTA [R] - (kelvins) <Default = 0.>
Minimum absolute change in any compartment temperature that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. If this quantity is zero, then the temperature check will be a pure relative test.

DELTR [R] - <Default = .01>
Minimum relative change in any compartment temperature that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. If this quantity is zero, then the temperature check will be a pure absolute test.

DELXA [R] - <Default = .001>
Minimum absolute change in any gas mole fraction that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. If this quantity is zero, then the mole fraction check will be a pure relative test.

DELXR [R] - <Default = 0.>
Minimum relative change in any gas mole fraction that will result in new values of heat-transfer timestep variables being written to units UOH and UOA. If this quantity is zero, then the mole fraction check will be a pure absolute test.

DELTHT [R] - <Default = .1>
Maximum fraction of the total simulation time (TRUN) that can elapse from a previous heat-transfer timestep variable output before new values of heat-transfer timestep variables will be written to units UOH and UOA. If this quantity is set to zero, then new values of heat-transfer timestep variables will be written on every heat-transfer timestep.

DELVA [R] - (meters per second) <Default = .1>
Minimum absolute change in any flow junction velocity that will result in new values of flow timestep variables being written to unit UOF. If this quantity is zero, then the velocity check will be a pure relative test.

DELVR [R] - <Default = .01>
Minimum relative change in any flow junction velocity that will result in new values of flow timestep variables being written to unit UOF. If this quantity is zero, then the velocity check will be a pure absolute test.

DELTFL [R] - <Default = .1>
Maximum fraction of the total simulation time (TRUN) that can elapse from a previous flow timestep variable output before new values of flow timestep variables will be written to unit UOF. If this quantity is set to zero, then new values of flow timestep variables will be written on every flow timestep.

4.2.3.6.3 Timestep Control Variables

DPRSMX [R] - (pascals) <Default = 10132.5>
Maximum absolute pressure change allowed in a compartment during a heat-transfer timestep.

DTMPMX [R] - (kelvins) <Default = 10.>
Maximum absolute temperature change allowed in a compartment during a heat-transfer timestep.

FLOMAX [R] - <Default = .95>
Maximum fraction of a compartment's gas volume that is allowed to flow out into other compartments during a flow timestep.

PCHMAX [R] - (pascals) <Default = 300.>
Maximum absolute pressure change allowed in a compartment during a flow timestep.

DTHTMN [R] - (seconds) <Default = .00001>
Minimum allowed timestep for heat-transfer calculations. This number must be greater than or equal to DTFLMN.

DTHTMX [R] - (seconds) <Default = 2.>
Maximum allowed timestep for heat-transfer calculations. This number must be greater than or equal to DTFLMX.

DTFLMN [R] - (seconds) <Default = .000001>
Minimum allowed timestep for intercompartment gas flow calculations. This number must be less than or equal to DTHTMN.

DTFLMX [R] - (seconds) <Default = 2.>
Maximum allowed timestep for intercompartment gas flow calculations. This number must be less than or equal to DTHTMX.

4.2.3.6.4 Miscellaneous Variables

NEXTRD [R] - (seconds) <Default = 1.0E+10>
The absolute time in the simulation that must be reached before additional pseudo-NAMELIST-type input can be read. This is useful for changing the values of certain parameters during the course of a run. This additional input will be read from unit UIC, must follow the $ ending this section of NAMELIST entries, and in turn must be terminated with a $ in column 1. At this point, NEXTRD can be set again, to an even later time in the simulation, so that when HECTR reaches this new time set point, more pseudo-NAMELIST-type input can be read. See also the discussion of TIMZER. As an example of the use of NEXTRD, suppose you wish to change the hydrogen ignition limits 1000 seconds into a calculation. The input would appear as follows:

```
XHMNIG = 1.0 !No combustion allowed
NEXTRD = 1000.
$End of NAMELIST INPUT
XHMNIG = 0.06 !Turn on igniters at
              !1000 seconds
$End of additional NAMELIST INPUT
```

FANS [A] - <Default = OFF>
Determines the mode of fan operation. Set this variable to

OFF	if there are no fans operating
ON	if the fans are to be turned on immediately (they will remain on for TFRUN seconds)
AUTO	if the fans are to be turned on after one of the previously specified set points (PSETF or TSETF) has been exceeded in any compartment (excluding the drywell if a suppression pool is included in the model). The fans will come on after a specified delay, DELAYF, and then remain on for TFRUN seconds.

Note that NEXTRD can be used to change the mode of fan operation (for example, from AUTO to OFF) at a specified time during a calculation.

HTEXCH(i) [A] - <Default = OFF>
Determines the mode of sump heat exchanger operation. Set this variable to

OFF	if there is no heat exchanger operating for sump i
ON	if the heat exchanger for sump i is to be turned on immediately (it will remain on for THERUN(i) seconds)
AUTO	if the heat exchanger for sump i is to be turned on after one of the previously specified set points (PSETH(i) or TSETH(i)) has been exceeded in any compartment (excluding the drywell if a suppression pool is included in the model). The sump heat exchanger will come on after a specified delay, DELAYH, and then remain on for THERUN(i) seconds.

Note that NEXTRD can be used to change the mode of sump heat exchanger operation (for example, from AUTO to OFF) at a specified time in a run.

SPRAYS [A] - <Default = OFF>
Determines the mode of spray operation. Set this variable to

OFF	if there are no sprays operating
ON	if the sprays are to be turned on immediately (they will remain on for TSPRUN seconds)
AUTO	if the sprays are to be turned on after one of the previously specified set points (PSET or TSET) has been exceeded in any compartment (excluding the drywell if a suppression pool is included in the model).

The sprays will come on after a specified delay, DELAY, and then remain on for TSPRUN seconds.

Note that NEXTRD can be used to change the mode of spray operation (for example, from AUTO to OFF) at a specified time in a run.

CHTICE [R] - <Default = 5.>
Factor to account for basket roughness and liquid layers in the definition of the Nusselt number for an ice-condenser surface (STYPE = 4 or 5). (See Section A.2.5 and Eq. A.50.)

MRCHSC [I] - <Default = 0>
The number of the compartment into which external (MARCH) sources are injected. The external (MARCH) input will be read in from unit UMI. If MRCHSC is zero, then it is assumed that there are no external (MARCH) inputs.

RECIRC [L] - <Default = TRUE>
If FALSE, then the sprays will turn off after the injection phase has completed (there will be no recirculation phase).

SCDOF(i) [R] - <Default = 0.>
Surface condensation drain-off factor. This quantity is multiplied with a mass flux for surface i based on a vertical plate, laminar flow calculation to determine the condensation runoff from the surface. This factor is used only for slab and lumped-mass surfaces. (See Section A.2.5 and Eq. A.59.)

TIMZER [R] - (seconds) <Default = 0.>
The initial time in a HECTR run. Note that some of the HECTR variables (e.g., TDNRUP, TIMHE(i), and NEXTRD) refer to absolute times rather than time that has passed since the start of the calculation. Resetting TIMZER may also require resetting these parameters.

WFTMX(i) [R] - (meters) <Default = .001>
Maximum water film thickness resulting from condensation that is allowed on surface i. This term is used only for slab and lumped-mass surfaces (STYPE = 1 or STYPE = 2).

Remember to enter a $ in column 1 at the end of the NAMELIST-type input!

4.3 Input File for the Output Processor (ACHILES)

ACHILES processes the time-dependent variable output (compartment pressures, flow junction velocities, surface temperatures, etc.) produced by HECTR. This output is divided into three categories: major heat-transfer timestep variables, flow timestep variables, and additional heat-transfer timestep variables. The values of these variables are read from the ACHILES units UHD, UHF, and UHA, respectively. ACHILES can create tables and graphs of this data. For example, consider surface temperatures. Often, the user may be interested only in the temperature histories of certain surfaces. Other times, the user may want temperature information on all surfaces. The procedures for selecting some, all, or none of the surfaces (or any other item) is explained in detail in Section 4.3.2. Following this explanation are lists of the possible variables that can be tabulated or plotted as functions of time. Prior to the input specifying which tables and graphs are to be produced, a NAMELIST-type input is required. This input can be used to change default values of various table and plot parameters.

ACHILES uses the DISSPLA graphics package [14] to produce plots. This package must reside on the user's computer system for plots to be possible. If DISSPLA is not available, then tables can still be produced, but the user will need to generate new plotting routines for the available system.

4.3.1 NAMELIST-Type Input

This section of the input is in a pseudo-NAMELIST-type format. See Section 4.1.1 for a description of the form of this input. This data is read from unit 5. Default values are provided for all of the variables in this section (as shown by the quantities within the angle brackets), and new values need be assigned only for those variables, if any, that need to be changed. Input is terminated with a dollar sign ($) placed in column 1. ACHILES input and output can be controlled using NAMELIST-type variables. The units for reading and writing data can be specified similarly to those discussed previously for HECTR in Section 4.2. In addition, NAMELIST-type variables can be used to control the amount of data

printed in the tables and the format of plots. If any plotting is to be done, care should be taken that the computer word length is defined appropriately by setting either the CMPUTR or the LENWRD variable.

>>>

4.3.1.1 Input Control Variables

BATCH [L] - <Default = FALSE>
If TRUE, then all input will be echoed unless the units UOM and UOT are the same. This will normally be desirable when running ACHILES in batch (non-interactive) mode and undesirable when running ACHILES interactively. See also CMPUTR.

CMPUTR [A] - <Default = VAX>
Type of computer on which ACHILES is running. The effects of the possible values of this variable are

CDC	sets BATCH to TRUE, UOT to 6, and sets internal variables that are affected by the computer word length (which is 10 bytes for a CDC computer)
CYBER	same as for CDC
CRAY	sets BATCH to TRUE, UOT to 6, and sets internal variables that are affected by the computer word length (which is 8 bytes for a CRAY)
VAX	sets BATCH to FALSE, UOT to 10, and sets internal variables that are affected by the computer word length (which is 4 bytes for a VAX)

The calls to the DISSPLA plot package for graph titling require knowledge of the computer word length in order to convert character-data-type titles into Hollerith, since DISSPLA is not ANSI standard FORTRAN 77 (as of January 1, 1984). These actions are desirable in the computing environment available at SNLA, but they may not be optimal at other installations.

LENWRD [I] - <Default = 4>
Computer word length in bytes. The calls to the DISSPLA plot package for graph titling require knowledge of the computer word length in order to convert character-data-type titles into Hollerith, since DISSPLA is not ANSI standard FORTRAN 77 (as of January 1, 1984). Usually, an appropriate value is 4 for DEC and IBM computers, 8 for CRAY computers, and 10 for CDC (CYBER) computers. Setting CMPUTR above will automatically set LENWRD to the correct value.

UAR [I] - <Default = 5>
The unit to which user input to ACHILES for specifying desired tables and plots is entered.

UHD [I] - <Default = 7>
The unit from which the values of major variables defined on heat-transfer timesteps are read (in unformatted READs). The HECTR output unit corresponding to UHD is UOH (which defaults to 7).

UHF [I] - <Default = 8>
The unit from which the values of major variables defined on flow timesteps are read (in unformatted READs). The HECTR output unit corresponding to UHF is UOF (which defaults to 8).

UHA [I] - <Default = 9>
The unit from which the values of additional variables defined on heat-transfer timesteps are read (in unformatted READs). The HECTR output unit corresponding to UHA is UOA (which defaults to 0--no output).

4.3.1.2 Output Control Variables

UOM [I] - <Default = 6>
The unit to which output messages produced by ACHILES are written.

UOT [I] - <Default = 10>
The unit to which output tables are written. See also CMPUTR above.

UAO [I] - <Default = 10>
The unit to which ACHILES summary output is written. If UOT is set to a number different than UAO, and BATCH is set to TRUE, then the ACHILES Summary information (and nothing else) will be written to UAO. This can be useful, for example, if is it desired to write the tables produced by ACHILES directly to microfiche and also create a hard copy of the ACHILES summary information.

4.3.1.3 Plot Control Variables (See Section 5.2.3)

COMBXF(i)* [L] - <Default = FALSE>
If TRUE, then the mole fraction plots for compartment i are combined into a single graph with each mole fraction curve indicated by a different line type. Setting COMBXF(i) to TRUE will set PLTXS(i), PLTXN2(i), PLTXO2(i), and PLTXH2(i) to FALSE. If it is desired to plot some of the mole fractions individually, as well as on a combined plot, then the appropriate PLT variables must be reset to TRUE after COMBXF(i) has been set to TRUE.

LEGCXF [L] - <Default = TRUE>
If TRUE, then for combined mole fraction plots, a legend identifying the different mole fraction curves will be placed in the upper right hand corner. In some cases the legend may overlap the curves making it desirable to omit the legend. The gas species indicated by each line type as recorded in the legend are

———— (solid)	steam	(H_2O)
—.—.—.— (chain dot)	nitrogen	(N_2)
— — — — — (chain dash)	oxygen	(O_2)
- - - - - - - (dashed)	hydrogen	(H_2)

NYTIKS [I] - <Default = 5>
Number of tick marks per step to be displayed on the vertical axis of all graphs.

TRPLEX [L] - <Default = FALSE>
If TRUE, then the DISSPLA triplex (fancy, publication quality) alphabet will be used to label the graphs.

PLTDEN(i)* [L] - <Default = TRUE>
If FALSE, then the density versus time graph for compartment i will not be plotted.

PLTPRS(i)* [L] - <Default = TRUE>
If FALSE, then the pressure versus time graph for compartment i will not be plotted.

PLTTMP(i)* [L] - <Default = TRUE>
If FALSE, then the temperature versus time graph for compartment i will not be plotted.

PLTXS(i)* [L] - <Default = TRUE>
If FALSE, then the steam mole fraction versus time graph for compartment i will not be plotted. See also COMBXF(i).

PLTXN2(i)* [L] - <Default = TRUE>
If FALSE, then the nitrogen mole fraction versus time graph for compartment i will not be plotted. See also COMBXF(i).

PLTXO2(i)* [L] - <Default = TRUE>
If FALSE, then the oxygen mole fraction versus time graph for compartment i will not be plotted. See also COMBXF(i).

PLTXH2(i)* [L] - <Default = TRUE>
If FALSE, then the hydrogen mole fraction versus time graph for compartment i will not be plotted. See also COMBXF(i).

*Note that plots for this variable will be produced only if this NAMELIST variable is set to TRUE and the plot is requested in the ACHILES input read from unit UAR.

PMIN [R] - (kilopascals) <Default = 50.>
Minimum pressure displayed on the vertical scale of pressure versus time graphs.

PSTEP [R] - (kilopascals) <Default = 50.>
Pressure stepsize used on the vertical scale of pressure versus time graphs.

PMAX [R] - (kilopascals) <Defaults to an internal calculation>
Maximum pressure displayed on the vertical scale of pressure versus time graphs. If this quantity is not specified, then an appropriate value will be determined directly from the data.

TMIN [R] - (kelvins) <Default = 200.>
Minimum temperature displayed on the vertical scale of temperature versus time graphs.

TSTEP [R] - (kelvins) <Default = 200.>
Temperature stepsize used on the vertical scale of temperature versus time graphs.

TMAX [R] - (kelvins) <Defaults to an internal calculation>
Maximum temperature displayed on the vertical scale of temperature versus time graphs. If this quantity is not specified, then an appropriate value will be determined directly from the data.

4.3.1.4 Table Control Variables

SHOWPT(i) [I] - <Default = 1>
Letting n = SHOWPT(i), entries for the pressure/temperature/density/mole fraction table for compartment i will be printed only on every nth timestep that ACHILES has read from unit UHD.

SHOWSV [I] - <Default = 1>
Letting n = SHOWSV, sump volumes will be printed only on every nth timestep that ACHILES has read from unit UHD.

SHOWWT [I] - <Default = 1>
Letting n = SHOWWT, surface temperatures will be printed only on every nth timestep that ACHILES has read from unit UHD.

SHOWHF [I] - <Default = 1>
Letting n = SHOWHF, heat and mass fluxes will be printed only on every nth timestep that ACHILES has read from unit UHD or UHA.

SHOWSR [I] - <Default = 1>
Letting n = SHOWSR, source information will be printed only on every nth timestep that ACHILES has read from unit UHD.

SHOWSY [I] - <Default = 1>
Letting n = SHOWSY, spray information will be printed only on every nth timestep that ACHILES has read from unit UHD or UHA.

SHOWIC [I] - <Default = 1>
Letting n = SHOWIC, ice-condenser information will be printed only on every nth timestep that ACHILES has read from unit UHD or UHA.

SHOWJV [I] - <Default = 1>
Letting n = SHOWJV, flow junction velocities will be printed only on every nth timestep that ACHILES has read from unit UHF.

SHOWFN [I] - <Default = 1>
Letting n = SHOWFN, fan volumetric flow rates will be printed only on every nth timestep that ACHILES has read from unit UHF.

SHOWSP [I] - <Default = 1>
Letting n = SHOWSP, suppression pool information will be printed only on every nth timestep that ACHILES has read from unit UHF.

Remember to enter a $ in column 1 at the end of the NAMELIST type input!

4.3.2 Tables and Plots

This data is read from unit UAR (UAR is defined in Section 4.3.1.1).

For each type of table that can be produced or graph that can be plotted, it is usually necessary to specify which compartments, flow junctions, surfaces, etc., are to be included. Consider, for example, plots of compartment spray heat-removal rates. Entering an input line beginning with the word ALL will select all possible compartments. Entering an input line beginning with the word NONE will choose no compartments (and so none of these plots will be produced). Often, plots for only some compartments will be desired. These compartments are indicated by numbers read in consecutive I3 formats. For example, if the input line is

```
  1  3  4  5  6  8  9 11 12 13 14 15
```

then compartments 1, 3 through 6, 8, 9, and 11 through 15 are selected. The special symbol ==> (meaning "through") can be used as a shorthand notation so that

```
  1  3==>  6  8  9 11==> 15
```

will choose the same compartments as the previous specification (note that everything is still written in consecutive I3 formats). If in the HECTR simulation there are sprays only in the first ten compartments, then ACHILES will not produce graphs from compartments numbered 11 and above (so that graphs for compartments 11 through 15 in the above example will not appear). If there are no sprays at all in the HECTR run, then no plots of this variable will be created. Similarly, no flow junction velocity tables or graphs will be produced for a single compartment case, etc. The ACHILES input for these items are still required, however. The same comments are generally applicable to all tables and plots. Entering an input line beginning with QUIT will cause ACHILES to quit processing further input (i.e., ACHILES execution will be terminated, and no further tables or plots will be produced). If the input line begins with SKIP, then the input processing will proceed immediately to the beginning of the next section (there are three major sections under both Tables and Plots: Major Heat-Transfer Timestep Variables, Flow Timestep Variables, and Additional Heat-Transfer Timestep Variables). If the input line begins with the word PLOT then the input processing will proceed immediately to the plotting segment of ACHILES. Lines that begin with an exclamation mark (!) are always treated as comments as is any text following an exclamation mark located anywhere in an input line.

4.3.2.1 Tables

The possible tables that can be produced, in order of required input (except when SKIPping or PLOTting), are listed below. See the discussion above for the method used to specify each line of input.

4.3.2.1.1 Major Heat-Transfer Timestep Variables (from unit UHD)

>>>
[1] For each compartment desired, display the pressure (kilopascals), temperature (kelvins), and the various gas mole fractions that were present at the beginning of each timestep. Also, note when combustion was occurring in each compartment by printing a T under the column labeled 'Burn?' (or F, if there were no combustion). In addition, display the overall gas density (kilograms per cubic meter), the total rate (kilograms per second) of hydrogen and steam injected into each compartment, and the quality of the steam injected.

>>>
[2] For each sump desired, display its volume (cubic meters) versus time.

>>>
[3] For each surface desired, display its temperature (kelvins) and note whether water was condensing on it, evaporating from it, or whether the surface was dry (indicated by a C, E, or D respectively).

>>>
[4] For each surface desired, display the condensation rate (kilograms per second) and the liquid film thickness (meters) versus time.

>>>
[5] Display

(1) the total containment injection rates (kilograms per second) for each source gas
(2) the total accumulated masses (kilograms) of each injected source gas
(3) external (MARCH) steam and hydrogen source information (the rate [kilograms per second] that water is transferred to the ECC system; the rate [kilograms per second], quality and total accumulated mass [kilograms] of injected steam; the rate [kilograms per second] and total accumulated mass [kilograms] of injected hydrogen)

versus time. Either 'ALL' or some combination of the numbers in parentheses may be specified.

>>>

[6] For each specified compartment, display the mass-evaporation rate (kilograms per second) from the sprays and the heat-removal rate (watts) by the sprays versus time.

>>>

[7] If desired, display the fraction of the initial ice mass remaining in the ice condenser versus time. Either 'All' or ' 1' are valid entries.

4.3.2.1.2 Flow Timestep Variables (from unit UHF)

>>>

[8] For each flow junction desired, display the gas velocity through it (meters per second) at the beginning of each timestep and note whether the junction was closed and whether flow through the junction was choked (indicated by the two letters following the velocity--a T indicates that a condition was true and an F indicates that a condition was false).

>>>

[9] For each fan connection desired, display the fan volumetric flow rate (cubic meters per second) versus time.

>>>

[10] If desired, display suppression pool information: vent gas volumetric flow rates (cubic meters per second) where 1 is the top vent, 2 is the middle vent, and 3 is the bottom vent; and vertical distances (meters) that the surface of the suppression pool is above the centerline of the bottom vent in the drywell and in the wetwell all versus time. Either 'All' or ' 1' are valid entries.

4.3.2.1.3 Additional Heat-Transfer Timestep Variables (from unit UHA)

>>>

[11] For each surface desired, display the net total heat flux to it (watts per square meter) versus time.

>>>

[12] For each surface desired, display the net radiative heat flux to it (watts per square meter) versus time.

>>>

[13] For each surface desired, display the convective heat flux (including effects due to condensation) to it (watts per square meter) versus time.

>>>

[14] For each surface desired, display the water drainage rate from it (kilograms per second) versus time.

>>>

[15] For each initiating spray compartment desired, display the emitted spray drop temperature (kelvins) versus time.

>>>
[16] If desired, display ice-condenser information: melting rate for each of the ice surfaces (kilograms per second), total rate (kilograms per second) of water falling into the lower plenum, drain temperature (kelvins), condensation rate (kilograms per second) on the water falling through the lower plenum atmosphere, and heat-transfer rate (watts) due to condensation on water falling through the lower plenum atmosphere, all versus time. Either 'ALL' or ' 1' are valid entries.

4.3.2.2 Plots

The possible plots that can be produced, in order of required input (except when SKIPping), are listed below. See the discussion at the beginning of this section for the method used to specify each line of input.

4.3.2.2.1 Major Heat-Transfer Timestep Variables (from unit UHD)

>>>
[1] For each compartment desired, plot the pressure (kilopascals), temperature (kelvins), gas density (kilograms per cubic meter), and the mole fractions of steam, nitrogen, oxygen, and hydrogen versus time.
>>>
Enter data describing the horizontal (time) axis for all graphs. This input must always be entered immediately after the input to [1] above unless the input was QUIT (even if the input was NONE or SKIP).

XMIN [R] - (seconds)
Minimum time to be displayed on each graph.

XSTEP [R] - (seconds)
Timestep size used on the horizontal scale of each graph.

XMAX [R] - (seconds)
Maximum time to be displayed on each graph.

NXTIKS [I] - Number of tick marks per step to be displayed on the horizontal axis of each graph.

>>>
[2] For each sump desired, plot its volume (cubic meters) versus time.

>>>
[3] For each surface desired, plot its temperature (kelvins) versus time.
>>>
[4] For each surface desired, plot the condensation rate on it (kilograms per second) versus time.
>>>
[5] For each surface desired, plot the film thickness on it (meters) versus time.
>>>
[6] Plot

(1) the total containment injection rates (kilograms per second) for each source gas
(2) the total accumulated masses (kilograms) of each injected source gas
(3) external (MARCH) steam and hydrogen source information: the rate (kilograms per second) that water is transferred to the emergency core cooling system; the rate (kilograms per second), quality and total accumulated mass (kilograms) of injected steam; the rate (kilograms per second) and total accumulated mass (kilograms) of injected hydrogen

versus time. Either 'ALL' or some combination of the numbers in parentheses may be specified
>>>
[7] For each compartment desired, plot the mass-evaporation rate (kilograms per second) from the sprays versus time.
>>>
[8] For each compartment desired, plot the heat-removal rate (watts) by the sprays versus time.
>>>
[9] If desired, plot the fraction of the initial ice mass remaining in the ice condenser versus time. Either 'ALL' or ' 1' are valid entries.

4.3.2.2.2 Flow Timestep Variables (from unit UHF)

>>>
[10] For each flow junction desired, plot the velocity (meters per second) versus time.
>>>
[11] For each fan connection desired, plot the volumetric flow rate through it (cubic meters per second) versus time.
>>>
[12] Plot suppression pool information

(1) top vent gas volumetric flow rate (cubic meters per second)
(2) middle vent gas volumetric flow rate (cubic meters per second)

(3) bottom vent gas volumetric flow rate (cubic meters per second)
(4) vertical distance (meters) the surface of the suppression pool is above the centerline of the bottom vent in the drywell
(5) similar to (4), except in the wetwell

versus time. Either 'ALL' or some combination of the numbers in parentheses may be specified.

4.3.2.2.3 Additional Heat-Transfer Timestep Variables (from unit UHA)

>>>
[13] For each surface desired, plot the net total heat flux to it (watts per square meter) versus time.
>>>
[14] For each surface desired, plot the net radiative heat flux to it (watts per square meter) versus time.
>>>
[15] For each surface desired, plot the convective heat flux (including effects due to condensation) to it (watts per square meter) versus time.
>>>
[16] For each surface desired, plot the water drainage rate from it (kilograms per second) versus time.
>>>
[17] For each initiating spray compartment desired, plot the emitted spray drop temperature (kelvins) versus time.
>>>
[18] For each of the four ice surfaces (in an ice condenser) desired, plot its melting rate (kilograms per second) versus time.
>>>
[19] Plot ice-condenser information

(1) total rate (kilograms per second) of water falling into the lower plenum
(2) drain temperature (kelvins)
(3) condensation rate (kilograms per second) on water falling through the lower plenum atmosphere
(4) heat-transfer rate (watts) due to condensation on water falling through the lower plenum atmosphere

versus time. Either 'ALL' or some combination of the numbers in parentheses are valid entries.

4.4 External Interface to Primary System Models (MARCH)

4.4.1 Introduction

As discussed in Section 4.2.3, HECTR can use input tables describing source terms consisting of any of the four gas species treated by the code. However, if a large number of scenarios are being considered, then providing this input may become very time-consuming. Because of this problem, we have developed an interface to a primary system model that allows a much more convenient treatment of sources and ECC recirculation.

The particular interface in HECTR was developed for the MARCH code, but the same approach can be used for other primary system codes. The approach used is relatively straightforward. The primary system code simply produces a file containing the pertinent information that HECTR then reads. It is not required that the codes be intimately coupled and run in parallel. This assumes that the containment response does not affect the primary system response. The details of the interface are provided below.

4.4.2 Details of the External Interface

The HECTR subroutines IMARCH and MARCHI act as the interface for source term input provided by external primary system computer codes. These subroutines read an output file written in a specific format that has been generated by one of these codes. Normally, the user will have to modify the primary system code to create this file. This section will describe the format of the file required by HECTR and additional details regarding the usage of the external interface.

The first line of the external file is assumed to be a title identifying the contents of the file. IMARCH reads this label and then prints it out noting that this line is "FROM MARCH". IMARCH then initializes the variables for the interface. The rest of the file should consist of a time history of steam and hydrogen source terms being injected into the containment from the primary system, their corresponding enthalpies, and the rate of water being recirculated into the emergency core cooling system (ECCS) from a designated containment sump. The actual variables read by HECTR, in order, are

NTIME [R] - (seconds)
The absolute time specifying the end time for this step (see discussion below).

NDNH2 [R] - (kilograms per second)
Rate of injection of hydrogen from the primary system for this step.

NDNH2O [R] - (kilograms per second)
Rate of injection of steam from the primary system for this step.

NHH2 [R] - (joules per kilogram)
Enthalpy of the hydrogen source for this step. This enthalpy is based on steam tables (i.e., the enthalpy is zero at 273.15 K or 0°C).

NHH2O [R] - (joules per kilogram)
Enthalpy of the steam source for this step. This enthalpy is based on steam tables (i.e., the enthalpy is zero at 273.15 K or 0°C).

NECCRR [R] - (kilograms per second)
The rate at which water is recirculated into the emergency core cooling system from containment. This water is drawn from the spray recirculation sump (SPRSRC, defined in Section 4.2.2.10).

The external file represents a set of step functions with time as the abscissa. The value taken for each variable at a time within a given step is the value it has at the end of the step. The variables are read as needed in list-directed format in the subroutine MARCHI. MARCHI is entered on every flow timestep at the simulation time specified by the HECTR variable TIME. If TIME is greater than NTIME, then new values of the variables will be read and the old values will be saved in the variables OTIME, ODNH2, ODNH2O, OHH2, OHH2O, and OECCRR. This last action will be repeated until a value of NTIME is encountered that is greater than or equal to TIME. The new values of the variables are then used in the HECTR conservation equations until the next step is crossed. This method of choosing values is appropriate for output received from the MARCH computer code, but may have to be modified by the user for output received from other primary systems codes (for example, the user may wish to interpolate the values between OTIME and NTIME). If an end-of-file occurs, then the last values read by MARCHI will be used for HECTR times greater than the last time read into NTIME.

By default, HECTR assumes that there is no external input. This assumption can be overridden by assigning a nonzero value to the pseudo-NAMELIST variable MRCHSC (see Section 4.2.3.6.4). A positive integer is used to indicate the number of the compartment into which the external source is to be injected. A second pseudo-NAMELIST variable, UMI (see Section 4.2.1.1), specifies the unit from which the external source input is to be read. The value of this variable

defaults to 1. Appendix C shows some examples of control language on various computers that can be used to access an external source file.

4.4.3 An Example External Source File

In this section, we present a sample external source file. The number of entries in the table has been greatly reduced for simplicity from what would normally be expected in a file generated by a primary system code. This external source file is the same one that was used in the sample problem presented in Section 6.2. These values are fairly typical of what one would expect for a small-break LOCA in a PWR with ECC failure. Notice that the steam source starts at zero seconds, while the hydrogen source does not start until 3000 seconds later (remember that the value of a quantity over a table interval is the value that it has at the end of the interval).

```
***  EXAMPLE EXTERNAL SOURCE FILE  ***
0.0     0.     90.    0.            1.376E+06   0.
2000.   0.     85.    0.            1.339E+06   0.
2500.   0.     20.    0.            2.712E+06   0.
3000.   0.     24.    0.            2.845E+06   0.
4000.   0.1    15.    1.2649E+07    2.847E+06   0.
5000.   0.4    20.    5.9449E+06    2.670E+06   0.
6000.   0.1    6.0    4.1966E+06    2.617E+06   0.
7000.   0.05   2.0    3.9140E+06    2.689E+06   0.
```

5. OUTPUT DESCRIPTION

5.1 HECTR Output

The output produced by HECTR can be classified into several major categories. There is the output generated by echoing the HECTR input when the pseudo NAMELIST variable BATCH has been set equal to TRUE. There are error (and warning) messages, informative messages, and a final run summary. In addition, HECTR creates data files containing the time histories of important variables. These files are processed by ACHILES in order to produce tables and plots. The HECTR output is discussed in the following subsections.

5.1.1 Error and Warning Messages

HECTR has many internal checks throughout the program. These checks are designed to give the user indications of trouble as it occurs and to terminate HECTR (with the usual run summary information printed) before a FORTRAN fatal error occurs. HECTR will print a message if a fatal error occurs and will print a warning if a nonfatal error occurs. Warnings (if there are any) are summarized at the end of a run. Fatal errors will cause HECTR to terminate, but a traceback will be produced listing the name of each program unit that was in the calling sequence of the program unit where the error occurred. Following the traceback, a summary of the run (see Section 5.1.3) up to the point where the fatal error occurred will be produced.

The warning and error messages that can be produced by HECTR are shown below. Each message is reproduced exactly as it would appear if printed by HECTR. Real numbers, integers, and character strings that are determined at run time are indicted by strings of lower case x's, y's, z's, w's, and v's; n's, m's, and k's; and a's, b's, and c's, respectively. All of the messages identify the program unit that wrote them and have been listed below alphabetically by program unit. Following each message is a short discussion of the error. This discussion may include possible causes and remedies for the error as well as an explanation of the message (if it is not obvious).

5.1.1.1 CHECK

*** CHECK: TRYING TO DUMP RUNOFF FROM SURFACE nnn
INTO A NONEXISTENT SUMP (mmm) ***

The user specified that the water running off surface nnn should be transferred to a sump that does not exist. This is probably due either to forgetting to define a sump or to mistyping. Note that this message will not appear if zero is specified as the sump number. Zero is an acceptable input that causes the runoff to disappear from the system.

5.1.1.2 CONTRL

*** CONTRL: AT TIME = xxxxx.xxx SECONDS, NMOLES(nn,m) =
yy.yyyyyyy ***

The number of moles of component m (1 = steam, 2 = nitrogen, 3 = oxygen, 4 = hydrogen) in compartment nn was calculated to be less than zero at the time indicated. The calculation was being performed with the minimum timestep specified by the user. This is probably the result of computer roundoff error. Try repeating the calculation on a computer with greater accuracy. This error may also occur if the final fraction of hydrogen to be left at the end of a burn in this compartment (FNLFH2(nn)) has been set to zero (each burn is 100% complete) and HECTR extrapolated the new number of moles near the end of a burn too low. In this case, it is necessary to reset FNLFH2(nn) to a small but nonzero value and rerun the problem.

*** CONTRL: BULK TEMPERATURE IN COMPARTMENT nn IS OUT OF THE
PROPERTY TABLE RANGE - TNEW = xx.xxxxxxxxx ***

The new compartment temperature was greater than 4000 K or less than 200 K. Since this is outside the HECTR table range, the calculation was stopped.

*** CONTRL: CONVERGENCE FAILURE ON TEMPERATURE ITERATION ***

The iteration used to calculate the compartment temperature from the internal energy of the compartment failed to converge. This error should not be encountered and indicates a logic error in HECTR.

*** CONTRL: FLOW REVERSAL PROBLEM AT TYME = xxxxx.xxx
SECONDS IN CONNECTION nnn OLD AND NEW FLOWS =
yy.yyyyyyyy AND zz.zzzzzzzz ***

Five attempts were made to calculate a new solution using the minimum timestep, but the flow directions assumed to exist at the end of the timestep did not match the calculated directions. One possible solution is to reduce the minimum flow timestep.

*** CONTRL: FLOW TIME STEP IS SMALLER THAN yy.yyyyyyyy MORE
THAN 1000 TIMES TYME = xxxxx.xxx SECONDS ***

The flow timesteps used by HECTR have been smaller than the minimum flow timestep specified by the user (DTFLMN) more than 1000 times. Either reduce the minimum timestep or loosen the constraints governing the step size.

*** CONTRL: HEAT TRANSFER TIME STEP IS SMALLER THAN
yy.yyyyyyyy MORE THAN 1000 TIMES - TYME =
xxxxx.xxx SECONDS ***

The heat-transfer timesteps used by HECTR have been smaller than the minimum heat-transfer timestep specified by the user (DTHTMN) more than 1000 times. Either reduce the minimum timestep or loosen the constraints governing the step size.

*** CONTRL: IFLUG FROM FZERO = nn, TYME = xxxxx.xxx,
JUNCTION = mmm ***

An error has occurred in trying to calculate the door angle for flow junction mmm. The door angle is determined by solving for the root of Eq. A-17 (this equation is specified by the function DOOR). The status code returned by the root finder (FZERO) and the current simulation time are displayed.

*** CONTRL: KCNT = 50 FOR COMPARTMENT nn - PPS = xx.xxxxxxxxx
PP = yy.yyyyyyyyy, POLD = zz.zzzzzzzzz, PNEW =
ww.wwwwwwwww ***

The iteration used to calculate the steam partial pressure failed to converge after 25 passes using a replacement method and 50 passes using a bisection method.

*** CONTRL: TNEW(nn) IS LESS THAN 273.15 AND THE HEAT TRANSFER TIME STEP (xx.xxxxxxx) IS LESS THAN OR EQUAL TO ITS MINIMUM (yy.yyyyyyy) ***

The new compartment temperature was less than 273.15 K using the minimum heat-transfer timestep. This may occur at the beginning of calculations in ice condensers. Try increasing the initial temperature slightly or including the gravity heads in the initial pressures (see Chapter 3). In some cases, it may help to tighten the flow timestep constraints governing the amount of outflow from a compartment.

5.1.1.3 CONVCT

*** CONVCT: RANGE OF PHYSICAL DATA EXCEEDED AT TIME = xxxxx.xxx SECONDS FOR SURFACE nn IN COMPARTMENT mm OF TYPE kk SURFACE TEMP = yyyyyy.yyy FOR LIQUID SURFACE ***

A pool or liquid film temperature has exceeded the maximum allowed value of 470 K.

*** CONVCT: RANGE OF PHYSICAL DATA EXCEEDED AT TIME = xxxxx.xxx SECONDS FOR SURFACE nn IN COMPARTMENT mm OF TYPE kk TI = yyyyyy.yyy, TBULK = zzzzzz.zzz, PPS = ww.wwwwwwwww ***

One of the listed parameters is outside the allowable bounds. This message will appear when TI < 273, TBULK > 2500, or PPS > 1455000.

5.1.1.4 GET

*** GET: ERROR ON READING ITEM NUMBER nn OF mm REQUESTED VALUES *** >aaaaaaaaaa<

The nnth of mm values on a numerical user-input record was not a number. The input line in which this error was detected is displayed below the message.

*** GET: INVALID USE OF AN ASTERISK IN THE LAST INPUT LINE *** >aaaaaaaaaa<

A replication factor was formed improperly on the numerical user input (see Section 4.1). The line in which this error occurred is displayed below the message.

*** GET: UNEXPECTED END-OF-FILE ON UNIT nn ***

An end-of-file occurred unexpectedly on the numerical user input.

*** GET: WARNING - EXCESS VALUES ON THE LAST INPUT LINE ***
>aaaaaaaaaa<

The last numerical user-input record contained more values than expected. These excess values will be ignored. The input line in which this problem was detected is displayed below the message. This problem is often a result of entering too few values for an earlier input request (or ignoring a request entirely) so that HECTR will have started reading the next input record to fill in the missing values, causing all subsequent input to be misaligned.

5.1.1.5 HECTR

*** HECTR: ERROR ON TRYING TO OPEN UNIT nn
ERROR MESSAGE NUMBER = mmmmm ***

An error has occurred in opening one of the HECTR input or output units 5, URD, UIC, or UOM (these are defined in Section 4.2.1). This is often the result of a missing file or of not declaring or attaching the file properly in the control language. The meaning of the error message number can usually be found in a system messages manual.

*** HECTR: RETURN FROM FZERO WITH IFLAG = nn
AT TIME = xxxxx.xxx SECONDS IN COMPARTMENT mm ***

An error has occurred in trying to find the equilibrium temperature for spray drops falling through compartment mm. The equilibrium temperature is determined by solving for the root of Eq. A-72 when it is set equal to zero (this equation is specified by the function TLAST). The status code returned by the root finder (FZERO) and the current simulation time are displayed.

5.1.1.6 IMARCH

*** IMARCH: ERROR ON TRYING TO OPEN UNIT nn
ERROR MESSAGE NUMBER = mmmmm ***

An error has occurred in opening the unit from which external (MARCH) input is read (UMI). This is often the result of a missing file or of not declaring or attaching the file properly in the control language. The meaning of the error message number can usually be found in a system messages manual.

5.1.1.7 INIOUT

*** INIOUT: ERROR ON TRYING TO OPEN UNIT nn
ERROR MESSAGE NUMBER = mmmmm ***

An error has occurred in opening one of the HECTR output units UOH, UOF, or UOA (these are defined in Section 4.2.1.2). This is often the result of a missing file or of not declaring or attaching the file properly in the control language. The meaning of the error message number can usually be found in a system messages manual.

5.1.1.8 INITAL

*** INITAL: THE TOTAL NUMBER OF WALL NODES REQUESTED THROUGH SURFACE nn HAS EXCEEDED THE MAXIMUM AVAILABLE (mmmm) ***

The total number of nodes available for all slab surfaces has been exceeded by the number needed for surfaces 1 through nn. This limit is controlled by the symbolic parameter NWN. See Section B.2.7.

5.1.1.9 INPUT1

*** INPUT1: ERROR ON CREATING ICE CONDENSER COMPARTMENTS ***

The maximum number of compartments, flow junctions, or surfaces allowed by HECTR has been exceeded by HECTR while attempting to generate the compartmentalization for the ice-bed region in an ice-condenser containment. The actual limit that was exceeded is indicated by an appropriate message (see below).

*** INPUT1: MAXIMUM ALLOWED NUMBER OF COMPARTMENTS (nn) HAS BEEN EXCEEDED ***

The maximum allowed number of compartments has been exceeded by the input. This limit is controlled by the symbolic parameter NC. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF COMPARTMENTS ORIGINATING SPRAYS (nn) HAS BEEN EXCEEDED ***

The maximum allowed number of compartments in which sprays originate has been exceeded by the input. This limit is controlled by the symbolic parameter NSC. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF DOORS (nn) HAS BEEN EXCEEDED ***

The maximum allowed number of inertial valve flow junctions (doors) has been exceeded by the input. This limit is controlled by the symbolic parameter ND. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF DRAINS (n) HAS BEEN EXCEEDED ***

The maximum allowed number of drains between the upper and lower compartments in an ice-condenser containment has been exceeded by the input. This limit is controlled by the symbolic parameter NDR. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF DROP SIZES (nn) HAS BEEN EXCEEDED IN COMPARTMENT mm ***

The maximum allowed number of spray drop sizes has been exceeded by the input for the indicated compartment. This limit is controlled by the symbolic parameter NDS. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF FAN HEAD CURVE ENTRIES (11) HAS BEEN EXCEEDED ***

The maximum allowed number of entries for the user-specified fan head curve table has been exceeded.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF FANS (nn) HAS BEEN EXCEEDED ***

The maximum allowed number of fan paths has been exceeded by the input. This limit is controlled by the symbolic parameter NF. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF FLOW JUNCTIONS (nnn) HAS BEEN EXCEEDED ***

The maximum allowed number of flow junctions has been exceeded by the input. This limit is controlled by the symbolic parameter NJ. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF SUMPS (nn) HAS BEEN EXCEEDED ***

The maximum allowed number of sumps has been exceeded by the input. This limit is controlled by the symbolic parameter NSMP. See Section B.2.7.

*** INPUT1: MAXIMUM ALLOWED NUMBER OF SURFACES (nnn) HAS BEEN EXCEEDED ***

The maximum allowed total number of surfaces has been exceeded by the input. This limit is controlled by the symbolic parameter NS. See Section B.2.7.

*** INPUT1: THE NUMBER OF SLAB LAYERS FOR SURFACE nn HAS EXCEEDED THE MAXIMUM ALLOWABLE NUMBER (mm) ***

The maximum allowed number of layers per slab surface has been exceeded by the input for the indicated surface. This limit is controlled by the symbolic parameter NLAYER. See Section B.2.7.

*** INPUT1: WARNING - ROW nnn OF THE VIEW FACTOR MATRIX HAS A SUM OF x.xxxxx **

The entries in the nnnth row of the radiation view factor matrix do not add up to within .001 of 1. If the sum of the entries in any given row of this matrix does not add up to 1 (or very close to 1), HECTR will not conserve energy in the radiation calculations and can produce unphysical behavior. See Section 3.7.

5.1.1.10 INPUT2

*** INPUT2: MAXIMUM ALLOWED NUMBER OF LEAK ENTRIES (nnn) HAS BEEN EXCEEDED BY SUMP mm ***

The maximum allowed number of entries for a water leakage table has been exceeded by the entries for sump mm. This limit is controlled by the symbolic parameter NSE. See Section B.2.7.

*** INPUT2: MAXIMUM ALLOWED NUMBER OF SOURCE ENTRIES (nnn) HAS BEEN EXCEEDED IN LOCATION mmm FOR GAS SPECIES k ***

The maximum allowed number of entries in the source array of gas species k (k = 1 for steam, 2 for nitrogen, 3 for oxygen, and 4 for hydrogen) has been exceeded by the source term entries for compartment mmm (all of the source tables from various compartments are stacked together in a single array for each gas species). This limit is controlled by the symbolic parameter NSE. See Section B.2.7. Note that if mmm is negative, then -mmm is actually the number of a sump.

5.1.1.11 LOOK

```
*** LOOK: NUMBER OUT OF RANGE   xxxxxxx.xxxx <=
          yyyyyyy.yyyy < zzzzzzz.zzzz VARIABLE aaaaaa
          IN ROUTINE bbbbbb ***
```

The value yyyyyyy.yyyy cannot be used by LOOK to interpolate the property table aaaaaa because it lies outside the range of the property table (the range is from xxxxxxx.xxxx to zzzzzzz.zzzz). LOOK was called from the program unit bbbbbb. This error is a symptom of other problems in HECTR that caused yyyyyyy.yyyy (usually a gas temperature) to be outside its normal range.

5.1.1.12 MELTHT

```
*** MELTHT: TBULK < TICE.  TBULK = xx.xxxxxxxx,
            TICE = yy.yyyyyyyy ***
```

The model that calculates the heat transfer to the liquid that drains into the lower plenum from the ice bed assumes that the lower-plenum temperature is greater than the ice temperature. If this assumption is violated, the calculation cannot be performed without revising HECTR.

5.1.1.13 NAMLST

```
*** NAMLST: bbbbbb HAS THE WRONG NUMBER OF SUBSCRIPTS (SHOULD
            EITHER HAVE n OR NONE) ***
>aaaaaaaaaa<
```

The pseudo-NAMELIST variable indicated has the wrong number of subscripts (it should either have the number indicated or no subscripts at all). The entry in which this error occurred is displayed below the message.

```
*** NAMLST: BAD INDEX OR VALUE FOR ENTRY ***
>aaaaaaaaaa<
```

A subscript or a "numerical" value that was supposed to be assigned to a pseudo-NAMELIST variable was not a number. The entry in which this error occurred is displayed below the message.

*** NAMLST: EITHER NICEC IS LESS THAN OR EQUAL TO ZERO OR
NICEC IS GREATER THAN THE MAXIMUM ALLOWED NUMBER
OF ICE COMPARTMENTS (n) ***

The pseudo-NAMELIST variable specifying the number of compartments to be automatically generated by HECTR for the ice-bed region of an ice condenser (NICEC) must not be set to a value less than one or greater than the value of the symbolic parameter NICE (see Section B.2.7).

*** NAMLST: ENTRY HAS MORE THAN THE MAXIMUM ALLOWED NUMBER OF
SUBSCRIPTS (n) ***
>aaaaaaaaaa<

The pseudo-NAMELIST entry has too many subscripts to be processed. The pseudo-NAMELIST variables in HECTR currently have at most one subscript. The entry is displayed below the error message.

*** NAMLST: ENTRY IS IMPROPERLY FORMED ***
>aaaaaaaaaa<

The pseudo-NAMELIST entry was improperly formed. The entry is displayed below the error message.

*** NAMLST: IMPROPER VARIABLE NAME => bbb ***
>aaaaaaaaaa<

The pseudo-NAMELIST variable name is missing or is longer than 6 characters. The entry in which this error occurred is displayed below the message.

*** NAMLST: INVALID STATUS (cccc) FOR bbbbbb ***
>aaaaaaaaaa<

The pseudo-NAMELIST variable indicated was not assigned the value OFF, ON, or AUTO. The entry in which this error occurred is displayed below the message.

*** NAMLST: LOGICAL VARIABLE (bbbbbb) MUST HAVE A VALUE OF
EITHER "TRUE" OR "FALSE" ***
>aaaaaaaaaa<

The logical pseudo-NAMELIST variable indicated was not assigned a value of TRUE or FALSE. The entry in which this error occurred is displayed below the message.

*** NAMLST: UNKNOWN COMPUTER TYPE => bbbbb ***
>aaaaaaaaaa<

The pseudo-NAMELIST variable CMPUTR was not assigned the value CDC, CYBER, CRAY, or VAX. The entry in which this error occurred is displayed below the message.

*** NAMLST: UNRECOGNIZED NAME => bbbbbb ***
>aaaaaaaaaa<

The name of the pseudo-NAMELIST variable was not one of the names expected (see Sections 4.2.1 and 4.2.3 for lists of the pseudo-NAMELIST variables in HECTR). The entry in which this error occurred is displayed below the message.

5.1.1.14 NUMBER

*** NUMBER: BAD NUMBER FOUND ON INPUT: aaa ***

NUMBER was given a character string to translate instead of a number. This error can result from deleting lines from or adding extra lines to the input (so that a word was read where a number was expected) as well as from mistyping.

*** NUMBER: NUMBER IS MORE THAN 20 CHARACTERS LONG:
aaaaaaaaaaaaaaaaaaaa ***

NUMBER cannot process numbers with string representations that are greater than 20 characters long. This error can result from deleting lines from or adding extra lines to the input (so that a word was read where a number was expected) as well as from mistyping.

5.1.1.15 NUMSTR

*** NUMSTR: BAD ARGUMENT (nnnnn) ***

NUMSTR cannot process numbers less than or equal to zero or greater than or equal to 1000. This error should not occur and indicates a HECTR logic error.

5.1.1.16 RADIAT

*** RADIAT: SYSTEM OF RADIOSITY EQUATIONS IS SINGULAR

The linear system of equations that determine the radiosities (Eq. A-44) is singular. The radiosities are used in the radiant heat exchange calculations.

*** RADIAT: TEMPERATURE IN COMPARTMENT nn (xxxx.x) IS < 273 ***

The gas temperature in the indicated compartment is less than 273 K. The Cess-Lian correlation for steam emittance, used by the HECTR radiative heat-transfer model (see Table A-3), is not defined for temperatures less than 273 K.

5.1.1.17 SOLVE

*** SOLVE: RCOND = y.yyyyyyy AT TIME = xxxxx.xxx ***

The reciprocal condition number of the matrix A (defined in Eq. A-13) is less than or equal to 10^{-10} at the indicated time in the simulation. The linear system of equations A dy = b is the linearized implicit formulation of the conservation equations used in HECTR. If the reciprocal condition number of A is very small (and so the condition number of A is very large), then A is ill-conditioned and there may be a loss of accuracy in the solution of the linear system of equations.

5.1.1.18 SPHE

*** SPHE: 1000 ITERATIONS REQUIRED ***

The iterative heat exchanger model has not converged after 1000 iterations. It is likely that unreasonable numbers are being passed into subroutine SPHE. Check the heat exchanger input parameters and the sump temperature.

*** SPHE: EXCESSIVE TEMPERATURE FOR TS2 (xxxxxx.xxx) ***

The exit temperature for the secondary side water in the heat exchanger has exceeded the maximum allowed value of 454 K. Check the heat exchanger input parameters and the sump temperature.

5.1.1.19 SPOOL

*** SPOOL: RCOND = x.xxxxxxx FROM SGECO ***

The reciprocal condition number is less than or equal to 10^{-10} for the matrix that defines the linear system of equations that is solved to give the rate of change of the suppression pool velocities. This means that the matrix is ill-conditioned and there may be a loss of accuracy in solving for the suppression pool water velocities.

5.1.1.20 SPRAY

*** SPRAY: DROP TEMPERATURE (yyyyyy.yyy) > SATURATION
TEMPERATURE (zzzzzz.zzz) EVALUATED AT THE
BULK PRESSURE AT TIME = xxxxx.xxx SECONDS IN
COMPARTMENT nn FOR DROP SIZE mm ***

The drop temperature is such that boiling or flashing should occur, and the spray model is no longer valid.

*** SPRAY: IDID = nnn, ISPR = mm, INT = k, TIME = xxxxx.xxx
VALUE(1) = yy.yyyyyyy ***

A problem has occurred integrating the ordinary differential equations that describe a falling spray drop. The status code returned by the integrator (DERKF), the index of the drop in the spray drop distribution, the integration strategy currently being used, the current simulation time, and the value of the drop mass returned by the integrator are displayed. The integration strategy can have one of three values: 2 if integrating drop mass and temperature equations simultaneously, 1 if integrating the drop mass equation only (the drop has come to an equilibrium temperature), and 0 if integrating the transformed drop mass equation (see Eq. A-74 and discussions in Chapter 3).

*** SPRAY: MODEL IS NOT VALID IN COMPARTMENT nn AT TIME =
xxxxx.xxx SECONDS WITH XS = y.yyyy ***

The spray model is valid for air/steam mixtures only. Pure steam models are not provided, and the calculation will terminate when the mole fraction of steam (XS) exceeds 0.99.

*** SPRAY: PRESSURE IS OUT OF RANGE AT TIME = xxxxx.xxx
SECONDS IN COMPARTMENT nn - P = yy.yyyyyyyy,
PPS = zz.zzzzzzzz ***

The bulk pressure has exceeded 2000000 Pa, which is the limit for the spray model.

5.1.1.21 SPRAY2

*** SPRAY2: YP(1) = 0 AT Z = xx.xxxxxxx, Y(1) = yy.yyyyyyy
Y(2) = zz.zzzzzzz ***

The derivative of the mass (and temperature) of a spray drop with respect to the distance it has fallen is zero. The current values of the fall distance, the drop's mass, and its temperature are displayed. If these two derivatives are zero, then the ordinary differential equation solver that is integrating the equations in SPRAY2 (DERKF) may not operate as efficiently and correctly as it should.

5.1.1.22 SUBC

*** SUBC: ICNT = 1000 - TSAT = xx.xxxxxxxxxxx, TBULK(nn) =
yy.yyyyyyyyyyy TSATN = zz.zzzzzzzzzzz, TNEW =
ww.wwwwwwwwwww, X = vv.vvvvvvvvv ***

The routine that removes excess steam from a supersaturated compartment (nn) has failed to converge after 1000 iterations. TSAT is the saturation temperature based on the original amount of steam, TBULK is the original gas temperature, TSATN and TNEW are the saturation temperature and gas temperature after removing the specified amount of steam, and X is the fraction of steam removed from the compartment (the variable of iteration).

*** SUBC: KCNT = 50 - PPNEW = xx.xxxxxxxxxx, PZ =
yy.yyyyyyyyyy, I = nn TNEW = zz.zzzzzzzzzz,
PL = ww.wwwwwwwwww, PR = vv.vvvvvvvvvv ***

The iteration used to calculate the steam partial pressure failed to converge after 25 passes using a replacement method and 50 passes using a bisection method.

*** SUBC: PPNEW = xx.xxxxxxxxxx, PP(nn,1) =
yy.yyyyyyyyyy ***

The partial pressure of steam has been reduced to 611 Pa or less, but the atmosphere is still supersaturated. HECTR will not remove any more steam at this point. This problem should occur only when the gas temperature is below about 274 K.

5.1.1.23 SUMPUP

*** SUMPUP: FLASHING IN SUMP nn CAUSES VOLUME IN COMPARTMENT
TO CHANGE MORE THAN 5 PERCENT - NEED TO UPGRADE
HECTR MODELS BEFORE THIS CASE CAN BE RUN ***

The sump model assumes that if some sump water is boiled, the amount will be small enough to give less than a 5% change in the compartment volume. If a larger volume change is predicted on a timestep, the calculation cannot be completed. Possible solutions are reducing the timestep size, charging the compartmentalization, or upgrading HECTR.

** SUMPUP: GOT INTO INFINITE LOOP DURING SUMP OVERFLOW ***

This error indicates that there was a problem when spilling water from one sump into another. This most likely results from specifying a recursive overflow path (e.g., Sump 1 overflowing into Sump 2, which overflows into Sump 3, which is allowed to overflow back into Sump 1).

*** SUMPUP: MNEW LESS THAN 0 BECAUSE ADDING TOO MUCH ENERGY
MNEW = xx.xxxxxxxx ***

A negative value was calculated for a sump mass because the amount of energy added to the sump during the timestep was larger than the amount needed to boil all of the water in the sump. This error should not occur and indicates a HECTR logic error.

*** SUMPUP: MNEW LESS THAN 0 BECAUSE REMOVING TOO MUCH MASS
MNEW = xx.xxxxxxxx ***

A negative value was calculated for a sump mass because too much water was removed from the sump. This error should not occur and indicates a HECTR logic error.

*** SUMPUP: SUMP nn IS BELOW FREEZING AT TIME = xxxxx.xxxx
SECONDS WITH TSNEW = yy.yyyyyyyy ***

A sump temperature was calculated to be less than 273 K at the indicated time.

5.1.1.24 TLAST

*** TLAST: SPRAY MODEL IS NOT VALID FOR XS = x.xxxx ***

The spray model is valid for air/steam mixtures only. Pure steam models are not provided, and the calculation will terminate when the mole fraction of steam (XS) exceeds 0.99.

5.1.2 Informative Messages

HECTR will write informative messages whenever important events occur. The informative messages that can be produced by HECTR are shown below. Each message is reproduced exactly as it would appear if printed by HECTR. Real numbers, integers, and character strings that are determined at run time are indicated by strings of lower case x's, y's, and z's; n's; and a's, respectively. The messages are listed below alphabetically by topic, except that those describing initial conditions are presented first. Following each message is a short discussion of its meaning. Additional informative messages, providing a run summary, are produced at the end of a HECTR run. This summary is discussed separately in Section 5.1.3.

********** FROM MARCH **********
aaaaaaaaaa
****

The first line read from the external (MARCH) source file is displayed. This line will normally be a title identifying the contents of the file. This message will appear only if MRCHSC has been set to a compartment number in the NAMELIST-type input (Section 4.2.3.6).

INITIAL COMPARTMENT CONDITIONS AT xxxxx.xxx SECONDS ARE:

COMP # TEMP PRESSURE XH2O XN2 XO2 XH2

The initial gas temperature (K), pressure (kPa), and gas mole fractions present in each compartment are displayed. The initial time is TIMZER.

INITIAL SURFACE TEMPERATURES (K) ARE:

The initial surface temperatures (K) are displayed.

BURN INITIATED IN COMPARTMENT nn AT TIME = xxxxx.xxx SECONDS

COMPARTMENT CONDITIONS AT xxxxx.xxx SECONDS ARE:

COMP # TEMP PRESSURE XH2O XN2 XO2 XH2

A burn has started (either through ignition or propagation) in compartment nn at the indicated time in the simulation. The gas temperature (K), pressure (kPa), and gas mole fractions present in each compartment at this time are displayed.

BURN COMPLETED IN COMPARTMENT nn AT TIME = xxxxx.xxx SECONDS

COMPARTMENT CONDITIONS AT xxxxx.xxx SECONDS ARE:

COMP # TEMP PRESSURE XH2O XN2 XO2 XH2

A burn was completed in compartment nn at the indicated time in the simulation. The gas temperature (K), pressure (kPa), and gas mole fractions present in each compartment at this time are displayed.

****

* DETONABLE CONCENTRATION PRESENT IN COMPARTMENT nn AT TIME = xxxxx.xxx

****

A detonable concentration (hydrogen mole fraction > .14, oxygen mole fraction > .09, and steam mole fraction < .30) is present in compartment nn at the indicated time in the simulation. HECTR does not treat detonations other than to note when detonable concentrations are present.

*** DETONABLE CONCENTRATION NO LONGER PRESENT IN COMPARTMENT nn (TIME = xxxxx.xxx SECONDS) ***

A detonable concentration (see previous message) is no longer present in compartment nn at the indicated time in the simulation.

****
* FAILURE PRESSURE (yyyy.y KPA) EXCEEDED IN COMPARTMENT nn AT TIME = xxxxx.xxx
****

The user-specified failure pressure has been exceeded by the pressure in compartment nn at the indicated time in the simulation. This message will not be printed more than once in a run. HECTR will take no action if the failure pressure is exceeded other than to print this message.

FANS WILL BE ACTIVATED AT xxxxx.xxx SECONDS DUE TO TBULK = yyyy.y AND PKPA = zzzz.z IN COMPARTMENT nn

The fans will be activated at the indicated time (time triggered plus delay time) due to the temperature or the pressure in compartment nn exceeding a user-specified set point. This action will occur only if the fans are in AUTO mode.

HEAT EXCHANGER FOR SUMP mm WILL BE ACTIVATED AT xxxxx.xxx SECONDS DUE TO TBULK = yyyy.y AND PKPA = zzzz.z IN COMPARTMENT nn

The heat exchanger for sump mm will be activated at the indicated time (time triggered plus delay time) due to the temperature or the pressure in compartment nn exceeding a user-specified set point. This action will occur only if the heat exchanger is in AUTO mode.

SPRAYS WILL BE ACTIVATED AT xxxxx.xxx SECONDS DUE TO TBULK = yyyy.y AND PKPA = zzzz.z IN COMPARTMENT nn

The sprays will be activated at the indicated time (time triggered plus delay time) due to the temperature or the pressure in compartment nn exceeding a user-specified set point. This action will occur only if the sprays are in AUTO mode.

SPRAYS WILL BE SWITCHED TO RECIRCULATION AT xxxxx.xxx SECONDS (yyyyy.yyy SECONDS AFTER BEING ACTIVATED)

The sprays will be switched to recirculation mode at the indicated time. The second number is the time that the sprays spend in injection phase (TINJ). This message immediately follows the previous message.

5.1.3 Run Summary

At the end of each run, HECTR will produce a summary of final conditions, maximums, and totals that occurred during the run. This summary is presented below. All messages are reproduced exactly as they appear when printed from HECTR. Real numbers, integers, and character strings that are determined at run time are indicated by strings of lower case x's, n's, and a's, respectively. Examples of run summaries can be found in Chapter 6.

The beginning of the run summary is indicated by the message

```
################################################################################
########################## END OF HECTR RUN ###################################
################################################################################
```

This is followed by a table that lists the number of burns that ignited or propagated into each compartment.

SUMMARY OF BURNS:

nnn BURN(S) OCCURRED IN COMPARTMENT nnn

. . .

The entries for any compartments in which there were no burns will not be printed. If there were no burns in any compartment, then HECTR will print the message

NO BURNS OCCURRED IN ANY COMPARTMENT

The global pressure and gas temperature maximums that were produced during the run and the times at which they occurred are shown next.

```
>>> GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS <<<

>>> xxxxx.xxx SECONDS              xxxx.x KPA <<<
>>> xxxxx.xxx SECONDS              xxxx.x K   <<<
```

If the failure pressure was exceeded anytime during the run, then the message

*** THE FAILURE PRESSURE (xxxx.x KPA) WAS EXCEEDED DURING THIS RUN ***

will be printed. The number in parentheses is the failure pressure. HECTR will next produce a set of three tables. The first two tables list, by compartment, the maximum pressures and gas temperatures that occurred during the run.

COMPARTMENT PRESSURE MAXIMUMS (KPA):

1. xxxx.x 2. xxxx.x 3. xxxx.x 4. xxxx.x 5. xxxx.x
. . .

COMPARTMENT TEMPERATURE MAXIMUMS (K):

1. xxxx.x 2. xxxx.x 3. xxxx.x 4. xxxx.x 5. xxxx.x
. . .

The third table shows the maximum surface temperatures (listed for each surface) that were achieved during the run.

SURFACE TEMPERATURE MAXIMUMS (K):

1. xxxx.x 2. xxxx.x 3. xxxx.x 4. xxxx.x 5. xxxx.x
. . .

A table is produced next that provides information about the masses of the HECTR components.

TOTAL MASSES	WATER+ICE	STEAM	NITROGEN	OXYGEN	HYDROGEN
INITIAL	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx
INJECTED SOURCE	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx
INJECTED SPRAY	x.xxxxxxx	0.000E+00	0.000E+00	0.000E+00	0.000E+00
FINAL	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx	x.xxxxxxx

The total masses (in kilograms) of liquid water and ice, steam, nitrogen, oxygen, and hydrogen are displayed in this table. The first row lists the initial masses present. The second row shows the masses injected by both regular and external sources. Note that any H_2O (liquid or vapor) injected into a sump will be recorded in the "Water & Ice" column. The third row presents the amount of mass (water only) injected by the sprays while in injection mode. The last row lists the final masses of each component present in the geometry. Note that the values on the bottom row might be slightly different than the sum of the entries in the previous three rows. Only four significant digits of each

number are printed in this table (so that it will fit in 80 columns). Also, burns will create steam at the expense of reductions in oxygen and hydrogen. Finally, if the user has specified zero instead of the number of a sump for certain input variables (ISV(i), ISSP(i), DUMPTO(is), ISS(i)), then liquid water may disappear from the system in certain situations.

The next table produced by HECTR is a list of the final volumes of each sump.

```
FINAL SUMP VOLUMES (M**3):

    1. xxxxx.xxx
       . . .
```

If an ice-condenser PWR was being modeled, then the fraction of the initial ice mass remaining in the ice bed at the end of the run will be shown next.

```
*** FINAL ICE FRACTION = x.xxx ***
```

HECTR will then produce a set of tables providing details about the timesteps that were taken during the run. The first table lists the number of heat-transfer and flow timesteps that were taken (first and third entries) and the total number of flow timesteps that were attempted.

```
NUMBER OF TIME STEPS TAKEN:

    HEAT TRANSFER    =      nnnn
    FLOW             =      nnnn
    SUCCESSFUL FLOW  =      nnnn
```

The next table lists the number of flow timesteps that had to be repeated for various reasons.

```
NUMBER OF FLOW TIME STEPS REPEATED AND REASON:

        nnnn    FLOW REVERSAL
        nnnn    CHOKING
        nnnn    EXCESSIVE PRESSURE CHANGE
        nnnn    TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
        nnnn    NEGATIVE MOLES
        nnnn    TEMPERATURE OFF TABLES
        nnnn    TEMPERATURE TOO LOW
        nnnn    EXCESSIVE PRESSURE OR TEMPERATURE CHANGE FOR
                HEAT TRANSFER
```

A flow timestep is repeated if a flow reversal or choked flow occurs in any flow junction during the timestep, or if the pressure change in any compartment or the fraction of any compartment's volume flowing out into other compartments during the timestep is too large (these last limits are set by

the pseudo-NAMELIST variables PCHMAX and FLOMAX, respectively--see Section 4.2.3.6.3). A flow timestep will also be repeated if the value for the number of moles of any gas species in any compartment is predicted to be negative at the end of the timestep, if the gas temperature predicted for the end of the timestep in any compartment will be outside the range of HECTR's tables (200 to 4000 K), if the value for the temperature in any compartment is predicted to be less than 273.15 K at the end of the timestep, or if the total change in pressure or temperature in any compartment during the heat-transfer timestep containing the flow timestep is too large (these last limits are set by the pseudo-NAMELIST variables DPRSMX and DTMPMX, respectively--see Section 4.2.3.6.3). The third table lists which factors were controlling the choice of new flow timesteps and how often each of these factors was responsible for determining the size of a new timestep.

FLOW TIME STEP CONTROLLING FACTORS AND TIMES USED:

nnnn	PRESSURE CHANGE
nnnn	TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
nnnn	MAXIMUM STRETCH FACTOR
nnnn	MINIMUM STEP SIZE
nnnn	MAXIMUM STEP SIZE
nnnn	MATCHING HEAT TRANSFER UPDATING TIME

The factors that control the length of a new flow timestep are the maximum compartment pressure change that occurred on the previous timestep, the maximum fraction of a compartment's volume that flowed out to other compartments during the previous timestep, the requirement that a timestep can not be more than 1.5 times the previous timestep, the user-defined minimum and maximum flow timestep sizes (DTFLMN and DTFLMX), and forcing a flow timestep to end at the same time as the heat-transfer timestep that contains it.

The next table produced in the run summary specifies the compartment conditions at the end of the run (which occurred at the indicated time).

FINAL COMPARTMENT CONDITIONS AT xxxxx.xxx SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
nn	xxxx.x	xxxx.x	x.xxxx	x.xxxx	x.xxxx	x.xxxx
			. . .			

The final gas temperature (K), pressure (kPa), and gas mole fractions present in each compartment are displayed. Finally, if any nonfatal error messages (warnings) were produced during the run, then the number of these messages generated by each program unit is indicated.

*** NON-FATAL ERRORS (WARNINGS) PRODUCED DURING THIS RUN ***

nnnn FROM PROGRAM UNIT aaaaaa

. . .

Here, aaaaaa represents the name of a program unit. This last table is convenient for checking for nonfatal errors without having to search through the rest of the HECTR output.

5.1.4 Data Files

Three different output files can be produced that contain the transient values of HECTR variables. These files are produced by writing the values of selected variables to the HECTR units UOH, UOF, and UOA (using unformatted write statements). The file written on unit UOH contains basic information about the HECTR calculation, followed by the transient values of variables describing compartment and surface conditions. The variables that describe the flows between compartments are written on unit UOF. The third file, written on unit UOA, contains additional HECTR variables that are used less often than the variables on the other two files, but are needed in some analyses. The transient variables written to each of the three units are listed in Table 5-1.

The three HECTR output files are processed by the computer program ACHILES to produce tables and plots of the desired variables. ACHILES can be run immediately after HECTR (during the same computer job), or the HECTR output files can be saved and ACHILES can process them during a subsequent job.

5.1.5 HECTR Output Control Variables

The HECTR output control variables are defined in Sections 4.2.1 and 4.2.3 (in the pseudo-NAMELIST input). In Section 4.2.1, the output units UOH, UOF, and UOA are defined. These are the units to which the various timestep variable histories are written, as was discussed in the previous section. Any of these units can be set to zero to suppress the output to the corresponding file. If the user sets UOH to zero, HECTR will automatically set UOF and UOA to zero as well, and no data output files will be produced. UOA defaults to zero and must be reset (normally to 9) for variables to be written to the file that corresponds to this unit.

Variables are not necessarily written to the output files at each timestep. Output will be written at every timestep during the portions of the calculation in which variables are changing rapidly, but will be written less often during slowly changing portions. If the calculation is near a significant event (initiation of sprays or fans, switching to recirculation mode for sprays, or burning in any compartment), output will be written at every timestep. Otherwise,

Table 5-1

HECTR Output Variables

Unit UOH
Introductory information
Time (s)

For each compartment:
- Pressure (kPa)
- Temperature (K)
- Mole fractions:
  - Steam
  - Nitrogen
  - Oxygen
  - Hydrogen
- Burning status
- Density (kg/m^3)

For each sump:
- Volume (m^3)

For each surface:
- Wall temperature (K)
- Condensation mode
- Condensing mass flux (kg/s)
- Film thickness (m)

For each ice condenser:
- Fraction of ice still in ice bed

For each MARCH source:
- ECC flow rate (kg/s)
- Steam injection:
  - Flow rate (kg/s)
  - Accumulated mass (kg)

For each compartment with sprays:
- Spray mass evaporation rate (kg/s)
- Heat-transfer rate (W)

For each compartment that water is injected into:
- Steam injection rate (kg/s)
- Water injection rate (kg/s)

For each compartment that hydrogen is injected into:
- Hydrogen injection rate (kg/s)

Table 5-1 (Continued)

HECTR Output Variables

Unit UOF
Time (s)

For each junction:
- Velocity (m/s)
- Open/close flag
- Choking flag

For each fan:
- Flow rate (m^3/s)

For each suppression pool:
- For each vent:
  - Gas flow rate (m^3/s)
- Drywell side water level (m)
- Wetwell side water level (m)

Unit UOA
Time (s)

For each surface:
- Net heat flux (W/m^2)
- Radiative heat-flux incident on surface (W/m^2)
- Water runoff rate (kg/s)

For each spray ring:
- Injection temperature (K)

For each ice condenser:
- Water falling through lower plenum:
  - Heat flux to water (W)
  - Condensation rate on water (kg/s)
- Drain temperature (K)
- Sum of ice melting rates and condensation on ice surfaces (kg/s)

For each ice surface:
- Melting rate (kg/s)

output will be written only if selected variables have changed significantly since the last file write or if a specified time has elapsed. The variables checked when writing to units UOH and UOA are pressure, temperature, and gas mole fractions. The only variable checked when writing to unit UOF is gas velocity. The criterion used to determine if any of the variables have changed sufficiently is

$$|z - zold| > DELzR\ |z| + DELzA \qquad (5\text{-}1)$$

where

- z = variable (P for pressure, T for temperature, X for gas mole fraction, or V for gas velocity)
- zold = value of variable z at the last file write
- DELzR = relative change in z that will force a file write (see Section 4.2.3.6.2)
- DELzA = absolute change in z that will force a file write (see Section 4.2.3.6.2)

Output is also written whenever a specified time has elapsed since the last file write. This time span can be different when writing to units UOH and UOA than when writing to unit UOF. The criterion used is

$$deltime > delt * tcalc \qquad (5\text{-}2)$$

where

- deltime = time elapsed since the last file write to the specified unit
- delt = fractional change in tcalc before output will be written (specified by the pseudo-NAMELIST variable DELTHT when writing to units UOH or UOA and DELTFL when writing to unit UOF)
- tcalc = length of the calculation

5.2 ACHILES Output

ACHILES, the output processor for HECTR, produces several types of output. ACHILES will echo the input if the pseudo-NAMELIST variable BATCH has been set equal to TRUE (unless the output units UOM and UOT are the same--see Section 4.3.1). ACHILES will also provide a summary of the HECTR run, make tables and plots of various HECTR variables versus time, and produce error messages if problems occur. This output is discussed in the following subsections.

5.2.1 Error and Warning Messages

The warning and error messages that can be produced by ACHILES are shown below. Each message is reproduced exactly as it would appear if printed by ACHILES. Integers and character strings are indicated by strings of lower case n's and m's, and a's and b's, respectively. All of the messages identify the program unit that wrote them and have been listed below alphabetically by program unit. Following each message is a short discussion of the error. This discussion may include possible causes and remedies for the error as well as an explanation of the message (if it is not obvious).

5.2.1.1 ACHILE

```
*** ACHILE: ERROR ON TRYING TO OPEN UNIT nn
            ERROR MESSAGE NUMBER =      mmmmm ***
```

An error has occurred in opening one of the ACHILES input or output units. This is often the result of a missing file or of not declaring or attaching the file properly in the control language. The meaning of the error message number can usually be found in a system messages manual.

```
*** ACHILE: 'PLOT' INVALID IN THIS CONTEXT - YOU WERE ALREADY
            PLOTTING! ***
```

A command to go to the plotting portion of ACHILES was issued when ACHILES was already there. This is usually due to miscounting tables.

5.2.1.2 CHEQUE

```
*** CHEQUE: VALUE FOR aaaaaa (= nnn) EXCEEDS THE MAXIMUM
            ALLOWED VALUE (bbb = mmm) AS SET IN PARAMETER
            STATEMENTS IN ACHILES ***
```

The value of a basic maximum HECTR problem parameter (such as NCOMPS, the number of compartments actually used in a HECTR run) is greater than the value assigned to the corresponding symbolic constant (NC, if comparing with NCOMPS) in the ACHILES PARAMETER statements. The value of the symbolic constant, which defines array sizes, must be increased in all the PARAMETER statements in ACHILES, which define this constant. See Section B.3.7.

5.2.1.3 FETCH

*** FETCH: UNEXPECTED END-OF-FILE ON UNIT nn ***

An end-of-file occurred unexpectedly on reading the HECTR generated file that contains the basic introductory information about a run (this file is read through unit UHD). Often, this indicates an empty file, which may result from HECTR being terminated abnormally while reading input or from improperly attaching the file in the control language (or not attaching it at all).

5.2.1.4 GET

*** GET: ERROR ON READING ITEM NUMBER nn OF mm REQUESTED VALUES ***
>aaaaaaaaaa<

The nnth of mm values on a numerical user-input record was not a number. The input line in which this error was detected is displayed below the message.

*** GET: INVALID USE OF AN ASTERISK IN THE LAST INPUT LINE ***
>aaaaaaaaaa<

A replication factor was formed improperly on the numerical user input (see Section 4.1). The line in which this error occurred is displayed below the message.

*** GET: UNEXPECTED END-OF-FILE ON UNIT nn ***

An end-of-file occurred unexpectedly on the numerical user input.

*** GET: WARNING - EXCESS VALUES ON THE LAST INPUT LINE ***
>aaaaaaaaaa<

The last numerical user-input record contained more values than expected. These excess values will be ignored. The input line in which this problem was detected is displayed below the message.

5.2.1.5 INTER

*** INTER: KMAX (= nnn) IS NOT SUFFICIENTLY LARGE -
SOME TABLES OR PLOTS WILL BE LOST ***

The temporary storage array INDEXX in INTER was not dimensioned large enough. This error is not fatal although some requested tables or plots may not be produced. The size of this array (and the value of KMAX) should be increased before the next ACHILES run.

5.2.1.6 NAMLST

*** NAMLST: bbbbbb HAS THE WRONG NUMBER OF SUBSCRIPTS
(SHOULD EITHER HAVE n OR NONE) ***
>aaaaaaaaaa<

The pseudo-NAMELIST variable indicated has the wrong number of subscripts (it should either have the number indicated or no subscripts at all). The entry in which this error occurred is displayed below the message.

*** NAMLST: BAD INDEX OR VALUE FOR ENTRY ***
>aaaaaaaaaa<

A subscript or a "numerical" value that was supposed to be assigned to a pseudo-NAMELIST variable was not a number. The entry in which this error occurred is displayed below the message.

*** NAMLST: ENTRY HAS MORE THAN THE MAXIMUM ALLOWED NUMBER OF
SUBSCRIPTS (n) ***
>aaaaaaaaaa<

The pseudo-NAMELIST entry has too many subscripts to be processed. The pseudo-NAMELIST variables in ACHILES have at most one subscript. The entry is displayed below the error message.

*** NAMLST: ENTRY IS IMPROPERLY FORMED ***
>aaaaaaaaaa<

The pseudo-NAMELIST entry was improperly formed. The entry is displayed below the error message.

```
*** NAMLST: IMPROPER VARIABLE NAME => bbb ***
>aaaaaaaaaa<
```

The pseudo-NAMELIST variable name is missing or is longer than 6 characters. The entry in which this error occurred is displayed below the message.

```
*** NAMLST: LOGICAL VARIABLE (bbbbbb) MUST HAVE A VALUE OF
            EITHER "TRUE" OR "FALSE" ***
>aaaaaaaaaa<
```

The logical pseudo-NAMELIST variable indicated was not assigned a value of TRUE or FALSE. The entry in which this error occurred is displayed below the message.

```
*** NAMLST: UNKNOWN COMPUTER TYPE => bbbbb ***
>aaaaaaaaaa<
```

The pseudo-NAMELIST variable CMPUTR was not assigned the value CDC, CYBER, CRAY, or VAX. The entry in which this error occurred is displayed below the message.

```
*** NAMLST: UNRECOGNIZED NAME => bbbbbb ***
>aaaaaaaaaa<
```

The name of the pseudo-NAMELIST variable was not one of the names expected (see Section 4.3.1 for a list of the pseudo-NAMELIST variables in ACHILES). The entry in which this error occurred is displayed below the message.

5.2.1.7 NUMBER

```
*** NUMBER: BAD NUMBER FOUND ON INPUT: aaa ***
```

NUMBER was given a character string to translate instead of a number. This error can result from deleting lines from or adding extra lines to the input (so that a word was read where a number was expected) as well as from mistyping.

```
*** NUMBER: NUMBER IS MORE THAN 20 CHARACTERS LONG:
            aaaaaaaaaaaaaaaaaaaa ***
```

NUMBER cannot process numbers with string representations that are greater than 20 characters long. This error can result from deleting lines from or adding extra lines to the input (so that a word was read where a number was expected) as well as from mistyping.

5.2.1.8 NUMSTR

*** NUMSTR: BAD ARGUMENT (nnnnn) ***

NUMSTR cannot process numbers less than or equal to zero or greater than or equal to 1000. This error should not occur and indicates a logic error.

5.2.1.9 WHICH

*** WHICH: ERROR INTERPRETING INPUT LINE ***
aaa
==>

The input that allows the user to select which compartments, surfaces, etc., he or she wishes to include for tables or plots of various variables versus time was entered incorrectly. For example, the input may not have been strictly entered in I3 format, or a number may have been mistyped. The erroneous input line is displayed with an arrow below it that points to the beginning of the 3-character-wide section where WHICH detected trouble.

5.2.2 Summary of HECTR Run

ACHILES reads basic introductory information about the HECTR run in process from the file connected to the unit UHD (defined in Section 4.3.1.1). ACHILES then counts the number of data points in each of the files connected to units UHD, UHF, and UHA and determines maximum values for compartment pressures and temperatures from this data. Next, ACHILES writes header information to units UOT and UAO. This header information includes the basic introductory information and a series of tables that will describe the basic model geometry and accident scenario for the HECTR run that ACHILES is currently processing.

The ACHILES header section is presented below. All messages are reproduced exactly as they appear when printed from ACHILES. Real numbers, integers, and character strings that are determined from the HECTR data are indicated by strings of lower case x's, y's, z's, w's, v's, and u's; n's, m's, k's, i's, and j's; and a's, b's, and c's, respectively. An example of a header section can be found in Section 6.1.4 where the ACHILES header section for the simple two compartment sample problem is reproduced.

The header section first identifies the version of HECTR that was used to produce the data ACHILES is currently processing.

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                      $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
```

ACHILES then prints the contents of the HECTR variables LTITLE (which is underlined below) and TEXT(i) (see Section 4.2.2: General).

```
    aaaaaaaaaa
    ----------

bbbbbbbbbb
  . . .
```

This is followed by a table that lists the number of compartments, flow junctions, surfaces, fan paths, and sumps that were in the HECTR geometry.

```
>>> nnn COMPARTMENT(S) mmm FLOW JUNCTION(S) kkk SURFACE(S) <<<
>>> iii FAN(S)          jjj SUMP(S)                        <<<
```

The modes of spray and fan operation are indicated next.

```
    SPRAYS WERE aaaa          FANS WERE bbbb
```

aaaa and bbbb will each be either OFF, ON, or AUTO. A table presenting timestep information is printed next.

```
MINIMUM HEAT TRANSFER TIME STEP       = x.xxxxxxx SECONDS
MAXIMUM HEAT TRANSFER TIME STEP       = y.yyyyyyy SECONDS
MINIMUM FLOW TIME STEP                = z.zzzzzzz SECONDS
MAXIMUM FLOW TIME STEP                = w.wwwwwww SECONDS
MAXIMUM TIME STEP PRESSURE CHANGE     = vv.vvvv   KPA
MAXIMUM TIME STEP TEMPERATURE CHANGE  = uu.uuuu   K
```

The values displayed are those of the HECTR variables DTHTMN, DTHTMX, DTFLMN, DTFLMX, DPRSMX, and DTMPMX (defined in Section 4.2.3.6.3). The last two values are the maximum absolute pressure and temperature changes allowed in a compartment during a heat-transfer timestep. Following the timestep information table is a table showing the hydrogen ignition and (upward, sideways, and downward) propagation limits for each compartment.

```
HYDROGEN LIMITS FOR  IGNITION  PROPAGATION  PROPAGATION  PROPAGATION
                               UPWARDS      SIDEWAYS     DOWNWARDS

COMPARTMENT   1       xxx.x%     yyy.y%       zzz.z%       www.w%
                                  . . .
```

If the failure pressure (PFAIL) has a positive value less than 10000 kPa, it will be printed next.

FAILURE PRESSURE = xxxx.x KPA

The compartments in the HECTR geometry are then listed, identified by the compartment descriptors COMPID(i) that were specified in HECTR.

COMPARTMENTS:

1. aaaaaaaaaa
2. bbbbbbbbbb
   (LOWER PLENUM)
3. cccccccccc
   . . .

Certain special compartments will be identified by ACHILES if they occur in this list, such as the lower plenum and upper plenum of an ice-condenser PWR, the drywell and wetwell of a Mark III BWR, and compartments generated by HECTR to model the ice-bed region in an ice-condenser PWR.

Next, ACHILES prints a list of the surfaces in the HECTR geometry, identified by the surface descriptors SURFID(i).

SURFACE TYPE KEY:
1. SLAB
2. LUMPED MASS
3. POOL
4. ICE
5. ICE CONDENSER WALL

SURFACES (BY COMPARTMENT NUMBER - SURFACE TYPE - NUMBER OF LAYERS IF A SLAB) FOLLOWED BY THE SURFACE NUMBER (AND THE SUMP NUMBER IF A SUMP):

(nnn-j-m)	1.		aaaaaaaaaa
(nnn-j)	2.	(kk)	bbbbbbbbbb
			(LOWER PLENUM DRAIN)
(nnn-j)	3.		cccccccccc
	. . .		

A surface is further identified by the number of the compartment in which it is located (nnn), its type (j) as given in the key above (see also STYPE(i) in Section 4.2.2.4), and the number of layers it contains (m) if it is a slab (surface type 1). A surface of a pool (sump - surface type 3) will be further identified by the number of the sump (kk) to which it is attached (ISS(i)). Certain special sumps will be identified by ACHILES if they occur in this list, such as the sump that the lower plenum drains into in an ice-condenser PWR, the upper pool, drywell sump, and suppression pool in a Mark III BWR, and the spray source sump.

The next table lists the flow junctions in the HECTR geometry.

```
FLOW JUNCTIONS/COMPARTMENT INTERCONNECTIONS
    (INTERCONNECTION AREA IN M**2 - FLOW COEFFICIENT):

  1. nnn => mmm  aaaaaaaaaa      bbbbbbbbb (xxxxxx.xx - yyy.yy)
                          . . .
```

Following the junction number, the direction of positive flow through the junction is specified (from compartment nnn into compartment mmm). Next is a string (aaaaaaaaaa) specifying the flow junction type (2-way, 1-way check valve, 1-way inertial value, or an ice-condenser drain). This is followed by a string (bbbbbbbbb) that indicates that flame propagation through this junction, in the direction of positive flow, was either DOWNWARDS, SIDEWAYS, or UPWARDS. Finally, the interconnection area of the junction and the loss coefficient are displayed.

All the fan paths in the HECTR geometry are shown next.

```
FAN CONNECTIONS (VOLUMETRIC FLOW RATE IN M**3/S WITH A
                 NEGATIVE NUMBER INDICATING THE USE OF A
                 HEAD CURVE):

  1. nnn => mmm      aaaaaaaaa      (xxxxx.x)
                    . . .
```

The fan path number is followed by a specification of the direction of positive flow (from compartment nnn to compartment mmm). A string (aaaaaaaaa) occurs next, which indicates that flame propagation through the fan (in the positive flow direction) was either DOWNWARDS, SIDEWAYS, or UPWARDS. The absolute value of the last number on the right is the constant or maximum volumetric flow rate of the fan. If this number is negative, then a head curve was used to determine the actual volumetric flow rate through the fan.

At this point, ACHILES will print out information determined from the data points in the HECTR generated files. First, ACHILES will print the final time for the HECTR run.

```
*** THIS RUN ENDED AT xxxxx.xxx SECONDS ***
```

Next, the global pressure and gas temperature maximums determined from the data in the files, and the times at which they occurred, are shown.

```
APPROXIMATE GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS
====================================================

xxxxx.xxx SECONDS          yyyy.y KPA
zzzzz.zzz SECONDS          wwww.w K

====================================================
```

These maximums are labeled approximate because they are determined from the data in the HECTR created files. These files will not, in general, contain all the pressures and temperatures that were calculated at each timestep during the run, but rather will hold only those pressures and temperatures for which differences from previous output values were "significant" (see Section 5.1.5). It is possible that these maximums will not exactly match those tabulated in the HECTR run summary, but they should be very close. The pressure and temperature maximums for each compartment and the times at which they occurred are presented next. These maximums will also be "approximate."

APPROXIMATE COMPARTMENT PRESSURE AND TEMPERATURE MAXIMUMS

COMPARTMENT 1: xxxxx.xxx SECONDS yyyy.y KPA
zzzzz.zzz SECONDS wwww.w K
. . .

The last information that ACHILES will print in this header section is information about the output files created by HECTR for this run.

UOF = nn UOA = mm

NHT = kkkk NFL = iiii NAH = jjjj

The first line lists the values of the HECTR variables UOF and UOA (see Section 4.2.1.2). These variables define the output units that HECTR uses for writing the values of major variables defined on flow timesteps and values of additional variables defined on heat-transfer timesteps, respectively (see Section 5.2.3). If either of these units is zero, then the corresponding set of variables will not have been written to a file by HECTR, and so ACHILES will not be able to create tables or plots of these variables. The second line lists the number of data records read by ACHILES for each major type of variable (main heat-transfer timestep variables, flow timestep variables, and additional heat-transfer timestep variables). Thus, if UOF is zero, then NFL will also be zero, and if UOA is zero, then NAH will also be zero.

5.2.3 Tables and Plots

5.2.3.1 ACHILES Unit Numbers

The units used in ACHILES to read the corresponding HECTR output files are listed in Table 5-2. Also included in this table are the default unit numbers set in HECTR and ACHILES.

Table 5-2

HECTR and ACHILES Unit Numbers

Timestep Variables	HECTR Unit	Default Value	Corresponding ACHILES Unit	Default Value
Heat Transfer	UOH	7	UHD	7
Flow	UOF	8	UHF	8
Heat Transfer (additional)	UOA	0	UHA	9

The file read by the ACHILES unit UHD must exist for ACHILES to process any of the output variables. The introductory information on this file defines the problem geometry (number of compartments, flow junctions, etc.) necessary for ACHILES to read the data files. The HECTR files, which are read by ACHILES from units UHF and UHA, are used by ACHILES only if variables from these files are actually being tabulated or plotted.

5.2.3.2 ACHILES Table and Plot Control Variables

By using the ACHILES table and plot control variables, the user can control the size of tables printed by ACHILES or the number of plots produced. These variables are all NAMELIST-type variables and can be readily changed by the user. These variables are also described in Section 4.3.1.

Entries in the tables generated by ACHILES are written every n^{th} timestep recorded on the HECTR output file. "n" is defined separately for each table produced by ACHILES using the pseudo-NAMELIST variables SHOWxx defined in Section 4.3.1. "n" is 1 by default for all tables but can be increased if it is desired to print fewer points for a particular table(s).

ACHILES normally produces separate plots of pressure, temperature, gas mole fractions, and density for each compartment specified. To reduce the amount of output, the user can specify that all mole fractions for a compartment be plotted on a single graph (rather than plotting each separately) by setting the pseudo-NAMELIST variable COMBXF to TRUE for the desired compartment. In addition, any of the plots normally produced for a compartment can be eliminated by setting the appropriate pseudo-NAMELIST variable described in Section 4.3.1 (PLTxxx) to FALSE for the desired compartment.

The maximum number of points that will be plotted for each curve produced by ACHILES is specified by the symbolic parameter NPTS (see Section B.3.7). If more than NPTS timesteps are recorded on the HECTR output file being used, points will be plotted only at every n^{th} timestep, where n is defined by:

$$n = \text{int}\left(\frac{NTOT - 1}{NPTS - 1}\right) + 1$$

where

NTOT = total number of timesteps written on the file being used
int(x) = largest integer that is less than x.

Thus, the plots produced by ACHILES may not include all of the points recorded on the HECTR output files. This may result in the ACHILES plots not reflecting the actual maximum and minimum values for the variable being plotted.

For more information regarding the HECTR and ACHILES output, refer to the sample problems presented in Chapter 6.

6. EXAMPLE CASES

In this chapter, three example problems are presented. They describe (1) a simple two-compartment geometry, (2) an ice-condenser PWR containment, and (3) a Mark III BWR containment. The results presented here should be considered as examples only and not representative of any particular accident scenario.

6.1 Simple Two-Compartment Problem

This first sample problem is for a simple two-compartment geometry. Because many of the models in HECTR are used in this problem, running this case will not only give the user an understanding of how a sample set of HECTR input should look, but will also provide a good checkout of the implementation of HECTR on the user's computer. There may be some small differences in the numbers produced (depending primarily on the word length of the user's computer), but no major differences should occur. We have run this same case on a CRAY-1, a Control Data Corporation (CDC) CYBER 76, and a VAX-11. The results from the CRAY-1 and the CDC CYBER 76 were identical. The results from the VAX-11 varied slightly (<2%) after the sprays were turned on.

The simple two-compartment problem is based on a geometry in which a large steel-lined volume resides above a smaller concrete-lined compartment. A sump lies in the bottom of the lower compartment, and a hydrogen source is located in the lower compartment. The steel in the upper compartment is treated as a lumped mass, while the concrete in the lower compartment is modeled as a slab. The flow junction connecting the two compartments has been chosen so that flow from the lower to the upper compartment is in the positive direction. If the pressure or temperature in either compartment exceeds specified values, sprays in the upper compartment will be actuated. A small fraction of any unevaporated spray drops that reach the bottom of the upper compartment are allowed to carry over into the lower compartment. There is also a fan that, once actuated, will blow air from the lower compartment into the upper compartment; the actuation criteria for the fans is similar to that used for the sprays. Finally, since no ignition limits are specified, the default values are used. These allow combustion to begin in a compartment if the hydrogen mole fraction there is greater than or equal to 0.08 (and if additional constraints on the oxygen and steam mole fractions are met).

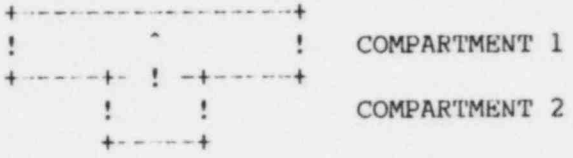
6.1.1 HECTR Input Data

The input data for the two-compartment problem is shown below. The first input defines the type of computer being used for the calculation (see Section 4.2.1).

```
! HECTR is being run on a CRAY
CMPUTR=CRAY
$ END OF NAMLST INPUT
```

The next section of input describes the geometry of the problem (see Section 4.2.2).

```
(S)IMPLE TWO COMPARTMENT PROBLEM$
THIS IS THE SITUATION OF TWO COMPARTMENTS, ONE STACKED ABOVE THE OTHER.
THE UPPER COMPARTMENT IS ABOUT THREE TIMES LARGER THAN THE LOWER COMPARTMENT.
```




```
0.        ! Failure pressure (Pa)
2         ! Number of compartments
!
! Compartment Data
!
UPPER COMPARTMENT
10603.    ! Volume (m**3)
10.       ! Elevation (m)
15.       ! Flame propagation length (m)
1         ! Number of surfaces
1         ! Water generated from subcooling goes into sump 1
1         ! Any spray not carried over falls into sump 1
LOWER COMPARTMENT
3534.     ! Volume (m**3)
0.        ! Elevation (m)
15.       ! Flame propagation length (m)
2         ! Number of surfaces
1         ! Water generated from subcooling goes into sump 1
1         ! Any spray carryover will go directly into sump 1
!
! Sump Data
!
1         ! Sump number
1000.     ! Capacity (m**3)
0         ! Sump overflow disappears from the system
$ END OF SUMPS
!
```

```
! Surface Data
!
UPPER COMPARTMENT STEEL
2           ! Surface type (lumped mass)
1.53E5      ! Mass (kg)
2121.       ! Area (m**2)
15.         ! Convective length (m)
460.5       ! Specific heat (J/kg-K)
.7          ! Emissivity
1           ! Any wall condensation will go directly into sump 1
LOWER COMPARTMENT CONCRETE
1           ! Surface type (slab)
1.          ! Mass (kg) - ignored for slabs
471.        ! Area (m**2)
5.          ! Convective length (m)
879.        ! Specific heat (J/kg-K)
.9          ! Emissivity
1           ! Any wall condensation will go directly into sump 1
! Layer information
1           ! Number of layers in slab
.762        ! Thickness of layer 1 (m)
5.5E-7      ! Thermal diffusivity of layer 1 (m**2/s)
1.385       ! Thermal conductivity of layer 1 (W/m-K)
! Slab mesh spacing control variables and back surface condition
0  0.       ! Let mesh spacing be chosen automatically
0.          ! Backside convective heat transfer coefficient (indicates an
            ! insulated back surface)
0.          ! Environmental temperature (indicates an insulated back surface)
LOWER COMPARTMENT POOL (SUMP)
3           ! Surface type (pool)
1000.       ! Mass (kg)
707.        ! Area (m**2)
15.         ! Convective length (m)
1.          ! Specific heat (J/kg-K) - ignored for pools
.94         ! Emissivity
1           ! This is the surface of sump number 1
!
! Flow Junction Data
!
2  1        ! Positive flow is from compartment 2 to compartment 1
1           ! Junction type (2-way flow)
300.        ! Interconnection area (m**2)
1.2         ! Flow coefficient
.015        ! Ratio of the flow length to the flow area (1/m)
1           ! Flow from compartment 2 to 1 is in the upward direction
5.          ! Junction elevation (m)
$ END OF FLOW JUNCTIONS
$ NO ICE CONDENSER INPUT
$ NO SUPPRESSION POOL INPUT
!
! Fan Data
!
```

```
350. 202650.      ! Temperature (K) and pressure (Pa) setpoints
18.               ! Time delay (s)
1.0E+06           ! Time that the fans remain on (s)
1  2              ! Fan blows from compartment 1 into compartment 2
50.               ! Constant volumetric flow rate (m**3/s)
1013.25           ! Shutoff head (Pa)
1.                ! Efficiency
-1                ! Flow from compartment 1 to 2 is in the downward direction
$ END OF FAN CONNECTIONS
$ USE DEFAULT HEAD CURVE
!
! Radiative Heat Transfer Data
!
! Beam lengths (m)
13.5  15.  15.
12.   12.
1.
! View factors
.667 .094 .239
.154 .423
.001
!
! Spray Data
!
1                 ! Number of compartments with spray sources
! Loop on compartments with spray sources
1                 ! Compartment where spray originates
330.37            ! Spray inlet temperature (K)
.5                ! Spray flow rate (m**3/s)
2                 ! Number of drop sizes
.95  309.         ! Frequency and diameter (um) of drops of the first drop size
.05  810.         ! Frequency and diameter (um) of drops of the second drop size
!
1 2  .02          ! 2 percent of sprays fall from comp. 1 into comp. 2
$ END OF SPRAY CARRYOVER DESCRIPTION
1 15.             ! Compartment and the spray fall height (m) in it
2 15.
$ END OF SPRAY FALL HEIGHTS
350. 202650.      ! Temperature (K) and pressure (Pa) setpoints
5.                ! Time delay (s)
1.0E+06           ! Time that the sprays remain on (s)
10.               ! Time spent in spray injection phase (s)
587.              ! Rated spray heat exchanger mass flow rate (kg/s)
3.74E+06          ! Rated spray heat exchanger effectiveness (W/K)
301.5             ! Spray heat exchanger secondary side inlet temperature (K)
755.              ! Spray heat exchanger secondary side mass flow rate (kg/s)
1                 ! Draw water from sump 1 when sprays are in recirculation mode
!
$ END OF HEAT EXCHANGERS
```

The next section of input describes the initial conditions and the accident scenario as described in Section 4.2.3.

```
60.          ! Simulation time (s)
!
! Compartment Data
!
300.         ! Initial temperature of the upper compartment (K)
3400.        ! Initial partial pressure of steam (Pa)
77000.       ! Initial partial pressure of nitrogen (Pa)
21000.       ! Initial partial pressure of oxygen (Pa)
0.           ! Initial partial pressure of hydrogen (Pa)
.3           ! Convective gas velocity (m/s)
!
300.         ! Initial temperature of the lower compartment (K)
3400.        ! Initial partial pressure of steam (Pa)
77000.       ! Initial partial pressure of nitrogen (Pa)
21000.       ! Initial partial pressure of oxygen (Pa)
0.           ! Initial partial pressure of hydrogen (Pa)
.3           ! Convective gas velocity (m/s)
!
! Source Terms
!
$ END OF STEAM SOURCES
$ END OF NITROGEN SOURCES
$ END OF OXYGEN SOURCES
2  -1  350.   ! Hydrogen source in compartment 2 with a constant temperature
              ! (indicated by the -1) of 350 K
0.   .8063    ! Time (s) and mass release rate (kg/s) at that time
70.  .8063    ! Release rate is linearly interpolated at intermediate values
75. 0.
$ END OF TABLE
$ END OF HYDROGEN SOURCES
$ NO WATER IS TO BE REMOVED FROM SUMPS FOR ECC RECIRCULATION
!
! Surface Temperatures (K)
!
300.  300.  302.6
!
! Namelist Type Input
!
SPRAYS=AUTO      ! Set the sprays on automatic
FANS=AUTO        ! Set the fans on automatic
KPROPJ(1)=.25    ! A burn can propagate through flow junction 1 after .25 of the
                 ! burn time in a burning compartment has elapsed
$ END OF NAMLST INPUT
```

6.1.2 ACHILES Input Data

The following is the input to the output processor (ACHILES) as described in Section 4.3.

```
!
! Namelist Type Input
!
CMPUTR=CRAY    ! ACHILES is being run on a CRAY
COMBXF=TRUE    ! Combine mole fraction plots into a single graph
$ END OF NAMLST INPUT
!
!   +--------+
!   ! Tables !
!   +--------+
!
! Main Heat Transfer Timestep Variables
!
ALL    ! Pressure, temperature, gas mole fractions, if burning, gas density,
       ! hydrogen and steam sources (by compartment)
NON    ! Sump volumes (by sump)
NON    ! Surface temperatures, if condensing, dry or evaporating (by surface)
NON    ! Condensation rates, film thicknesses (by surface)
NON    ! (1) Source injection rates, (2) accumulated injected source masses,
       ! (3) external (MARCH) steam and hydrogen source information
NON    ! Spray mass evaporation rates, spray heat removal rates (by compartment)
NON    ! Fraction of initial ice mass remaining in the ice condenser
!
! Flow Timestep Variables
!
ALL    ! Junction gas velocities, if closed or choked (by flow junction)
NON    ! Fan volumetric flow rates (by fan path)
NON    ! Suppression pool vent volumetric flow rates, suppression pool levels
!
! Additional Heat Transfer Timestep Variables
!
NON    ! Net total incident heat fluxes (by surface)
NON    ! Net incident radiation (by surface)
NON    ! Convective heat fluxes (by surface)
NON    ! Water drainage rates (by surface)
NON    ! Emitted spray drop temperatures (by compartment)
NON    ! Ice condenser information: melting rates, drain temperature, etc.
!
!   +-------+
!   ! Plots !
!   +-------+
!
! Main Heat Transfer Timestep Variables
!
ALL    ! Pressure, temperature, gas density, gas mole fractions (by compartment)
!
0 10 60 5    ! Minimum time (s), time stepsize (s), maximum time (s) and number
             ! of tick marks to be plotted per step
!
```

```
NON     ! Sump volumes (by sump)
NON     ! Surface temperatures (by surface)
NON     ! Condensation rates (by surface)
NON     ! Film thicknesses (by surface)
ALL     ! (1) Source injection rates, (2) accumulated injected source masses,
        ! (3) external (MARCH) steam and hydrogen source information
NON     ! Spray evaporation rates (by compartment)
NON     ! Spray heat removal rates (by compartment)
NON     ! Fraction of initial ice mass remaining in the ice condenser
!
! Flow Timestep Variables
!
ALL     ! Junction gas velocities (by flow junction)
NON     ! Fan volumetric flow rates (by fan path)
NON     ! (1) Top, (2) middle, (3) bottom vent volumetric flow rates
        ! (4) Drywell, (5) wetwell suppression pool levels
!
! Additional Heat Transfer Timestep Variables
!
NON     ! Net total incident heat fluxes (by surface)
NON     ! Net incident radiation (by surface)
NON     ! Convective heat fluxes (by surface)
NON     ! Water drainage rates (by surface)
NON     ! Emitted spray drop temperatures (by compartment)
NON     ! (1)-(4) Ice surface melting rates in an ice condenser
NON     ! (1) Mass rate of water flowing into lower plenum, (2) drain temperature
        ! (3) Condensation rate, (4) heat transfer rate to drops in lower plenum
```

6.1.3 HECTR Output

The HECTR (CRAY) output resulting from the sample input given above is shown below, except for the echoing of the input (see Section 5.1 for more details).

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                             $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

INITIAL COMPARTMENT CONDITIONS AT     0.000 SECONDS ARE:

COMP #  TEMP      PRESSURE    XH2O       XN2        XO2        XH2

 1      300.0       101.4    0.0336     0.7593     0.2071     0.0000
 2      300.0       101.4    0.0336     0.7593     0.2071     0.0000

INITIAL SURFACE TEMPERATURES (K) ARE:

    1.  300.0       2.  300.0       3.  302.6
```

```
BURN INITIATED IN COMPARTMENT  2 AT TIME =    31.318 SECONDS
-----------------------------------------------------------

COMPARTMENT CONDITIONS AT    31.318 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1       302.9       104.9      0.0336      0.7586      0.2069      0.0010
 2       307.0       105.1      0.0309      0.6961      0.1899      0.0832

SPRAYS WILL BE ACTIVATED AT    36.476 SECONDS DUE TO
TBULK =  357.2 AND PKPA =  110.4 IN COMPARTMENT  2

SPRAYS WILL BE SWITCHED TO RECIRCULATION AT    46.476 SECONDS
(   10.000 SECONDS AFTER BEING ACTIVATED)

FANS WILL BE ACTIVATED AT    49.476 SECONDS DUE TO
TBULK =  357.2 AND PKPA =  110.4 IN COMPARTMENT  2

BURN COMPLETED IN COMPARTMENT  2 AT TIME =    33.906 SECONDS
-----------------------------------------------------------

COMPARTMENT CONDITIONS AT    33.906 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1       379.8       156.0      0.0378      0.7501      0.2022      0.0098
 2      1101.3       156.0      0.1301      0.7219      0.1476      0.0004

BURN INITIATED IN COMPARTMENT  2 AT TIME =    52.679 SECONDS
-----------------------------------------------------------

COMPARTMENT CONDITIONS AT    52.679 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1       318.0       130.6      0.0719      0.7236      0.1946      0.0099
 2       593.4       130.7      0.1685      0.6136      0.1378      0.0801

BURN COMPLETED IN COMPARTMENT  2 AT TIME =    58.675 SECONDS
-----------------------------------------------------------

COMPARTMENT CONDITIONS AT    58.675 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1       334.8       151.2      0.1074      0.6965      0.1831      0.0130
 2      1136.7       151.3      0.2812      0.6207      0.0976      0.0005

################################################################################
################################## END OF HECTR RUN ############################
################################################################################


SUMMARY OF BURNS:

     2 BURN(S) OCCURRED IN COMPARTMENT   2
```

```
>>> GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS <<<

>>>    33.929 SECONDS              156.0 KPA <<<
>>>    58.554 SECONDS             1138.0 K   <<<


COMPARTMENT PRESSURE MAXIMUMS (KPA):

     1.  156.0      2.  156.0

COMPARTMENT TEMPERATURE MAXIMUMS (K):

     1.  379.8      2. 1138.0


SURFACE TEMPERATURE MAXIMUMS (K):

     1.  302.0      2.  365.7      3.  326.3
```

TOTAL MASSES	WATER+ICE	STEAM	NITROGEN	OXYGEN	HYDROGEN
INITIAL	1.000E+03	3.479E+02	1.223E+04	3.809E+03	0.000E+00
INJECTED SOURCE	0.000E+00	0.000E+00	0.000E+00	0.000E+00	4.845E+01
INJECTED SPRAY	4.880E+03	0.000E+00	0.000E+00	0.000E+00	0.000E+00
FINAL	5.101E+03	1.415E+03	1.223E+04	3.554E+03	1.631E+01

```
FINAL SUMP VOLUMES (M**3):

    1.     5.166


NUMBER OF TIME STEPS TAKEN:
   HEAT TRANSFER   =      275
   FLOW            =      584
   SUCCESSFUL FLOW =      532


NUMBER OF FLOW TIME STEPS REPEATED AND REASON:
          6    FLOW REVERSAL
          0    CHOKING
          7    EXCESSIVE PRESSURE CHANGE
          0    TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
          0    NEGATIVE MOLES
          0    TEMPERATURE OFF TABLES
          0    TEMPERATURE TOO LOW
         30    EXCESSIVE PRESSURE OR TEMPERATURE CHANGE FOR HEAT TRANSFER
```

```
FLOW TIME STEP CONTROLLING FACTORS AND TIMES USED:
        478    PRESSURE CHANGE
          0    TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
         24    MAXIMUM STRETCH FACTOR
          0    MINIMUM STEP SIZE
          0    MAXIMUM STEP SIZE
         30    MATCHING HEAT TRANSFER UPDATING TIME
```

FINAL COMPARTMENT CONDITIONS AT 60.088 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	329.9	148.2	0.1075	0.6964	0.1830	0.0130
2	1034.0	148.3	0.2771	0.6117	0.1008	0.0105

There are several points to note about these results. First, due to the strong hydrogen source in the lower compartment, two burns occur there within the simulation time of one minute. The first burn begins at 31.318 seconds and ends at 33.906 seconds, yielding a burn time of 2.588 seconds. The temperature rise in the lower compartment during the first burn causes the sprays and fans to be activated. A few seconds after the first burn is complete, the sprays come on. After ten more seconds, the sprays switch to the recirculation mode, drawing water from the sump in the lower compartment. Three seconds after this event occurs, the fans also turn on. Note that the messages signaling the activation of these systems are printed when the systems are triggered rather than when the systems actually come on. A few seconds after the fans come on, a second burn occurs in the lower compartment.

Summary information is printed at the end of the run. For example, we can see that the maximum pressure rise occurs after the end of the first burn, while the maximum gas temperature rise is produced near the end of the second burn. The concrete slab surface in the lower compartment has the greatest temperature rise of the three surfaces in this problem. A total of 48.45 kg of hydrogen are injected during the run, and 32.14 (= 48.45 - 16.31) kg are combined with oxygen during the two burns to form steam. Note that the injected spray mass includes only mass injected prior to the switchover to the recirculation mode. During the run, approximately twice as many flow timesteps were taken as heat-transfer timesteps and about 11% of the flow timesteps had to be repeated. Most of the flow timesteps were repeated to prevent excessive pressure and/or temperature changes during the heat-transfer timesteps (most likely a result of

the rapid changes occurring at the beginning of the burns). The size of the flow timesteps was controlled principally by pressure changes with about 10% of the timesteps determined by pressure and/or temperature changes in the heat-transfer timesteps and by HECTR trying to stretch out the timesteps after each burn was completed. At the end of the summary, the final compartment conditions are printed. The title of this summary indicates that HECTR completed its last heat-transfer timestep at a fraction of a second past the specified 60-s simulation time.

6.1.4 ACHILES Output

The ACHILES (CRAY) initial header information for this sample problem is presented next (see Section 5.2 for more details).

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                             $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

    (S)IMPLE TWO COMPARTMENT PROBLEM$
    ----------------------------------------------------------------------------

THIS IS THE SITUATION OF TWO COMPARTMENTS, ONE STACKED ABOVE THE OTHER.
THE UPPER COMPARTMENT IS ABOUT THREE TIMES LARGER THAN THE LOWER COMPARTMENT.

                        +------------------+
                        !        ^         !    COMPARTMENT 1
                        +-----+- ! -+------+
                              !     !           COMPARTMENT 2
                              +-----+

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

>>>   2 COMPARTMENT(S)          1 FLOW JUNCTION(S)          3 SURFACE(S) <<<
>>>   1 FAN(S)                  1 SUMP(S)                                <<<

    SPRAYS WERE AUTO          FANS WERE AUTO

MINIMUM HEAT TRANSFER TIMESTEP        = 1.000E-05 SECONDS
MAXIMUM HEAT TRANSFER TIMESTEP        = 2.000E+00 SECONDS
MINIMUM FLOW TIMESTEP                 = 1.000E-06 SECONDS
MAXIMUM FLOW TIMESTEP                 = 2.000E+00 SECONDS
MAXIMUM TIMESTEP PRESSURE CHANGE      = 10.1325   KPA
MAXIMUM TIMESTEP TEMPERATURE CHANGE = 10.0000   K
```

```
HYDROGEN LIMITS FOR    IGNITION    PROPAGATION    PROPAGATION    PROPAGATION
                                     UPWARDS       SIDEWAYS       DOWNWARDS

COMPARTMENT   1          8.0%         4.1%           6.0%           9.0%
COMPARTMENT   2          8.0%         4.1%           6.0%           9.0%

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

COMPARTMENTS:

  1. UPPER COMPARTMENT
  2. LOWER COMPARTMENT

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

SURFACE TYPE KEY:
   1. SLAB
   2. LUMPED MASS
   3. POOL
   4. ICE
   5. ICE CONDENSER WALL


SURFACES (BY COMPARTMENT NUMBER - SURFACE TYPE -
          NUMBER OF LAYERS IF A SLAB) FOLLOWED BY THE SURFACE NUMBER
         (AND THE SUMP NUMBER IF A SUMP):

(  1-2)     1.       UPPER COMPARTMENT STEEL
(  2-1-1)   2.       LOWER COMPARTMENT CONCRETE
(  2-3)     3. ( 1) LOWER COMPARTMENT POOL (SUMP)
                     (SPRAY SOURCE SUMP)

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

FLOW JUNCTIONS/COMPARTMENT INTERCONNECTIONS (INTERCONNECTION AREA IN M**2 -
                                             FLOW COEFFICIENT):

  1.   2 =>   1    2-WAY                    UPWARDS      (   300.00 -   1.20)

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

FAN CONNECTIONS (VOLUMETRIC FLOW RATE IN M**3/S WITH A NEGATIVE
                 NUMBER INDICATING THE USE OF A HEAD CURVE):

  1.   1 =>   2     DOWNWARDS     (   50.0)

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

*** THIS RUN ENDED AT    60.088 SECONDS ***
```

```
APPROXIMATE GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS
====================================================

   33.929 SECONDS            156.0 KPA
   58.675 SECONDS           1136.7 K

====================================================

APPROXIMATE COMPARTMENT PRESSURE AND TEMPERATURE MAXIMUMS
---------------------------------------------------------

COMPARTMENT   1:        33.929 SECONDS      156.0 KPA
                        33.929 SECONDS      379.8 K

COMPARTMENT   2:        33.906 SECONDS      156.0 KPA
                        58.675 SECONDS     1136.7 K

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

UOF =  8          UOA =  0

NHT =      276          NFL =      120          NAH =        0
```

The ACHILES header information provides a useful summary of the geometry and some of the major parameters of the problem. Most of this information is self-explanatory, but a few points need to be made clear. The maximum timestep pressure and temperature changes refer to heat-transfer timesteps (these are the values of the HECTR variables DPRSMX and DTMPMX). The pressure and temperature maximums are labeled approximate because they are determined from the values in the HECTR output files. These files may not contain all the pressures and temperatures that were calculated at each timestep during the run, but rather will contain only those pressures and temperatures for which differences from previous output values were "significant" (see Section 5.1.5). It is possible that these maximums do not exactly match those tabulated in the HECTR output, but they should be very close. The next to last line indicates that flow timestep variables were written by HECTR to Unit 8, but no additional heat-transfer timestep variables were written. The final line lists the number of records read by ACHILES for each major type of variable (main heat-transfer timestep variables, flow timestep variables, and additional heat-transfer timestep variables, respectively). Since UOA was zero (the default condition), NAH should be zero. These last numbers can be compared to the number of timesteps taken to see what fraction of the results is being saved.

For the sample ACHILES input listed in Section 6.1.2, various tables and plots were produced. A portion of one of the tables is shown below.

COMPARTMENT 2

TIME (SECONDS)	PRESSURE (KPA)	TEMP (K)	XH2O	XN2	XO2	XH2	BURN?
0.000	101.4	300.0	0.0336	0.7593	0.2071	0.0000	F
1.609	101.7	300.4	0.0335	0.7559	0.2062	0.0045	F
2.463	101.8	300.6	0.0334	0.7541	0.2057	0.0068	F
3.744	101.9	300.9	0.0333	0.7514	0.2049	0.0104	F
5.667	102.1	301.4	0.0331	0.7474	0.2038	0.0156	F
7.630	102.4	301.8	0.0329	0.7434	0.2027	0.0210	F
9.594	102.6	302.3	0.0327	0.7393	0.2016	0.0263	F
11.560	102.8	302.7	0.0326	0.7353	0.2005	0.0316	F
13.528	103.0	303.2	0.0324	0.7313	0.1994	0.0369	F
15.498	103.3	303.6	0.0322	0.7273	0.1983	0.0422	F
17.469	103.5	304.0	0.0320	0.7233	0.1973	0.0474	F
19.442	103.7	304.5	0.0319	0.7194	0.1962	0.0526	F
21.417	103.9	304.9	0.0317	0.7154	0.1951	0.0577	F
23.393	104.2	305.3	0.0315	0.7115	0.1941	0.0629	F
25.372	104.4	305.7	0.0314	0.7077	0.1930	0.0680	F
27.352	104.6	306.2	0.0312	0.7038	0.1919	0.0731	F
29.334	104.8	306.6	0.0310	0.6999	0.1909	0.0781	F
31.318	105.1	307.0	0.0309	0.6961	0.1899	0.0832	F
31.341	107.4	315.4	0.0317	0.6964	0.1895	0.0825	T
31.369	107.1	323.3	0.0327	0.6966	0.1891	0.0816	T
31.401	106.8	332.3	0.0338	0.6970	0.1886	0.0806	T
31.425	108.3	340.5	0.0346	0.6972	0.1883	0.0799	T
31.447	109.8	348.2	0.0354	0.6974	0.1880	0.0792	T
31.476	110.4	357.2	0.0365	0.6977	0.1875	0.0783	T

This table shows the Compartment 2 (lower compartment) pressure, temperature, and gas mole fractions as a function of time (additional columns showing the density and injection rate of the hydrogen source into this compartment are not presented due to space limitations). The eighth column, labeled BURN?, displays the value of a logical variable that indicates whether a burn is occurring in the compartment at the beginning of a timestep. The first burn actually started at 31.318 seconds, but because of the particular order of calculations and output in HECTR, the beginning of the burn is not indicated in this table until one timestep later. The end of the burn is indicated properly, however.

A sampling of the plots produced by ACHILES for this case is shown in Figures 6-1 through 6-5. Figure 6-1 shows the upper compartment pressure versus time. The two sharp rises are due to the two hydrogen burns. The sharp drop at about 37 seconds is a result of the spray initiation. Figure 6-2

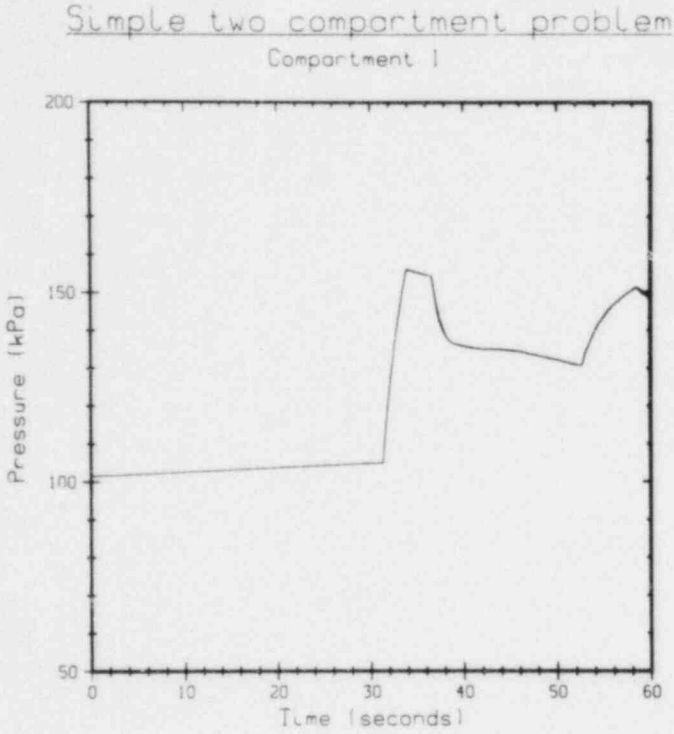


Figure 6-1. Upper Compartment Pressure

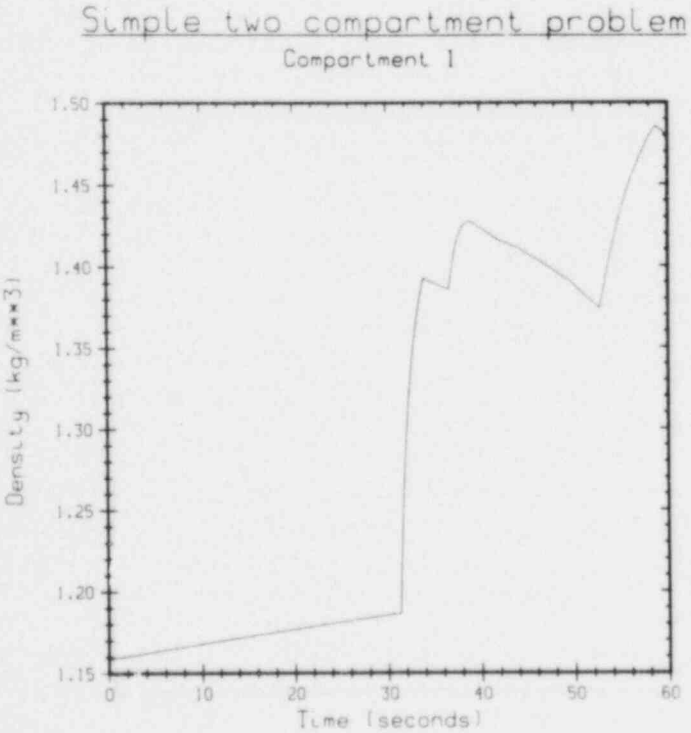


Figure 6-2. Upper Compartment Gas Density

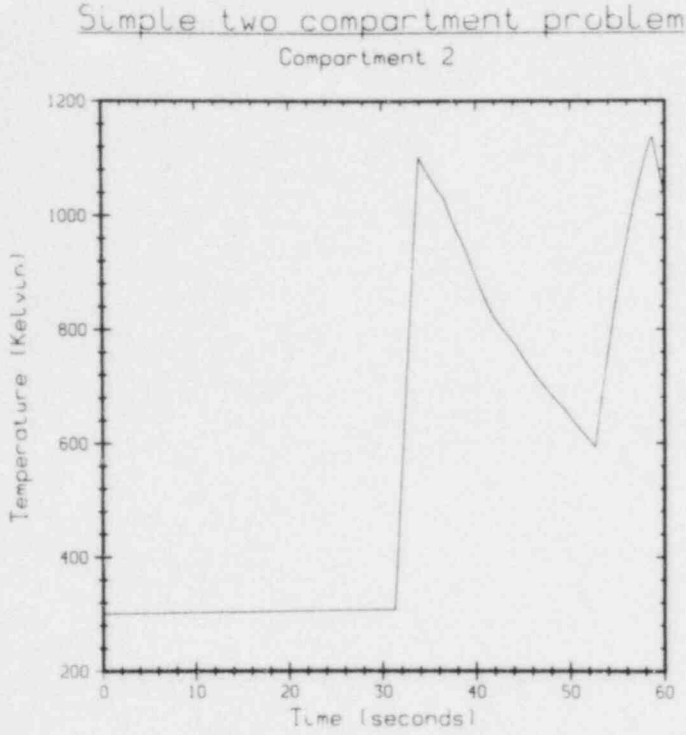


Figure 6-3. Lower Compartment Gas Temperature

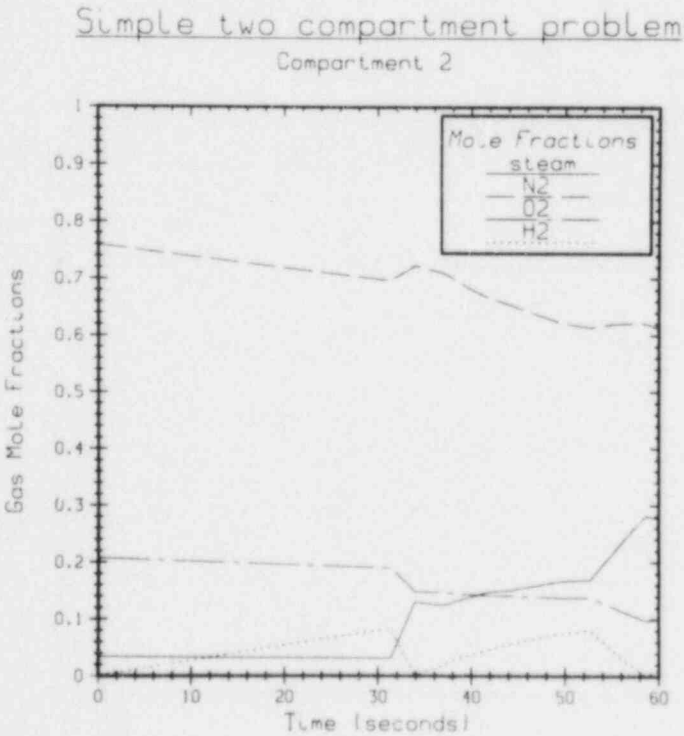


Figure 6-4. Lower Compartment Gas Composition

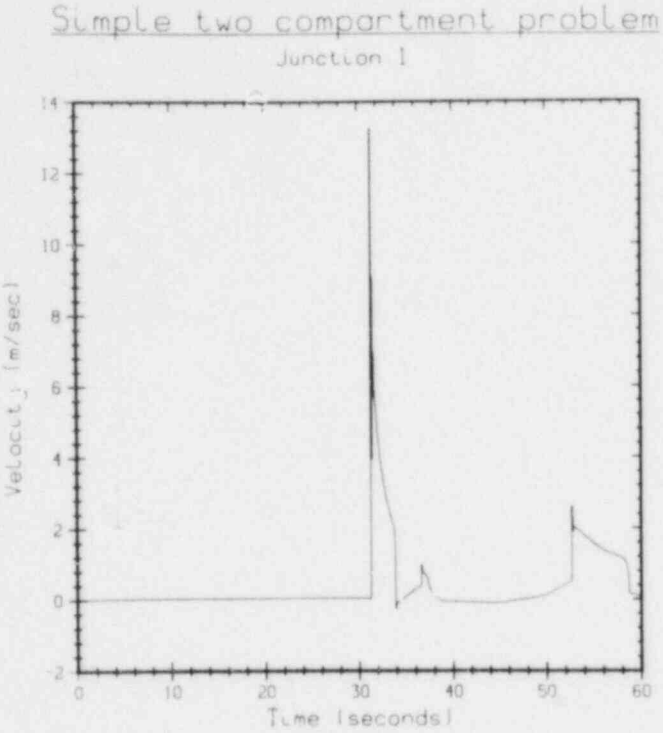


Figure 6-5. Gas Flow Velocity

shows the gas density history of the upper compartment. The two burns and the initiation of the sprays show up very clearly in this figure. The pressure in the lower compartment tracks the upper compartment pressure very closely, so that figure is not shown here. The gas temperature and the four gas mole fractions in the lower compartment versus time are displayed in Figures 6-3 and 6-4, respectively. Hydrogen is a source gas so its concentration rises until a burn occurs that causes both the hydrogen and the oxygen levels to drop and the steam level to rise. The sprays also cause an increase in the steam mole fraction, but the effect is not as large as that caused by a burn. The last figure (Figure 6-5) exhibits the gas velocity through the flow junction connecting the two compartments. Here, positive flow is in the upward direction (from the lower into the upper compartment). The two burns and the initiation of the sprays again show up very clearly. The change in slope at about 50 seconds is caused by the fans starting.

6.2 Ice-Condenser Containment Problem

6.2.1 Containment Description

The general arrangement of an ice-condenser containment is shown in Figure 6-6. Sequoyah is used as the reference plant for this calculation. The reactor coolant system is located in the lower compartment. During an accident, pressurization due to blowdown from the reactor coolant system causes the ice-condenser doors to open and gases to flow from the lower compartment through the ice condenser to the dome. As the gases flow through the ice regions, they are cooled and steam is condensed, thereby limiting containment pressurization.

The ice condenser is essentially a cold-storage room shaped in the form of a "C" with approximately 300 degrees of arc, a 16-m inside radius, and a 20-m outside radius. The ice condenser is approximately 24 m tall. It consists of three basic regions: the lower plenum, the ice region, and the upper plenum. The lower plenum doors are normally closed, but they open upon slight pressurization in the lower compartment, allowing gases to flow through the lower plenum and up into the ice region. The lower plenum doors are designed to reclose to block any downward gas flow through the ice condenser. The ice region contains perforated metal tubes or baskets that are filled with ice. Gases flow out of the ice region to the upper plenum via the intermediate deck doors. These doors are normally closed under the force of gravity, but they open upon pressurization from below to permit upward flow. They also reclose to prevent downward flow. An additional set of lightweight doors, the top deck doors, are located at the top of the upper plenum.

Two recirculation fans function to bring air from the dome to the lower compartment and to reduce the concentration of hydrogen in stagnant areas. The fans draw air from the dome, the steam generator enclosures, the pressurizer enclosure, the accumulator spaces, and the instrument room, and they exhaust into the lower compartment through the annular equipment areas. Forced circulation is maintained from the lower compartment through the ice condenser to the dome. The fans are actuated upon receipt of a high containment pressure signal (typically 122 kPa).

A containment spray system is provided for long-term containment heat removal. This system sprays water droplets into containment from spray rings at the top of the dome. Droplets that fall to the floor drain to the lowest portion of the dome compartment, the refueling canal. Two drains in the bottom of the refueling canal allow the water to drain into the recirculation sump, which is located in the lower compartment.

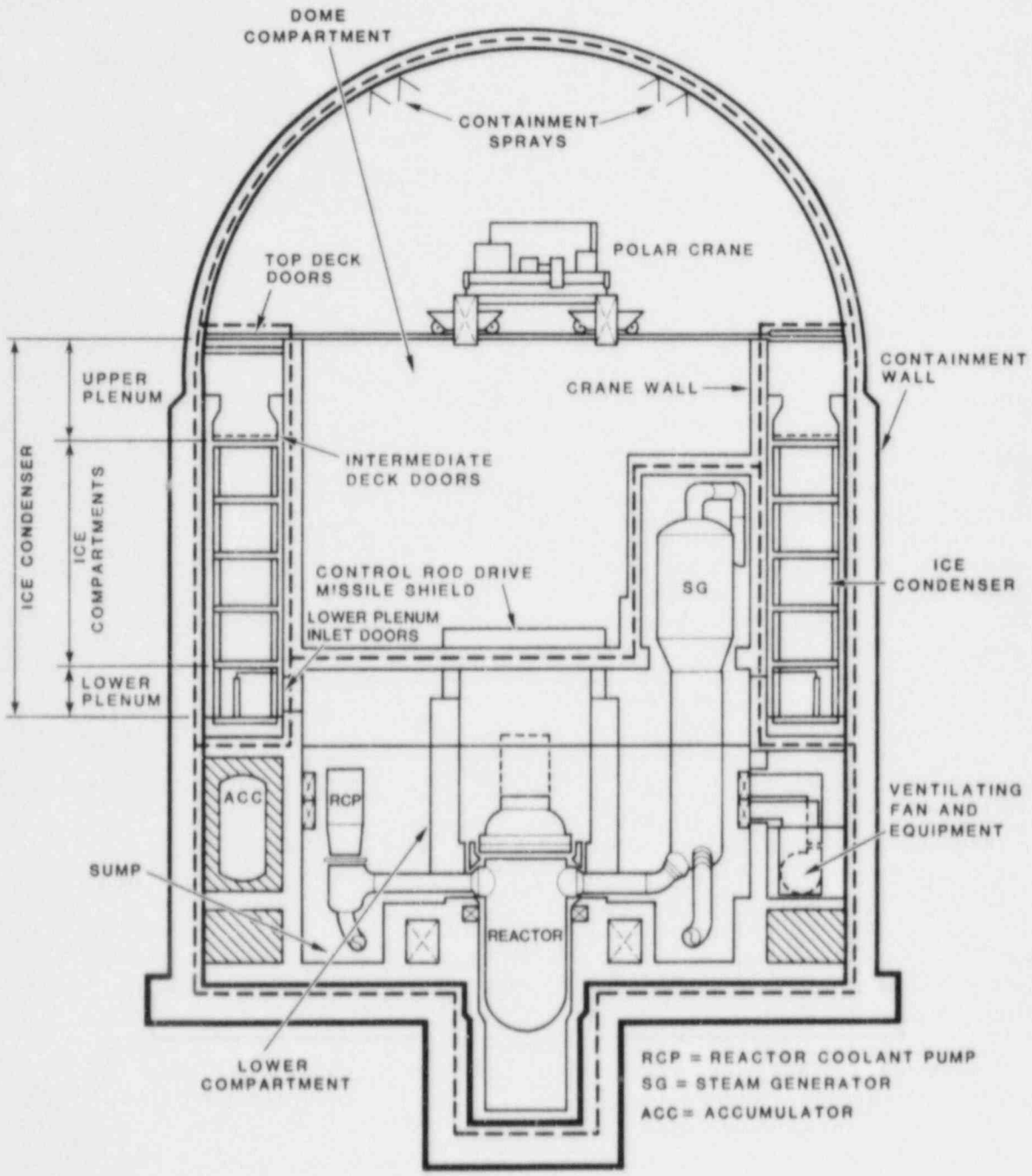


Figure 6-6. PWR Ice-Condenser Containment

Note that these drains can provide a gas flow path from the lower compartment to the dome that bypasses the ice condenser. However, when the sprays are operating, the refueling canal fills up with water to some steady-state depth such that flow through the drains roughly matches the flow rate of the sprays. Also, for any accident in which the inventory of the refueling water storage tank is injected into containment, the water level in the lower compartment will rise above the level of the drains. Thus, gas flow through these drains is precluded early in many accidents.

The spray system has two modes of operation, the injection mode and the recirculation mode. In the injection mode, the system draws water from the refueling water storage tank, which is located outside of containment. In the recirculation mode, water is drawn from the recirculation sump in the lower compartment and is cooled by a recirculation heat exchanger before being sprayed into the dome.

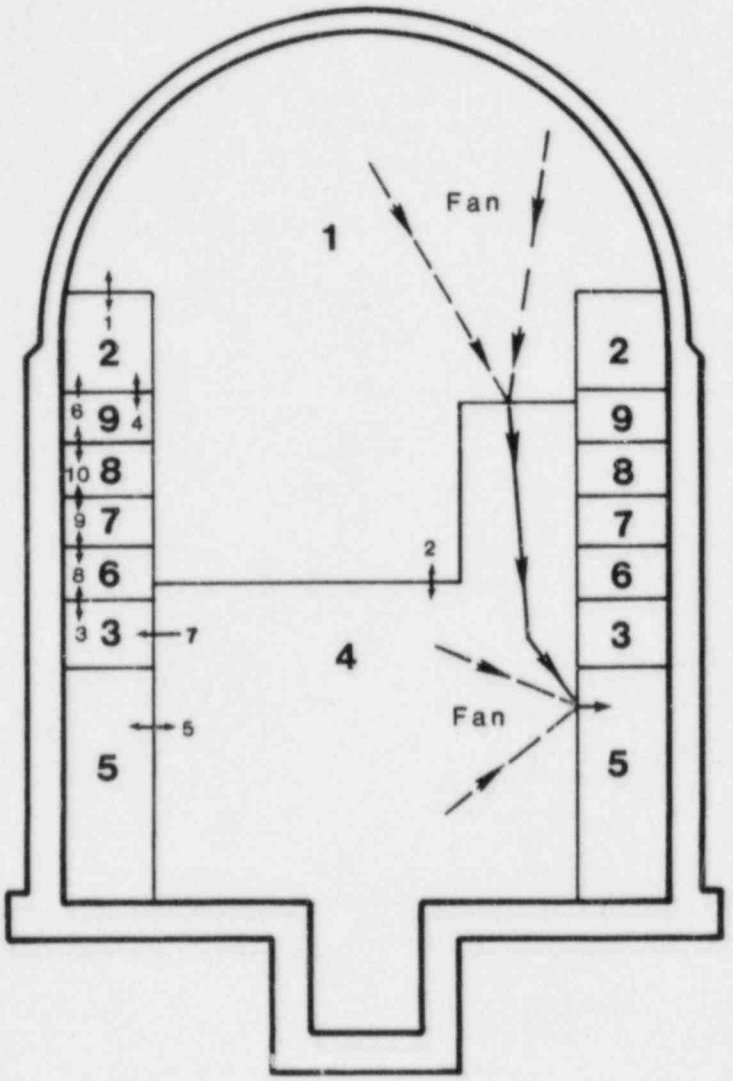
In some containments, deliberate ignition systems have been installed in an attempt to mitigate the effects of hydrogen combustion. Typically, these systems consist of igniters that are located in the upper plenum of the ice condenser, the dome, and throughout the lower regions of containment. The igniters are installed to improve the likelihood that ignition will occur early, before hydrogen accumulates to a level that could pose a threat to containment integrity. These igniters may not be available in some loss-of-power accidents.

6.2.2 Computational Model

The containment model used for this calculation is shown in Figure 6-7. A nine-compartment model was employed, including the dome (1), the upper plenum (2) and lower plenum (3) of the ice condenser, the lower compartment (4), a dead-ended region (5), and four ice compartments (6,7,8,9).

The ice condenser is represented by 6 Compartments. Compartment 2 represents the upper plenum, Compartment 3 the lower plenum, and Compartments 6 through 9 are four equal volumes containing ice. Volume changes caused by ice melting are included as well as heatup of the water falling through the lower plenum. The only igniters in the ice condenser are in the upper plenum. No igniters are present in the lower plenum or the ice compartments, and the only burns that can occur in these compartments are those that begin elsewhere and propagate in.

Two sumps are modeled for this case. The first sump is the large recirculation sump that is located in the lower compartment. Sprays that drain from the dome, surface condensate from Compartments 1, 4, and 5, and liquid from the



KEY

1 - Compartment Number

1 - Flow Junction Number

→ - One-way Flow Junction

↔ - Two-way Flow Junction

Note: Igniters Present in Compartments 1, 2, 4, and 5.

Compartment Descriptors

1. Dome
2. Upper Plenum
3. Lower Plenum
4. Lower Compartment
5. Dead-Ended Region
6-9. Ice Compartments

Figure 6-7. PWR Ice-Condenser Containment Model

primary system are all added to the inventory of this sump. Water drawn by the containment spray system when in the recirculation mode is subtracted from the sump inventory. The volume of the lower compartment is adjusted to account for changes in the free gas volume due to the accumulation of liquid. The second sump is located in the lower plenum. This sump collects melted ice and condensate from the ice condenser. A relatively small amount of water is allowed to collect in this sump before it overflows into the recirculation sump in the lower compartment.

Flow junctions are also indicated in Figure 6-7. Of particular importance are Junctions 2, 4, 6, and 7. Junction 2 represents the floor drains connecting the dome with the lower compartment. Gas flow through this junction is precluded in either of two situations. First, when the sprays are operating, drainage from the dome to the lower compartment through this junction will preclude simultaneous gas flow. Second, when sufficient water (750 m^3) accumulates in the recirculation sump, the liquid level is high enough to block gas flow through this junction. Junction 4 represents bypass flow around the ice-condenser intermediate deck doors, and Junctions 6 and 7 represent the intermediate deck doors and the lower plenum inlet doors, respectively. The top deck doors are not modeled in this example. Fans are assumed to transfer gas from the dome and the lower compartment into the dead-ended region, with the flow from the dome to the dead-ended region dominating.

Both the sprays and the fans are activated based on a pressure set point of 122 kPa. Once this containment pressure is reached, the sprays are activated after a 30-s delay, and the fans are activated after a 600-s delay.

HECTR Version 1.0 does not address the possible effects of stable diffusion flames or jets. Such burning might occur at the hydrogen release point if the local area is not steam-inerted. It may also be possible to establish stable flames in or just above the ice condenser, although non-steady gas flow caused by movement of the ice-condenser doors may make this unlikely.

6.2.3 Case Description and Input Listing

The case presented is a small-break loss-of-coolant accident in which emergency core cooling (ECC) fails, but the sprays and fans are assumed to function normally. All of the initial conditions and the geometric and containment system information is included in the input listing presented below. The default combustion parameters are used except for the propagation time through Junction 7. As discussed at the end of Section 3.6, using a longer propagation time may prevent propagation from the lower compartment into the

lower plenum of the ice condenser. For ice-condenser problems, we recommend some additional restrictions on the time-step control, as are shown in the pseudo-NAMELIST input. These restrictions are warranted because of the effects of the one-way ice-condenser doors on the fluid mechanics, and the effects of the heatup of melted ice and condensate in the lower plenum of the ice condenser. The source terms for this case are provided from an external file, as discussed in Section 4.4. Setting MRCHSC equal to 4 in the input indicates that these sources will be injected into Compartment 4. Additional calculations for an ice-condenser containment using a prerelease version of HECTR are presented in References 2 and 12.

INPUT LISTING FOR THE SAMPLE PROBLEM

This is the HECTR input section as described in Section 4.2.

```
! INITIAL NAMELIST TYPE INPUT
! THIS PROBLEM IS BEING RUN ON A CYBER 76.
CMPUTR=CYBER
UOA=9
$ END OF NAMELIST INPUT
!*********************************************
! PROBLEM GEOMETRY AND CONTAINMENT DESCRIPTION
!*********************************************
ICE-CONDENSER SAMPLE PROBLEM$

THIS IS A 9 COMPARTMENT SAMPLE PROBLEM DEALING WITH A
SMALL BREAK LOCA IN THE SEQUOYAH ICE-CONDENSER
CONTAINMENT.  THIS SAMPLE PROBLEM IS FOR ILLUSTRATION
PURPOSES ONLY AND SHOULD NOT BE CONSIDERED AS NECESSARILY
REPRESENTATIVE OF ANY PARTICULAR ACCIDENT SEQUENCE.



350000.  ! LOWER BOUND FAILURE PRESSURE (36 PSIG)
5 ! NUMBER OF COMPARTMENTS EXCLUDING ICE REGION
!
! FOR EACH COMPARTMENT: THE VOLUME, ELEVATION, FLAME PROPAGATION
! LENGTH, NUMBER OF SURFACES, AND INTEGERS SPECIFYING WHICH SUMP
! TO DUMP EXCESS WATER (FROM SUPERSATURATION) INTO AND WHICH SUMP
! THE SPRAYS FALL INTO.
!
UPPER COMPARTMENT
18435.
29.
17.5
3
1
1
```

```
UPPER PLENUM
1330.
29.
9.0
1
2
2
LOWER PLENUM
685.
10.
3.5
3
2
2
LOWER COMPARTMENT
8184.
0.
12.0
3
1
1
DEAD ENDED REGIONS
2662.
0.
6.0
2
1
1
! FOR EACH SUMP, SUMP NUMBER, MAXIMUM VOLUME, SUMP NUMBER THAT
! THIS SUMP OVERFLOWS TO
1 8184. 0
2 80. 1  ! THIS SUMP ALLOWS SOME HOLDUP IN THE LOWER PLENUM
         ! BEFORE FLOWING INTO THE LOWER COMPARTMENT SUMP
$
!
! FOR EACH SURFACE: TYPE OF SURFACE, MASS OF SURFACE, AREA OF
! SURFACE, CHARACTERISTIC LENGTH, SPECIFIC HEAT, EMISSIVITY,
! INTEGER INDICATING WHICH SUMP THE CONDENSATE GOES INTO.  FOR
! SLABS (STYPE = 1), THE NUMBER OF LAYERS IN THE SURFACE, AND FOR
! EACH, THE THICKNESS, THERMAL DIFFUSIVITY, AND THERMAL
! CONDUCTIVITY.  FINALLY, THE NODING INFORMATION AND BOUNDARY
! CONDITIONS ARE SPECIFIED (0'S INDICATE HECTR WILL DETERMINE
! THE VALUES INTERNALLY). NOTE THAT SOME OF THE NUMBERS SET TO 1.
! ARE NOT USED FOR THAT SURFACE TYPE.
!
! UPPER COMPARTMENT SURFACES
!
DOME
1 1. 1762. 8.0 1. .9 1
1
.0127 1.28E-5 47.25
0 0. 0. 0.
```

```
UPPER COMPARTMENT CONCRETE
1 1. 2333. 5. 1. .9 1
1
.414 5.8E-7 1.454
0 0. 0. 0.
UPPER COMPARTMENT STEEL
1 1. 2000. 1. 1. .9 1
1
.013 1.28E-5 47.25
0 0. 0. 0.
!
! UPPER PLENUM SURFACES
!
UPPER PLENUM STEEL
1 1. 1000. 5. 1. .9 2
1
.013 1.28E-5 47.25
0 0. 0. 0.
!
! LOWER PLENUM SURFACES
!
LOWER PLENUM WALLS
1 1. 280. 3. 1. .9 2
1
.013 1.28E-5 47.25
0 0. 0. 0.
ICE CONDENSER SUPPORT STRUCTURE
1 1. 2660. .2 1. .9 2
1
.0081 1.28E-5 47.25
0 0. 0. 0.
LOWER PLENUM SUMP
3 0. 310. 4. 1. .94 2
!
! LOWER COMPARTMENT SURFACES
!
LOWER COMPARTMENT STEEL
1 1. 3000. 2. 1. .9 1
1
.069 1.28E-5 47.25
0 0. 0. 0.
LOWER COMPARTMENT CONCRETE
1 1. 3569. 4. 1. .9 1
1
.1 5.8E-7 1.454
0 0. 0. 0.
SUMP SURFACE
3 0. 353. 6. 1. .94 1
!
! DEAD ENDED COMPARTMENT SURFACES
!
DEAD ENDED STEEL
1 1. 1834. 4. 1. .9 1
1
```

```
.031 1.28E-5 47.25
0 0. 0. 0.
DEAD ENDED CONCRETE
1 1. 3257. 4. 1. .9 1
1
.448 5.8E-7 1.454
0 0. 0. 0.
!
! FLOW JUNCTION DATA: COMPARTMENT ID'S, TYPE OF CONNECTION, FLOW
! AREA, LOSS COEFFICIENT, L/A RATIO, RELATIVE POSITION OF
! COMPARTMENTS, AND JUNCTION ELEVATION. COMPARTMENT ID OF 0
! INDICATES THE ICE CONDENSER. JUNCTIONS WITHIN THE ICE
! CONDENSER ARE SET UP INTERNALLY. ADDITIONAL INFORMATION
! IS PROVIDED FOR JUNCTION TYPES 3 AND 4.
!
2 1 1 186.   1.43 .015    1  30.8
4 1 4 .204   1.5  1.0     1  11.2
1 750.
3 0 1 167.   0.2  .044    1  11.2
0 2 1 1.8581 1.5  0.2     1  25.7
5 4 1 27.7   4.2  .007    0  0.0
0 2 3 91.3   0.2  .049    1  25.7
0. 263.4  3.791E4  1.56
4 3 3 78.    0.89 .0055   1  10.0
0. 0. 142.07 0.96
$
!
! ICE CONDENSER INPUT
!
! LOWER AND UPPER PLENUM COMPARTMENTS; SUMP THAT THE LOWER PLENUM
! CONDENSATE AND MELTED ICE DRAINS INTO.
3 2 2
! ICE DESCRIPTION: TOTAL MASS, AREA, TEMPERATURE, LENGTH,
! EMISSIVITY, VOLUME.
1.11E6 2.48E4 273.5 14.53 .94 2.0E3
! WALL AND STRUCTURES IN ICE CONDENSER (EXCLUDING BASKETS): MASS,
! AREA, SPECIFIC HEAT, EMISSIVITY
2.0E5 2058. 485.7 .9
! MASS OF BASKETS, AREA OF BASKETS, DRAIN TEMPERATURE.
1.47E5 9.92E3 310.
! ELEVATION OF BOTTOM OF ICE, FLOW AREA, LOSS COEFFICIENT FOR
! EACH ICE JUNCTION, TOTAL FREE GAS VOLUME
11.2 167. .2 2444.
!
$
!
! FAN DATA
! TEMP. AND PRESS. SETPOINTS, DELAY TIME, AND TIME THAT FANS
! REMAIN OPERATIVE AFTER INITIATION.
! HIGH VALUE FOR TEMP. SETPOINT INDICATES THAT VALUE WON'T BE
! USED.
10000.  121590.  600.  1.E10
! COMPARTMENT ID'S, FLOW RATE (- INDICATES USE OF HEAD CURVE),
! SHUTOFF HEAD (PA), EFFICIENCY, RELATIVE POSITION OF
```

```
! COMPARTMENTS.
1  5  -54.7  1327.3575  1.  -1
4  5  -1.17  1327.3575  1.   0
$
$
!
! RADIATIVE BEAM LENGTHS - UPPER RIGHT HALF OF MATRIX IS INPUT.
! ICE SURFACES ARE NOT INCLUDED HERE. (THEY ARE DONE INTERNALLY)
!
17.5 23. 20. 12. 0. 0. 0. 0. 0. 0. 0. 0.
10. 15. 0. 0. 0. 0. 0. 0. 0. 0. 0.
10. 10. 0. 0. 0. 0. 0. 0. 0. 0.
5. 0. 0. 0. 0. 0. 0. 0. 0.
8. 5. 5. 0. 0. 0. 0. 0.
5. 3. 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0.
3. 3. 5. 0. 0.
3. 5. 0. 0.
0. 0. 0.
3. 3.
3.
!
! VIEW FACTORS: UPPER RIGHT HALF OF MATRIX IS INPUT
! ICE SURFACES ARE NOT INCLUDED HERE.
!
.45 .3 .2 .05 0. 0. 0. 0. 0. 0. 0. 0.
.6 .173 0. 0. 0. 0. 0. 0. 0. 0. 0.
.597 .025 0. 0. 0. 0. 0. 0. 0. 0.
.862 0. 0. 0. 0. 0. 0. 0. 0.
.4 .3 .3 0. 0. 0. 0. 0.
.883 .085 0. 0. 0. 0. 0.
0. 0. 0. 0. 0. 0.
.441 .5 .059 0. 0.
.531 .0493 0. 0.
0. 0. 0.
.36 .64
.64
!
! SPRAY INPUT
! NUMBER OF COMPARTMENTS WITH SPRAYS, AND ID OF THOSE
! COMPARTMENTS. SPRAY TEMP DURING INJECTION PHASE, FLOW RATE
! (M**3/S), NUMBER OF DROP SIZES, FREQUENCY AND DIAMETER
! (MICRONS) FOR EACH DROP SIZE.
1
1 300.6 0.599 2
0.95 309.
0.05 810.
$
! COMPARTMENT ID AND SPRAY FALL HEIGHT FOR THAT COMPARTMENT.
1 16.
$
! TEMPERATURE AND PRESSURE SETPOINTS, DELAY TIME FOR SPRAYS,
! TIME THAT SPRAYS REMAIN OPERATIVE AFTER INITIATION.
```

```
! HIGH TEMPERATURE INDICATES THAT NUMBER WON'T BE USED.
10000. 121590. 30. 1.E10
! INJECTION TIME, RATED SPRAY FLOW RATE (KG/S), HEAT EXCHANGER
! RATED EFFECTIVENESS (W/K), SECONDARY SIDE INLET TEMP, RATED
! SECONDARY SIDE FLOW RATE (KG/S), SUMP THAT WATER IS DRAWN FROM.
2000. 587. 3.74E6 301.5 7.55E2 1
$
! ************************************************************
! ENTER INITIAL CONDITIONS AND ACCIDENT SCENARIO INFORMATION
! ************************************************************
! SIMULATION TIME
7500.
!
! COMPARTMENT INITIAL CONDITIONS: TEMP; PARTIAL PRESSURES OF
! STEAM, NITROGEN, OXYGEN, HYDROGEN; CONVECTIVE VELOCITY.
!
! UPPER COMPARTMENT
303.
345.  81187.  21424.   0.
.3
! UPPER PLENUM
273.5
620.  80912.   21424.   0.
.3
! LOWER PLENUM
273.5
620.  81105.   21475.   0.
.3
! LOWER COMPARTMENT
311.
620. 81000.   21447.     0.
.3
! DEAD ENDED COMPARTMENT
311.
620.  81200.  21500.     0.
.3
! ICE CONDENSER INITIAL CONDITIONS
273.5
620.  81200.  21500.    0.
!
! ADDITIONAL SOURCE TERMS (MASS FLOW IN KG/S AND ENTHALPY IN
!  J/KG IN JANAF TABLE UNITS).
$ ! NO WATER SOURCES
$ ! NO NITROGEN SOURCES
$ ! NO OXYGEN SOURCES
$ ! NO HYDROGEN SOURCES
$ ! NO WATER REMOVAL FROM SUMP
!
! INITIAL SURFACE TEMPERATURES
! UPPER COMPARTMENT
303. 303. 303.
! UPPER PLENUM
273.5
```

```
! LOWER PLENUM
273.5 273.5 273.5
! LOWER COMPARTMENT
311. 311. 311.
! DEAD ENDED COMPARTMENT
311. 311.
!
! NAMELIST INPUT
!
! SET IGNITION LIMITS TO 1. IN LOWER PLENUM AND ICE CONDENSER (NO
! IGNITERS).  DEFAULT VALUE OF 8% WILL BE USED ELSEWHERE.
XHMNIG(3)=1.
XHMNIG(6)=1.
XHMNIG(7)=1.
XHMNIG(8)=1.
XHMNIG(9)=1.
! PROPAGATION TIME BETWEEN L.C. AND L.P. EQUAL .1 TIMES THE BURN
! TIME. KPROPJ = .5 ELSWHERE.
KPROPJ(7)=0.1
! MAX HEAT TRANSFER TIME STEP.
DTHTMX=0.5
SPRAYS=AUTO
FANS=AUTO
! INSERT SOURCE TERMS FROM MARCH TAPE INTO COMPARTMENT 4
MRCHSC=4
$
```

This is the ACHILES input section as described in Section 4.3.

```
!
! Namelist Type Input
!
CMPUTR=CYBER  ! Problem is being run on a CYBER 76
COMBXF=TRUE   ! Combine mole fraction plots into a single graph
$ END OF NAMLST INPUT
!
!   +--------+
!   ! Tables !
!   +--------+
!
! Main Heat Transfer Timestep Variables
!
NON   ! Pressure, temperature, gas mole fractions, if burning,
      ! gas density, hydrogen and steam sources (by compartment)
NON   ! Sump volumes (by sump)
NON   ! Surface temperatures, if condensing, dry or evaporating
      ! (by surface)
NON   ! Condensation rates, film thicknesses (by surface)
NON   ! (1) Source injection rates, (2) accumulated injected
      ! source masses, (3) external (MARCH) steam and hydrogen
      ! source information
```

```
NON   ! Spray mass evaporation rates, spray heat removal rates
      ! (by compartment)
NON   ! Fraction of initial ice mass remaining in the ice condenser
!
! Flow Timestep Variables
!
NON   ! Junction gas velocities, if closed or choked (by flow
      ! junction)
NON   ! Fan volumetric flow rates (by fan path)
NON   ! Suppression pool vent volumetric flow rates, suppression
      ! pool levels
!
! Additional Heat Transfer Timestep Variables
!
NON   ! Net total incident heat fluxes (by surface)
NON   ! Net incident radiation (by surface)
NON   ! Convective heat fluxes (by surface)
NON   ! Water drainage rates (by surface)
NON   ! Emitted spray drop temperatures (by compartment)
NON   ! Ice condenser information: melting rates, drain
      ! temperature, etc.
!
!   +-------+
!   ! Plots !
!   +-------+
!
! Main Heat Transfer Timestep Variables
!
ALL   ! Pressure, temperature, gas density, gas mole fractions
      ! (by compartment)
!
0 1000 8000 4 ! Minimum time (s), time stepsize (s), maximum time
              ! (s) and number of tick marks to be plotted per step
!
ALL   ! Sump volumes (by sump)
NON   ! Surface temperatures (by surface)
NON   ! Condensation rates (by surface)
NON   ! Film thicknesses (by surface)
ALL   ! (1) Source injection rates, (2) accumulated injected
      ! source masses, (3) external (MARCH) steam and hydrogen
      ! source information
NON   ! Spray evaporation rates (by compartment)
NON   ! Spray heat removal rates (by compartment)
ALL   ! Fraction of initial ice mass remaining in the ice condenser
!
! Flow Timestep Variables
!
ALL   ! Junction gas velocities (by flow junction)
ALL   ! Fan volumetric flow rates (by fan path)
NON   ! (1) Top, (2) middle, (3) bottom vent volumetric flow
      ! rates, (4) Drywell, (5) wetwell suppression pool levels
!
```

```
! Additional Heat Transfer Timestep Variables
!
NON    ! Net total incident heat fluxes (by surface)
NON    ! Net incident radiation (by surface)
NON    ! Convective heat fluxes (by surface)
NON    ! Water drainage rates (by surface)
NON    ! Emitted spray drop temperatures (by compartment)
ALL    ! (1)-(4) Ice surface melting rates in an ice condenser
ALL    ! (1) Mass rate of water flowing into lower plenum, (2)
       ! drain temperature. (3) Condensation rate, (4) heat
       ! transfer rate to drops in lower plenum
QUIT
```

6.2.4 Results

The source terms for this calculation are shown in Figures 6-8 to 6-10. Initially, liquid water is injected into containment and flashes to a mixture of steam and liquid. The values shown in Figures 6-8 and 6-9 are based on a flashing calculation in HECTR. At around 2000 s, the liquid injection rate drops rapidly as the break uncovers, and from that point on most of the water injected is vapor. Hydrogen begins entering containment at about 3000 s.

The pressure response for the dome (Compartment 1) is shown in Figure 6-11. The sprays come on automatically at 130 s, and the fans come on automatically at 700 s, with the latter event resulting in a significant drop in pressure. The minor variations in pressure between 2000 and 3000 s are due to changes in the source terms and the switchover of the sprays to recirculation mode at 2130 s.

Combustion begins in the upper plenum (Compartment 2) when the hydrogen concentration reaches 8%, as shown in Figure 6-12. This burn produces the first, small pressure spike at 4172 s. The pressure rise is small, because the gases in the upper plenum expand into the large volume of the dome. Generally, it can be expected that combustion will be frequent in the upper plenum, because steam is removed as the gases pass through the ice condenser, and the resultant mixture will be richer in hydrogen and air. The largest pressure rises generally come from burns that propagate from the upper plenum into the dome, with the last, largest pressure rise coming from a burn that propagates into a 6.8% hydrogen concentration in the dome. The smallest pressure rises come from burns that are confined to the upper plenum, and the intermediate-sized pressure rises come from burns that begin in the upper plenum and propagate downward into the ice regions or into very lean mixtures in the dome.

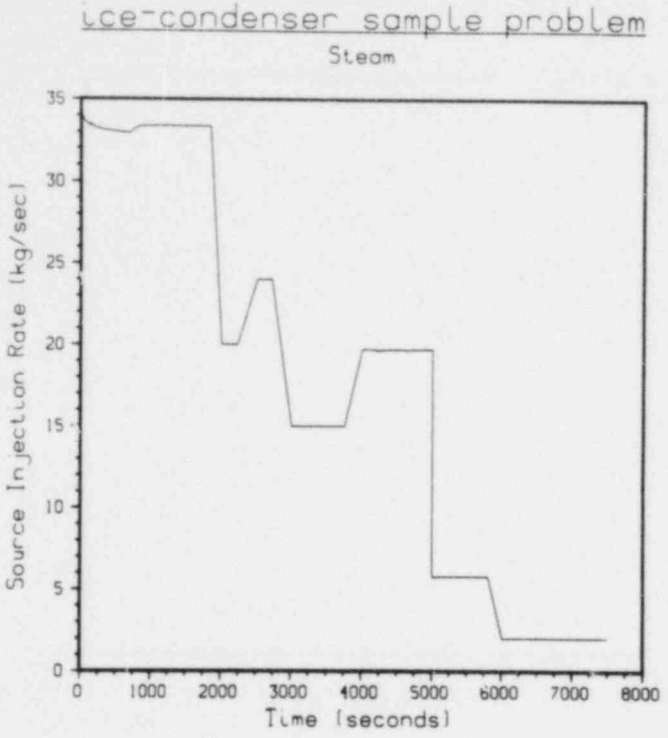


Figure 6-8. Steam Source Term for Ice-Condenser Sample Problem

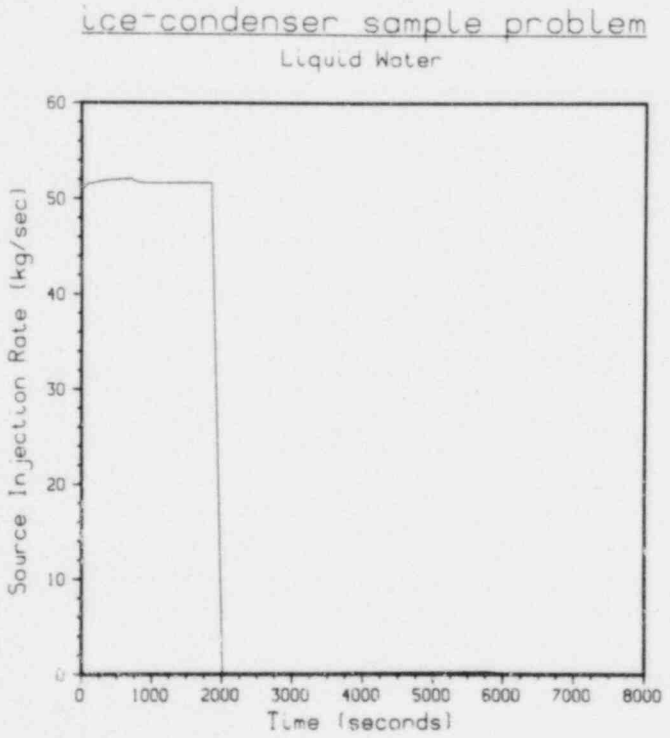


Figure 6-9. Liquid Source Term for Ice-Condenser Sample Problem

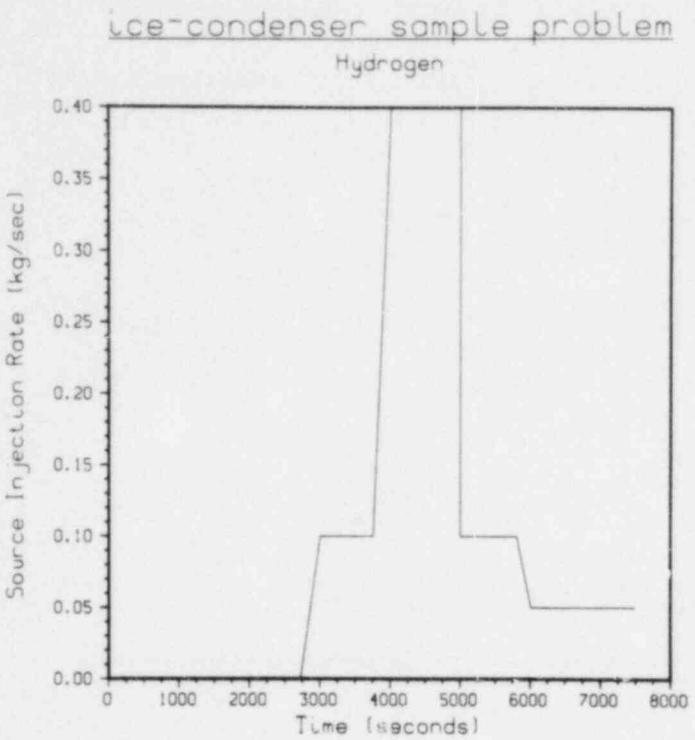


Figure 6-10. Hydrogen Source Term for Ice-Condenser Sample Problem

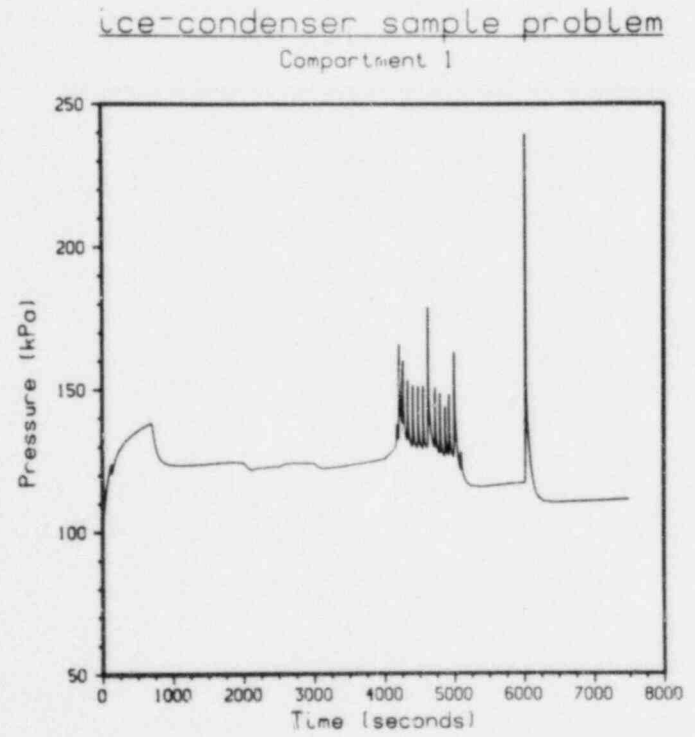


Figure 6-11. Dome Pressure Response for Ice-Condenser Sample Problem

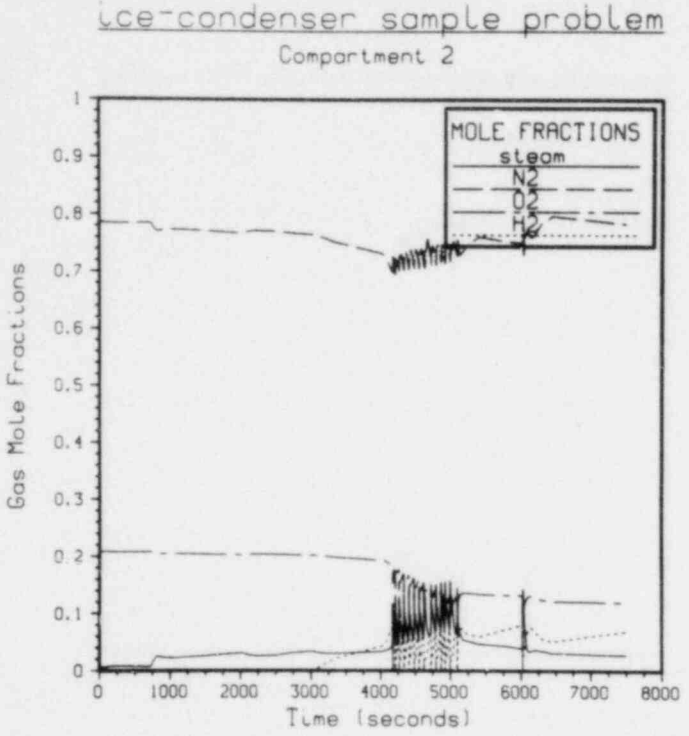


Figure 6-12. Upper Plenum Gas Composition for Ice-Condenser Sample Problem

Burns that take place in the lower regions of containment (none occurred in this case) tend to produce low pressure rises, because the gases can expand up through the ice condenser into the large volume of the dome. The ice-condenser doors prevent reverse flow (assuming that they survive) so that gas expansion for burns that occur in the upper regions of containment is prevented. Thus, burns in the upper regions of containment generally produce higher pressure rises than burns in the lower regions of containment.

In order to simulate 7500 s of accident time and process the output shown, as well as a great deal of additional output (as indicated in the ACHILES input), the following amount of CPU time was required on a CYBER 76 computer (which is about one-third to one-half as fast as a CRAY-1):

compile HECTR	8.2 s
run HECTR	2152 s
compile ACHILES	4.2 s
run ACHILES	285 s

The time spent running ACHILES can be increased or decreased by requesting more or less output. Additional information regarding this sample case may be obtained by studying the printed output from HECTR and ACHILES provided below.

HECTR OUTPUT

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                            $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

********************************* FROM MARCH ***********************************
**  EXAMPLE EXTERNAL SOURCE FILE  ***
********************************************************************************
```

INITIAL COMPARTMENT CONDITIONS AT 0.000 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	303.0	103.0	.0034	.7886	.2081	0.0000
2	273.5	103.0	.0060	.7859	.2081	0.0000
3	273.5	103.2	.0060	.7859	.2081	0.0000
4	311.0	103.1	.0060	.7859	.2081	0.0000
5	311.0	103.3	.0060	.7859	.2081	0.0000
6	273.5	103.3	.0060	.7859	.2081	0.0000
7	273.5	103.3	.0060	.7859	.2081	0.0000
8	273.5	103.3	.0060	.7859	.2081	0.0000
9	273.5	103.3	.0060	.7859	.2081	0.0000

INITIAL SURFACE TEMPERATURES (K) ARE:

1.	303.0	2.	303.0	3.	303.0	4.	273.5	5.	273.5
6.	273.5	7.	273.5	8.	311.0	9.	311.0	10.	311.0
11.	311.0	12.	311.0	13.	273.5	14.	273.5	15.	273.5
16.	273.5	17.	273.5	18.	273.5	19.	273.5	20.	273.5

SPRAYS WILL BE ACTIVATED AT 130.373 SECONDS DUE TO
TBULK = 353.6 AND PKPA = 121.6 IN COMPARTMENT 4

SPRAYS WILL BE SWITCHED TO RECIRCULATION AT 2130.373 SECONDS
(2000.000 SECONDS AFTER BEING ACTIVATED)

FANS WILL BE ACTIVATED AT 700.373 SECONDS DUE TO
TBULK = 353.6 AND PKPA = 121.6 IN COMPARTMENT 4

BURN INITIATED IN COMPARTMENT 2 AT TIME = 4171.397 SECONDS

COMPARTMENT CONDITIONS AT 4171.397 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	303.6	129.1	.0337	.7328	.1937	.0398
2	306.4	129.1	.0397	.6962	.1840	.0801
3	346.9	129.6	.2320	.5461	.1443	.0776
4	348.7	129.8	.3059	.4929	.1303	.0709
5	306.9	129.8	.0394	.7313	.1933	.0360
6	337.1	129.6	.1874	.5792	.1531	.0803

```
 7      328.3       129.6       .1282       .6230       .1647       .0841
 8      317.9       129.5       .0770       .6615       .1748       .0867
 9      306.9       129.5       .0425       .6885       .1820       .0870

BURN COMPLETED IN COMPARTMENT  2 AT TIME =  4173.096 SECONDS
-------------------------------------------------------------
COMPARTMENT CONDITIONS AT  4173.096 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1      311.9       137.6       .0376       .7296       .1924       .0404
 2      933.0       137.5       .1230       .7259       .1505       .0006
 3      350.2       135.8       .2128       .5598       .1480       .0794
 4      351.0       132.8       .3072       .4917       .1299       .0712
 5      308.9       132.8       .0395       .7311       .1932       .0362
 6      339.6       135.8       .1797       .5848       .1546       .0809
 7      328.8       135.8       .1153       .6325       .1672       .0850
 8      319.3       135.7       .0647       .6713       .1772       .0868
 9      349.2       135.7       .0424       .6954       .1810       .0812

(ADDITIONAL BURN INFORMATION NOT SHOWN HERE)

################################################################################
################################## END OF HECTR RUN ############################
################################################################################


SUMMARY OF BURNS:

     4 BURN(S) OCCURRED IN COMPARTMENT   1
    15 BURN(S) OCCURRED IN COMPARTMENT   2
     1 BURN(S) OCCURRED IN COMPARTMENT   3
     1 BURN(S) OCCURRED IN COMPARTMENT   6
    10 BURN(S) OCCURRED IN COMPARTMENT   7
    11 BURN(S) OCCURRED IN COMPARTMENT   8
    12 BURN(S) OCCURRED IN COMPARTMENT   9


>>> GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS <<<

>>>  6024.365 SECONDS              249.0 KPA <<<
>>>  4624.774 SECONDS             1109.2 K   <<<


COMPARTMENT PRESSURE MAXIMUMS (KPA):

     1.  249.0      2.  249.0      3.  211.9      4.  151.1      5.  151.1
     6.  211.8      7.  211.8      8.  211.7      9.  211.6

COMPARTMENT TEMPERATURE MAXIMUMS (K):

     1.  651.3      2. 1003.0      3. 1109.2      4.  377.4      5.  343.2
     6.  999.6      7.  956.8      8.  958.7      9.  951.3
```

SURFACE TEMPERATURE MAXIMUMS (K):

1.	311.7	2.	317.4	3.	311.8	4.	334.5	5.	348.7
6.	355.9	7.	373.9	8.	347.1	9.	371.3	10.	373.6
11.	312.3	12.	314.2	13.	273.5	14.	345.5	15.	273.5
16.	354.8	17.	273.5	18.	347.3	19.	273.5	20.	336.4

TOTAL MASSES	WATER+ICE	STEAM	NITROGEN	OXYGEN	HYDROGEN
INITIAL	1.110E+06	1.145E+02	3.062E+04	9.244E+03	0.
INJECTED SOURCE	1.040E+05	1.321E+05	0.	0.	6.749E+02
INJECTED SPRAY	1.192E+06	0.	0.	0.	0.
FINAL	2.531E+06	1.369E+03	3.062E+04	5.340E+03	1.829E+02

FINAL SUMP VOLUMES (M**3):

1.	2004.059
2.	80.000

*** FINAL ICE FRACTION = .409 ***

NUMBER OF TIME STEPS TAKEN:

HEAT TRANSFER	=	19001
FLOW	=	41465
SUCCESSFUL FLOW	=	33777

NUMBER OF FLOW TIME STEPS REPEATED AND REASON:

1922	FLOW REVERSAL
3643	CHOKING
1038	EXCESSIVE PRESSURE CHANGE
0	TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
0	NEGATIVE MOLES
0	TEMPERATURE OFF TABLES
0	TEMPERATURE TOO LOW
1017	EXCESSIVE PRESSURE OR TEMPERATURE CHANGE FOR HEAT TRANSFER

FLOW TIME STEP CONTROLLING FACTORS AND TIMES USED:

17666	PRESSURE CHANGE
0	TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
662	MAXIMUM STRETCH FACTOR
6	MINIMUM STEP SIZE

```
      14426     MAXIMUM STEP SIZE
       1017     MATCHING HEAT TRANSFER UPDATING TIME

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

FINAL COMPARTMENT CONDITIONS AT  7500.248 SECONDS ARE:

COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

 1       303.8       111.1       .0382       .7805       .1191       .0621
 2       299.8       111.1       .0278       .7835       .1196       .0691
 3       322.8       111.6       .0787       .7411       .1131       .0671
 4       323.1       111.7       .1106       .7153       .1092       .0649
 5       306.1       111.7       .0428       .7775       .1187       .0611
 6       318.6       111.5       .0706       .7479       .1142       .0674
 7       311.1       111.5       .0575       .7586       .1158       .0680
 8       304.4       111.5       .0413       .7720       .1178       .0689
 9       297.5       111.4       .0278       .7831       .1195       .0696

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

ACHILES OUTPUT

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                             $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

    ICE-CONDENSER SAMPLE PROBLEM$
    -----------------------------------------------------------------------


THIS IS A 9 COMPARTMENT SAMPLE PROBLEM DEALING WITH A
SMALL BREAK LOCA IN THE SEQUOYAH ICE-CONDENSER
CONTAINMENT.  THIS SAMPLE PROBLEM IS FOR ILLUSTRATION
PURPOSES ONLY AND SHOULD NOT BE CONSIDERED AS NECESSARILY
REPRESENTATIVE OF ANY PARTICULAR ACCIDENT SEQUENCE.

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

>>>    9 COMPARTMENT(S)          10 FLOW JUNCTION(S)          20 SURFACE(S) <<<
>>>    2 FAN(S)                   2 SUMP(S)                                 <<<

    SPRAYS WERE AUTO          FANS WERE AUTO
```

```
MINIMUM HEAT TRANSFER TIMESTEP       = 1.000E-05 SECONDS
MAXIMUM HEAT TRANSFER TIMESTEP       = 5.000E-01 SECONDS
MINIMUM FLOW TIMESTEP                = 1.000E-06 SECONDS
MAXIMUM FLOW TIMESTEP                = 5.000E-01 SECONDS
MAXIMUM TIMESTEP PRESSURE CHANGE     = 10.1325   KPA
MAXIMUM TIMESTEP TEMPERATURE CHANGE = 10.0000   K
```

HYDROGEN LIMITS FOR	IGNITION	PROPAGATION UPWARDS	PROPAGATION SIDEWAYS	PROPAGATION DOWNWARDS
COMPARTMENT 1	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 2	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 3	100.0%	4.1%	6.0%	9.0%
COMPARTMENT 4	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 5	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 6	100.0%	4.1%	6.0%	9.0%
COMPARTMENT 7	100.0%	4.1%	6.0%	9.0%
COMPARTMENT 8	100.0%	4.1%	6.0%	9.0%
COMPARTMENT 9	100.0%	4.1%	6.0%	9.0%

FAILURE PRESSURE = 350.0 KPA

COMPARTMENTS:

1. UPPER COMPARTMENT
2. UPPER PLENUM
   (UPPER PLENUM)
3. LOWER PLENUM
   (LOWER PLENUM)
4. LOWER COMPARTMENT
5. DEAD ENDED REGIONS
6. ICE COMPARTMENT 1
   (GENERATED ICE COMPARTMENT)
7. ICE COMPARTMENT 2
   (GENERATED ICE COMPARTMENT)
8. ICE COMPARTMENT 3
   (GENERATED ICE COMPARTMENT)
9. ICE COMPARTMENT 4
   (GENERATED ICE COMPARTMENT)

SURFACE TYPE KEY:

1. SLAB
2. LUMPED MASS
3. POOL
4. ICE
5. ICE CONDENSER WALL

SURFACES (BY COMPARTMENT NUMBER - SURFACE TYPE -
NUMBER OF LAYERS IF A SLAB) FOLLOWED BY THE SURFACE NUMBER
(AND THE SUMP NUMBER IF A SUMP):

(1-1-1)	1.		DOME
(1-1-1)	2.		UPPER COMPARTMENT CONCRETE
(1-1-1)	3.		UPPER COMPARTMENT STEEL
(2-1-1)	4.		UPPER PLENUM STEEL
(3-1-1)	5.		LOWER PLENUM WALLS
(3-1-1)	6.		ICE CONDENSER SUPPORT STRUCTURE
(3-3)	7.	(2)	LOWER PLENUM SUMP (LOWER PLENUM DRAIN)
(4-1-1)	8.		LOWER COMPARTMENT STEEL
(4-1-1)	9.		LOWER COMPARTMENT CONCRETE
(4-3)	10.	(1)	SUMP SURFACE (SPRAY SOURCE SUMP)
(5-1-1)	11.		DEAD ENDED STEEL
(5-1-1)	12.		DEAD ENDED CONCRETE
(6-4)	13.		ICE SURFACE 1
(6-5)	14.		ICE STRUCTURE 1
(7-4)	15.		ICE SURFACE 2
(7-5)	16.		ICE STRUCTURE 2
(8-4)	17.		ICE SURFACE 3
(8-5)	18.		ICE STRUCTURE 3
(9-4)	19.		ICE SURFACE 4
(9-5)	20.		ICE STRUCTURE 4

FLOW JUNCTIONS/COMPARTMENT INTERCONNECTIONS (INTERCONNECTION AREA IN M**2 -
FLOW COEFFICIENT):

1.	2 =>	1	2-WAY	UPWARDS	(	186.00 -	1.43)
2.	4 =>	1	DRAIN IN ICE CONDENSER	UPWARDS	(	.20 -	1.50)
3.	3 =>	6	2-WAY	UPWARDS	(	167.00 -	.20)
4.	9 =>	2	2-WAY	UPWARDS	(	1.86 -	1.50)
5.	5 =>	4	2-WAY	SIDEWAYS	(	27.70 -	4.20)
6.	9 =>	2	1-WAY INERTIAL VALVE	UPWARDS	(	0.00 -	.20)
7.	4 =>	3	1-WAY INERTIAL VALVE	UPWARDS	(	0.00 -	.89)
8.	6 =>	7	2-WAY	UPWARDS	(	167.00 -	.20)
9.	7 =>	8	2-WAY	UPWARDS	(	167.00 -	.20)
10.	8 =>	9	2-WAY	UPWARDS	(	167.00 -	.20)

FAN CONNECTIONS (VOLUMETRIC FLOW RATE IN M**3/S WITH A NEGATIVE
NUMBER INDICATING THE USE OF A HEAD CURVE):

1.	1 =>	5	DOWNWARDS	(	-54.7)
2.	4 =>	5	SIDEWAYS	(	-1.2)

*** THIS RUN ENDED AT 7500.248 SECONDS ***

APPROXIMATE GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS

6024.414 SECONDS	247.5 KPA
4624.770 SECONDS	1106.3 K

APPROXIMATE COMPARTMENT PRESSURE AND TEMPERATURE MAXIMUMS

COMPARTMENT	1:	6024.414 SECONDS	247.5 KPA
		6024.414 SECONDS	647.0 K
COMPARTMENT	2:	6024.414 SECONDS	247.5 KPA
		4209.774 SECONDS	1003.0 K
COMPARTMENT	3:	6025.862 SECONDS	211.8 KPA
		4624.770 SECONDS	1106.3 K
COMPARTMENT	4:	4218.562 SECONDS	151.0 KPA
		700.397 SECONDS	377.4 K
COMPARTMENT	5:	4218.562 SECONDS	151.1 KPA
		6040.045 SECONDS	343.2 K
COMPARTMENT	6:	6025.862 SECONDS	211.8 KPA
		4624.782 SECONDS	998.0 K
COMPARTMENT	7:	6025.862 SECONDS	211.7 KPA
		4623.998 SECONDS	956.8 K
COMPARTMENT	8:	6025.862 SECONDS	211.6 KPA
		4997.918 SECONDS	956.9 K
COMPARTMENT	9:	6025.862 SECONDS	211.6 KPA
		4926.532 SECONDS	949.3 K

UOF = 8 UOA = 9

NHT = 6937 NFL = 26640 NAH = 6937

6.3 Mark III BWR Containment Problem

6.3.1 Containment Description

A schematic of a BWR Mark III containment is shown in Figure 6-13. The containment is divided into two regions: (1) a central region called the drywell, and (2) an outer region, which consists of an annular region surrounding the drywell and a large, open region at the top of the containment called the dome. The central region, which contains the reactor vessel, is separated from the outer region by the drywell wall. A large pool of water called the suppression pool is located at the bottom of the containment in the annular region between the outer wall of the containment and a short wall, called the weir wall, which is located inside the drywell wall. Horizontal vents at the bottom of the drywell wall allow water in the suppression pool to flow between the drywell region of the suppression pool and the outer region.

The BWR Mark III containment was designed to limit the containment pressure following an accident by forcing the steam in the reactor vessel or the drywell through the suppression pool (where most of the steam should be condensed) before allowing it to enter the outer region of the containment. The safety relief valves (SRVs) from the reactor vessel discharge into the suppression pool, limiting pressure rises from accidents involving steam flow through the SRVs. For accidents involving pipe breaks in the drywell, steam is injected into the drywell until the pressure rises enough to depress the water level in the pool below the vents in the drywell wall. Steam can then flow from the drywell into the suppression pool. Any gases that are not condensed in the suppression pool will then flow into the annular region of the containment (the lowest section of this annular region is called the wetwell). Similarly, burns in the outer containment regions could cause flow of gases from the wetwell back into the drywell by depressing the level on the wetwell side of the suppression pool below the vents in the drywell wall. Depression of the water level on the wetwell side of the suppression pool (caused by burns, etc.) can cause the water in the suppression pool to rise above the weir wall and spill over onto the drywell floor.

Flow between the drywell and the outer region can also occur through the purge/vent system. The purge/vent system consists of compressors that circulate gases from the dome to the drywell and vacuum breakers that allow flow from the dome to the drywell if the dome pressure exceeds the drywell pressure.

A containment spray system is also provided to limit the containment pressure. The water for spray injection is drawn from the suppression pool, cooled in heat exchangers,

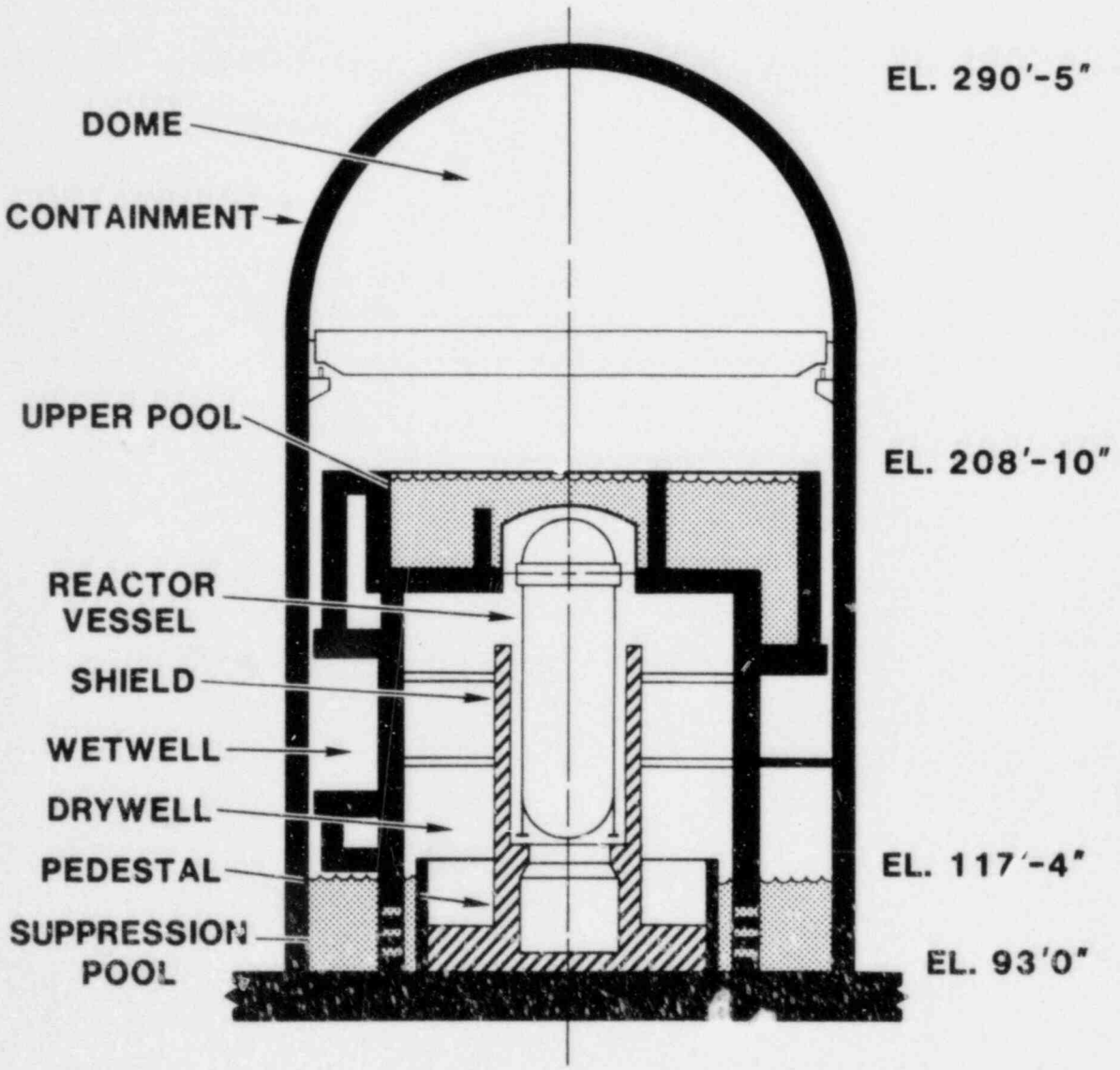


Figure 6-13. BWR Mark III Containment

and then injected into the containment through spray rings that are located at the top of the dome. The heat exchangers can also be used to cool the suppression pool, prior to spray initiation.

A pool of water called the upper pool is located at the bottom of the dome region (above the drywell). Water from this pool can be dumped to the suppression pool to increase the suppression pool water inventory.

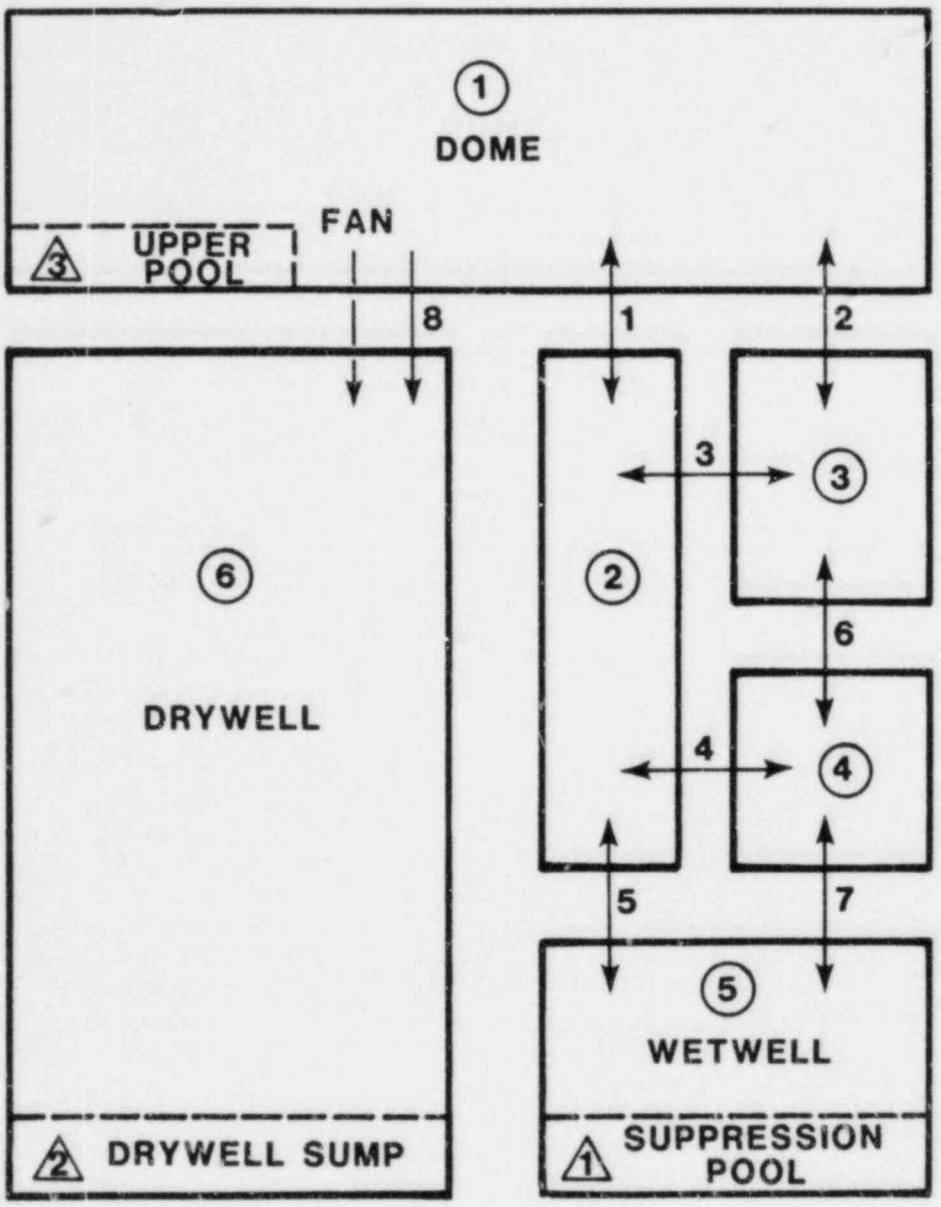
Mark III containments are equipped with deliberate ignition systems, consisting of hydrogen igniters (glow plugs) that are installed throughout the containment. These systems are intended to reduce the threats from hydrogen combustion by burning the hydrogen at low concentrations, rather than allowing it to accumulate to higher levels.

6.3.2 Computational Model

The HECTR containment model used for this calculation is shown in Figure 6-14. Six compartments are used to model the containment, and eight junctions are used to model flow between compartments. Compartment 1 represents the dome, Compartment 2 represents the vertical space where equipment can be transferred, Compartments 3 and 4 represent the remainder of the annular region of the containment above the wetwell, Compartment 5 represents the wetwell, and Compartment 6 represents the drywell. The suppression pool (Sump 1), upper pool (Sump 3), and drywell pool (Sump 2) are all included in the model. Spray water is drawn from the suppression pool, cooled by a heat exchanger, and injected into the dome region (Compartment 1). The heat exchangers used to cool the spray water are also used to cool the suppression pool before spray operation begins. The purge/vent system is modeled by including a fan that circulates air from the dome to the drywell and a check valve between the dome and the drywell (Junction 8).

6.3.3 Case Description

This example is included to show HECTR's capability to model accidents in Mark III containments. The example is intended to show the general containment response that would be expected for a drywell break. The steam and hydrogen sources used in the example were not actually calculated for a drywell break accident, so the calculated results are useful only as examples of typical containment responses and should not be considered predictions of any particular accident sequence. Prior to 1800 s, the sources were all injected into the drywell to model flow out of the break. The Automatic Depressurization System (ADS) was assumed to be actuated at 1800 s, so the sources were split between the



(1) COMPARTMENT NUMBER
1 JUNCTION NUMBER
△1 SUMP NUMBER

Figure 6-14. BWR Mark III Containment Model

suppression pool (to model flow out the SRVs) and the dry-well. The same combustion parameters were used for this case as for the ice-condenser calculation.

6.3.4 Input Listing

This is the HECTR input section as described in Section 4.2.

```
! INITIAL NAMELIST INPUT
!
CMPUTR=CRAY  ! PROBLEM IS BEING RUN ON A CRAY 1
!
$ END OF NAMELIST INPUT
BWR MARK III SAMPLE PROBLEM$


8% IGNITION
FANS ON AT 1200 SEC
SPRAYS AUTO, 1 TRAIN
SUPPRESSION COOLING AFTER 1800 SEC
PURGE/VENT SYSTEM - 1 VENT, 2 COMPRESSORS
70/30 SPLIT BETWEEN S/RV'S AND BREAK

496000. ! FAILURE PRESSURE
6 ! NUMBER OF COMPARTMENTS
!
! COMPARTMENT DATA
!
! FOR EACH COMPARTMENT:  THE VOLUME, ELEVATION, FLAME PROPAGATION
! LENGTH, NUMBER OF SURFACES, SUMP NUMBER TO DEPOSIT WATER FROM
! SUBCOOLING INTO AND SUMP NUMBER TO DEPOSIT EXCESS SPRAY INTO
DOME
23683. 39.78 19. 5 3 3
PIE SHAPED SECTION IN ANNULAR REGION
1654. 14.78 11.13 1 1 1
ANNULUS BETWEEN 161 AND 209
4480. 18.75 14.32 4 1 1
ANNULUS BETWEEN 135 AND 161
3278. 7.62 7.92 4 1 1
WETWELL
4341. 0. 3.67 5 1 1
DRYWELL
7649. 8.7 13. 4 2 2
!
! SUMP DATA
!
! FOR EACH SUMP:  THE SUMP NUMBER, CAPACITY, AND SUMP TO OVERFLOW INTO
1    0. 0 ! SUPPRESSION POOL
2 1416. 0 ! DRYWELL SUMP
3 1780. 1 ! UPPER POOL
$
!
```

```
! SURFACE DATA
!
! FOR EACH SURFACE:  TYPE OF SURFACE, MASS OF SURFACE (OR SUMP), AREA
! OF SURFACE, CHARACTERISTIC LENGTH, SPECIFIC HEAT, EMISSIVITY, AND
! EITHER SUMP NUMBER ( FOR POOL SURFACES) OR SUMP NUMBER THAT ACCEPTS
! RUNOFF FROM SURFACE FROM CONDENSATION.  FOR SLAB SURFACES, THIS IS
! FOLLOWED BY THE NUMBER OF LAYERS IN THE SLAB, THEN THE THICKNESS,
! THERMAL DIFFUSIVITY, AND THERMAL CONDUCTIVITY OF EACH LAYER.  AFTER
! ALL LAYERS ARE INPUT, NODALIZATION INPUT AND BACK SURFACE CONDITIONS
! ARE SPECIFIED.  DEFAULT CONDITIONS ARE USED FOR ALL SURFACES HERE.
!
! COMPARTMENT 1
CONCRETE FLOOR
1 1.      297.3  6.    879.  .9  3
1
.1524  5.5E-7  1.385
0 0. 0. 0.
STEEL POOL WALLS
1 1.      555.   .46   460.5 .7  3
1
.00747 1.17E-5 43.27
0 0. 0. 0.
UPPER POOL SURFACE
3 1.68E6   339.   6.    1.     .94 3
CRANE$
1 1.      1188.  1.    460.5 .7  3
1
.2152  1.17E-5 43.27
0 0. 0. 0.
DOME AND WETWELL WALLS
1 1.      3290.6 28.   460.5 .7  3
1
.00634 1.17E-5 43.27
0 0. 0. 0.
! COMPARTMENT 2
WETWELL WALL - COMP 2
1 1.      393.4  22.3 460.5 .7  1
1
.00634 1.17E-5 43.27
0 0. 0. 0.
! COMPARTMENT 3
WETWELL WALL - COMP 3
1 1.      950.   14.3 460.5 .7  1
1
.00634 1.17E-5 43.27
0 0. 0. 0.
DRYWELL WALL - COMP 3
1 1.      202.   14.3 879.  .9  1
1
.762   5.5E-7  1.385
0 0. 0. 0.
CONCRETE - COMP 3
1 1.      2103.  6.    879.  .9  1
1
```

```
.1524  5.5E-7  1.385
0 0. 0. 0.
MISCELLANEOUS STEEL - COMP 3
2 2.82E5 3960.  1.   460.5 .7  1
! COMPARTMENT 4
WETWELL WALL - COMP 4
1 1.     702.   7.9  460.5 .7  1
1
.00634 1.17E-5 43.27
0 0. 0. 0.
DRYWELL WALL - COMP 4
1 1.     487.   7.9  879.  .9  1
1
.762   5.5E-7  1.385
0 0. 0. 0.
CONCRETE - COMP 4
1 1.     396.   7.   879.  .9  1
1
.1524  5.5E-7  1.385
0 0. 0. 0.
MISCELLANEOUS STEEL - COMP 4
2 1.96E5 2079.  1.   460.5 .7  1
! COMPARTMENT 5
WETWELL WALL - COMP 5
1 1.     832.   7.3  460.5 .7  1
1
.00634 1.17E-5 43.27
0 0. 0. 0.
DRYWELL WALL - COMP 5
1 1.     557.   7.3  879.  .9  1
1
.762   5.5E-7  1.358
0 0. 0. 0.
CONCRETE - COMP 5
1 1.     308.   4.   879.  .9  1
1
.1524  5.5E-7  1.385
0 0. 0. 0.
MISCELLANEOUS STEEL - COMP 5
2 4.59E4 1127.  .045 460.5 .7  1
SUPRESSION POOL SURFACE
3 3.86E6 619.   6.   1.    .94 1
! COMPARTMENT 6
DRYWELL AND REACTOR SHIELD WALLS
1 1. 2530. 10. 879. .7 2
3
3.96E-6 1.82E-7 .36
.0105 1.32E-5 48.
.7 5.0E-6 2.1
0 0. 0. 0.
REACTOR PEDESTAL MAT AND WEIR WALL
1 1. 1035. 15. 879. .9 2
1
```

```
0.5 5.0E-6 2.1
0 0. 0. 0.
MISC STEEL - DW
1 1. 4308. 4. 461. .7 2
2
3.96E-6 1.82E-7 .36
.0046 1.32E-5 48.
0 0. 0. 0.
DRYWELL POOL
3 0. 292. 5. 0. .94 2
!
! JUNCTION DATA
!
! FOR EACH JUNCTION: SOURCE COMPARTMENT, RECEIVING COMPARTMENT,
! JUNCTION TYPE, AREA, LOSS COEFFICIENT, INERTIAL LENGTH OVER AREA,
! AND ORIENTATION FOR BURN PROPAGATION, ELEVATION
1 2 1  74.3     .75 0.1682 -1 26.2
1 3 1 152.1    1.5  0.0691 -1 26.2
2 3 1 135.64   1.5  0.1163  0 18.75

2 4 1 157.     1.5  0.1005  0  7.62
2 5 1  62.4     .75 0.1184 -1  3.66
3 4 1 228.8    1.5  0.0243 -1 11.58
4 5 1 144.4    1.5  0.0264 -1  3.66
1 6 2    .051  1.19 0.001  -1 26.2
$
$ ! NO ICE CONDENSER, SO NO INPUT IS NECESSARY
!
! SUPPRESSION POOL DATA
!
! DRYWELL COMPARTMENT, WETWELL COMPARTMENT, SUPPRESSION POOL SUMP
! NUMBER, UPPER POOL SUMP NUMBER, DRYWELL POOL SUMP NUMBER
6 5 1 3 2
! DISTANCE FROM WEIR WALL TO CENTER OF TOP ROW OF VENTS, DISTANCE
! BETWEEN TOP AND MIDDLE ROWS OF VENTS, DISTANCE BETWEEN MIDDLE AND
! BOTTOM VENTS, VENT LENGTH, INITIAL LEVEL OF WATER ABOVE CENTER OF
! TOP ROW OF VENTS
3.963 1.27 1.27 1.52 2.210
! CROSS SECTIONAL AREA OF DRYWELL SIDE OF SUPPRESSION POOL, SINGLE ROW
! OF VENTS, AND WETWELL SIDE OF SUPPRESSION POOL, VENT INLET AND OUTLET
! LOSS COEFFICIENTS FOR WATER FLOW, VENT LOSS COEFFICIENT FOR GAS FLOW,
! EQUIVALENT LOSS FOR VENT EXIT LOSSES
51.4 17.9 619. 3. 0.3 30. 0.85
! UPPER POOL DUMP INPUT.  MASS FLOW RATE, TIME TO BEGIN DRAINING,
! MASS OF WATER IN UPPER POOL AFTER IT IS DUMPED
3.42E3 1800. 6.5E5
!
! FAN DATA
!
! TEMPERATURE AND PRESSURE SET POINTS, DELAY, TIME TILL SHUT OFF
0. 0. 1200. 1.E6
! SOURCE COMPARTMENT, RECEIVING COMPARTMENT, RUN OUT FLOW RATE,
! SHUT OFF HEAD, EFFICIENCY, FAN ORIENTATION FOR BURN
! PROPAGATION
```

```
1 6 -0.55 1.16E5 1. 0
$
! FAN HEAD CURVE TABLE INPUT - NORMALIZED HEAD, NORMALIZED FLOW
0. 1.
.501 1.
.749 .928
.901 .817
.970 .723
1. .596
$
!
! RADIATION HEAT TRANSFER DATA
!
! BEAM LENGTHS
1.    1.    1.    15.24 21.55 18*1.
1.    10.   15.24 21.55 18*1.
1.    15.24 21.55 18*1.
0.3   21.55 18*1.
26.46 18*1.
20.61 17*1.
26.32 7.81  12.19  4.5  13*1.
1.    12.19 6.    13*1.
9.14  6.    13*1.
2.5   13*1.
21.85 7.5   6.42  4.5   9*1.
1.    5.36  4.5   9*1.
8.5   6.    9*1.
1.    9*1.
21.68 7.32  4.88  4.    4.88  4*1.
1.    4.69  3.    4.69  4*1.
1.    2.5   8.2   4*1.
2.    6.    4*1.
1.    4*1.
5.    10.   2.    10.
2.    10.   2.
2.    10.
1.
! VIEW FACTORS
.0     .0     .0     .1     .9     18*.0
.609   .1955  .01955 .17595 18*.0
.0     .068   .612   18*.0
.437   .5095  18*.0
.6421  18*.0
1.     17*.0
.05    .0851  .4     .4649  13*.0
.0     .20000 .4     13*.0
.25    .5501  13*.0
.576   13*.0
.05000 .3     .25    .4     9*.0
.0     .2     .3676  9*.0
.2     .1108  9*.0
.7577  9*.0
.08    .31    .14    .185   .285   4*.0
.0     .11    .2149  .212   4*.0
```

```
.0      .0829   .34     4*.0
.5934   .1411   4*.0
.0      4*.0
.3427   .0241   .6043   .0289
.7      .1      .1411
.6042   .0169
.0
!
! SPRAY DATA
!
! NUMBER OF SPRAY RINGS
1
! COMPARTMENT SPRAY IS INJECTED INTO, INITIAL DROP TEMPERATURE, FLOW
! RATE, NUMBER OF DROP SIZES
1 330.37 .356 2
! FRACTION OF DROPS OF EACH SIZE, DIAMETER
.95     309.
.05     810.
! SPRAY CARRYOVER FRACTION
1 2 .1
1 3 .2
$
! COMPARTMENT NUMBER, FALL HEIGHT
1 19.5
2 22.5
3  7.5
$
! TEMPERATURE AND PRESSURE SETPOINTS, TIME DELAY, AND TIME ON
358.15  163376.43  120. 1.E6
!
! SPRAY RECIRCULATION
!
! TIME IN INJECTION MODE, RATED FLOW, RATED EFFECTIVE HEAT REMOVAL RATE,
! SECONDARY INLET TEMPERATURE, SECONDARY FLOW RATE, SUMP THAT WATER IS
! DRAWN FROM
0. 470. 2.35E6 305.5 498. 1
!
! SUMP HEAT EXCHANGERS
!
! SUMP NUMBER, FLAG FOR TURNING OFF SUPPRESSION POOL COOLING WHEN SPRAYS
! ARE ACTIVATED, RATED FLOW RATE, RATED EFFECTIVE HEAT REMOVAL RATE,
! SECONDARY INLET TEMPERATURE, SECONDARY SIDE FLOW RATE, ACTUAL FLOW
! RATE OF WATER THROUGH PRIMARY SIDE
1 1 470. 2.35E6 305.5 498. 400.
! TEMPERATURE AND PRESSURE SETPOINTS, TIME DELAY, AND TIME ON
0. 0. 1800. 1.E6
$
! SIMULATION TIME
8000.
!
! COMPARTMENT INITIAL CONDITIONS
!
! FOR EACH COMPARTMENT:  TEMPERATURE, PARTIAL PRESSURE OF STEAM,
! NITROGEN, OXYGEN AND HYDROGEN, AND CONVECTIVE VELOCITY
```

```
300.
2068. 78460. 20753. 0.
.3
300.
2068. 78460. 20753. 0.
.3
300.
2068. 78460. 20753. 0.
.3
300.
2068. 78460. 20753. 0.
.3
300.
2068. 78460. 20753. 0.
.3
331.
8963. 73013. 19305. 0.
.3
!
! SOURCE TERMS
!
! STEAM
! COMPARTMENT (OR SUMP IF -) INJECTED INTO, TEMPERATURE OR ENTHALPY
! FLAG, TEMPERATURE OR ENTHALPY IF CONSTANT
6 3 0.
! TIME, INJECTION RATE, ENTHALPY
0.      99.77  2.749E6
602.    83.14  2.784E6
902.    85.37  2.796E6
1204.   59.01  2.807E6
1789.   55.69  2.817E6
1802.   54.79  2.819E6
1803. 16.44  2.819E6
2707. 10.18  2.894E6
2994.  6.58  3.003E6
3601.  3.77  3.228E6
3631.  4.15  3.226E6
4201.   .64  3.205E6
4504.   .33  3.108E6
4541.   .94  3.629E6
4858.   .94  4.301E6
5158.   .31  3.629E6
5458.   .019 3.356E6
5758.   .15  4.34E6
6058.   .014 3.563E6
6358.   .34  4.487E6
6359.   .58  3.612E6
7807.13 .58  3.612E6
7807.14 .0   3.612E6
$
-1 3 0.
! TIME, INJECTION RATE, ENTHALPY
0.      0.    2.749E6
1802.   0.    2.819E6
```

```
1803.   38.35   2.819E6
2707.   23.74   2.894E6
2994.   15.35   3.003E6
3601.    8.80   3.228E6
3631.    9.69   3.226E6
4201.    1.50   3.205E6
4504.     .76   3.108E6
4541.    2.20   3.629E6
4858.    2.18   4.301E6
5158.     .69   3.629E6
5458.     .045  3.356E6
5758.     .34   4.34E6
6058.     .032  3.563E6
6358.     .78   4.487E6
6359.    1.35   3.612E6
7807.13  1.35   3.612E6
7807.14  0.     3.612E6
$
$
! NITROGEN
$
! OXYGEN
$
! HYDROGEN
! COMPARTMENT (OR SUMP), TEMPERATURE OR ENTHALPY FLAG, TEMPERATURE OR
! ENTHALPY IF CONSTANT
6 1 0.
! TIME, INJECTION RATE, TEMPERATURE
0.      0.         290.
1803.   0.         547.
2707.   1.667E-9   547.
2995.   0.524E-6   592.
3295.   0.816E-4   641.
3601.     .00097   691.
3631.     .00121   694.
3901.     .00652   745.
4201.     .00661   674.
4541.     .0443    875.
4858.     .1417   1197.
5158.     .0667    872.
5458.     .0093    742.
5758.     .1384   1201.
6058.     .0757    833.
6358.     .1197   1265.
6359.     .1417   1260.
7807.13   .1417   1260.
7807.14   .0       290.
$
-1 1 0.
! TIME, INJECTION RATE, TEMPERATURE
0.      0.         290.
1803.   0.         547.
2707.   3.889E-9   547.
2995.   1.222E-6   592.
```

```
3295.  1.905E-4 641.
3601.    .00225  691.
3631.    .00283  694.
3901.    .01520  745.
4201.    .01543  674.
4541.    .1012   875.
4858.    .3306  1197.
5158.    .1558   872.
5458.    .0219   742.
5758.    .3231  1201.
6058.    .01765  833.
6358.    .2792  1265.
6359.    .3306  1260.
7807.13 .3306  1260.
7807.14 .0      290.
$
$
!
! WATER REMOVED FROM SUMP FOR ECC
!
$
!
! INITIAL WALL TEMPERATURES
!
300. 300. 325. 15*300. 333. 331. 331. 331. 300.
! NAMELIST INPUT
UOA=9
DTHTMX=1.
SPRAYS=AUTO
FANS  =AUTO
HTEXCH(1)=AUTO
$
```

This is the ACHILES input section as described in Section 4.3.

```
CMPUTR=CRAY
SHOWPT=10
SHOWWT=10
SHOWJV=10
COMBXF=TRUE
$
! **********
! * TABLES *
! **********
NON        ! COMPARTMENT INFORMATION
NON        ! SUMP
NON        ! SURFACE TEMPERATURES
NON        ! MASS FLUXES AND FILM THICKNESSES
NON        ! SOURCES
NON        ! SPRAYS
NON        ! ICE CONDENSER
NON        ! JUNCTION FLOWS
```

```
NON         ! FANS
NON         ! SUPPRESSION POOL
NON         ! NET HEAT FLUXES
NON         ! RADIATIVE HEAT FLUXES
NON         ! CONVECTIVE HEAT FLUXES
NON         ! MASS DRAINING TO SUMPS
NON         ! SPRAY TEMPERATURE
NON         ! ICE CONDENSER
! **********
! * PLOTS  *
! **********
  1  5  6       ! COMPARTMENTS
0 2000 8000 5   ! XMIN, XSTEP, XMAX, NXTIKS
ALL             ! SUMP
 16==> 23       ! WALL TEMPERATURES
 20==> 23       ! CONDENSATION RATE
 20==> 23       ! FILM THICKNESS
ALL             ! SOURCES
ALL             ! MVAP
ALL             ! HTSPR
NON             ! ICE FRACTION
ALL             ! JUNCTION VELOCITIES
ALL             ! FANS
ALL             ! SUPPRESSION POOL
 20==> 23       ! NET HEAT FLUX
NON             ! RADIATION
NON             ! CONVECTION
NON             ! SURFACE DRAINING RATES
ALL             ! SPRAY TEMPERATURE
NON             ! ICE CONDENSER
NON             ! ICE CONDENSER
```

6.3.5 Results

The pressure response for the dome is shown in Figure 6-15, and the gas compositions for the drywell, wetwell, and dome are shown in Figures 6-16 through 6-18, respectively. Nine burns occurred in this calculation. The burns all began in the wetwell and propagated upward into Compartment 2. Most of the burns continued to propagate through the other compartments in the outer containment and into the dome. No burns occurred in the drywell, because the oxygen concentrations there were low enough to prevent burning. The first two burns were so close together that it is difficult to detect two separate burns on the plots. The first burn started in the wetwell and propagated through all of the outer containment, including the dome. The hydrogen concentrations in the upper regions of the containment were higher for this burn than for any of the subsequent burns. Also, the sprays did not begin operating until the first burn was completed. These two effects caused the first burn to have a larger pressure rise than the remaining burns. The second burn followed the first burn so closely that the

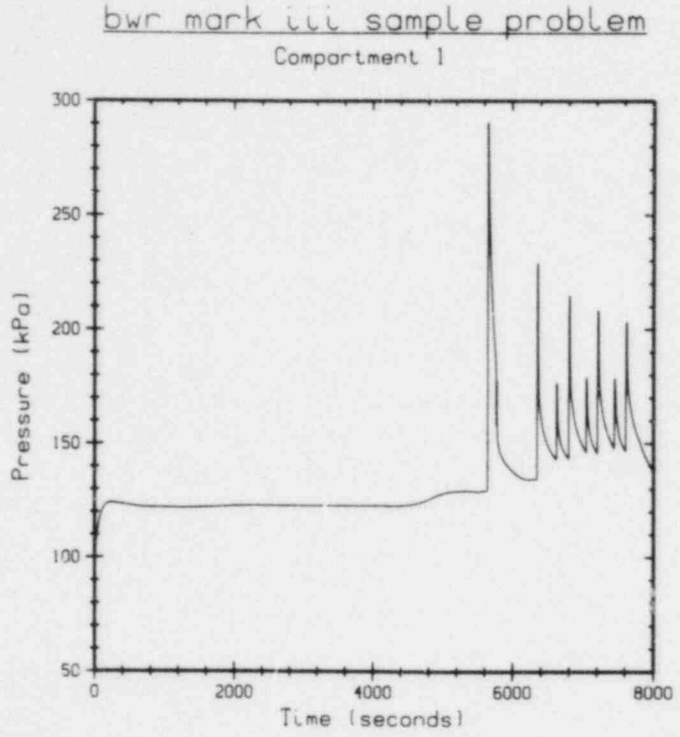


Figure 6-15. Dome Pressure Response for Mark III Sample Problem

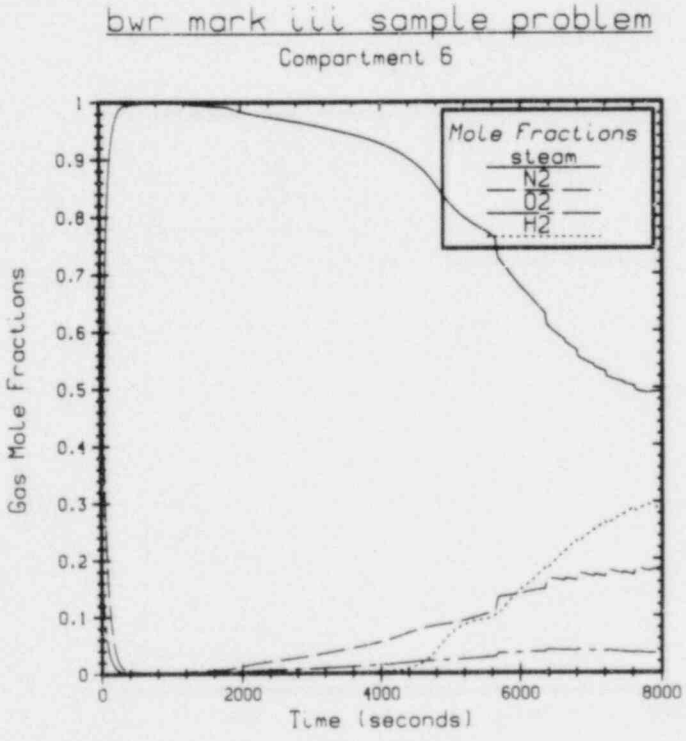


Figure 6-16. Drywell Gas Composition for Mark III Sample Problem

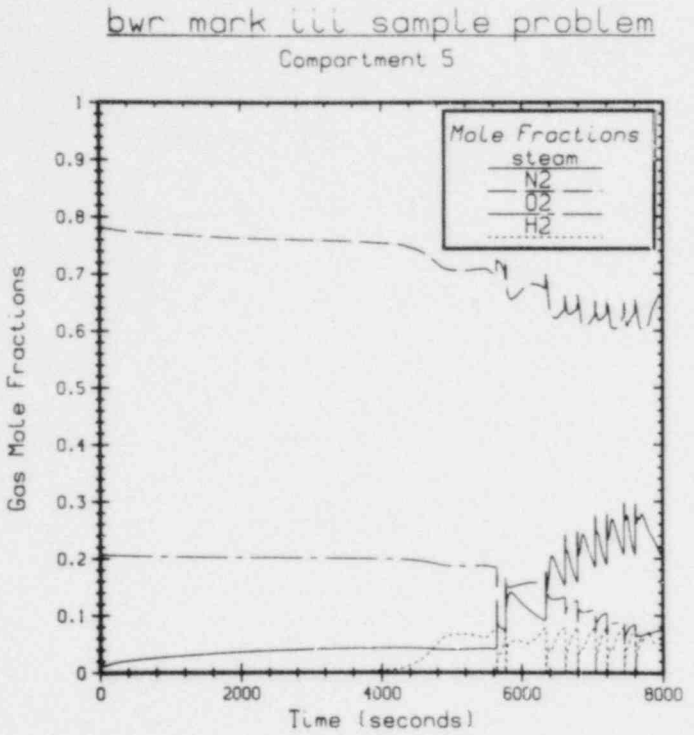


Figure 6-17. Wetwell Gas Composition for Mark III Sample Problem

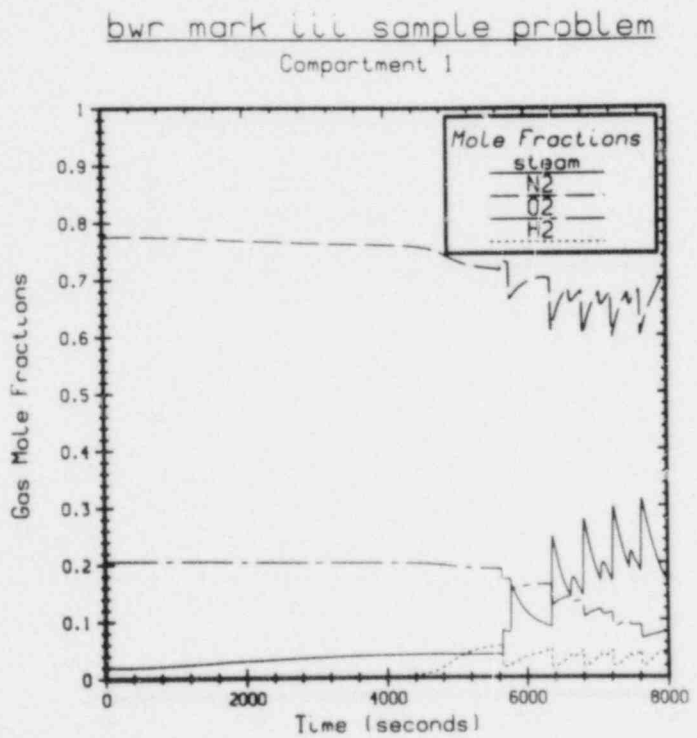


Figure 6-18. Dome Gas Composition for Mark III Sample Problem

hydrogen concentration was very low in all compartments except the wetwell and Compartment 2. Thus, the pressure rise was much smaller for the second burn than the first burn. Four of the remaining burns propagated all of the way into the dome (burns with the higher pressure rises in Figure 6-15) and the other three burns propagated into all compartments except the dome and drywell.

During the burns, the level on the wetwell side of the suppression pool was depressed, but not far enough to clear the vents. Thus, there was no pressure relief in the outer containment due to flow through the suppression pool. However, a small amount of pressure relief was provided by flow through the vacuum breakers.

Recent experiments by the Hydrogen Control Owners' Group have shown that, in some cases, the hydrogen may actually burn continuously in plumes above the suppression pool for this type of scenario, rather than in the discrete, volumetric burns calculated by the current HECTR burn models. Diffusion flame models to calculate this phenomena are being developed for HECTR, but are not currently available.

To simulate 8000 s of accident time and process the output shown, as well as some additional output (as indicated in the ACHILES input, only plots were requested for this run), the following amount of CPU time was required on a CRAY-1 computer:

compile HECTR	4.4 s
run HECTR	410 s
compile ACHILES	2.9 s
run ACHILES	77.6 s

Additional information regarding this sample case may be obtained by studying the printed output from HECTR and ACHILES provided below.

HECTR OUTPUT

```
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                              $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

 INITIAL COMPARTMENT CONDITIONS AT      0.000 SECONDS ARE:

 COMP #  TEMP      PRESSURE      XH2O        XN2         XO2         XH2

   1     300.0       101.3      0.0205      0.7746      0.2049      0.0000
   2     300.0       101.3      0.0205      0.7746      0.2049      0.0000
   3     300.0       101.3      0.0205      0.7746      0.2049      0.0000
   4     300.0       101.3      0.0205      0.7746      0.2049      0.0000
```

5	300.0	101.3	0.0205	0.7746	0.2049	0.0000
6	331.0	101.3	0.0887	0.7208	0.1906	0.0000

INITIAL SURFACE TEMPERATURES (K) ARE:

1.	300.0	2.	300.0	3.	325.0	4.	300.0	5.	300.0
6.	300.0	7.	300.0	8.	300.0	9.	300.0	10.	300.0
11.	300.0	12.	300.0	13.	300.0	14.	300.0	15.	300.0
16.	300.0	17.	300.0	18.	300.0	19.	333.0	20.	331.0
21.	331.0	22.	331.0	23.	300.0				

FANS WILL BE ACTIVATED AT 1200.000 SECONDS DUE TO
TBULK = 300.0 AND PKPA = 101.3 IN COMPARTMENT 1

HEAT EXCHANGER FOR SUMP 1 WILL BE ACTIVATED AT 1800.000 SECONDS DUE TO
TBULK = 300.0 AND PKPA = 101.3 IN COMPARTMENT 1

BURN INITIATED IN COMPARTMENT 5 AT TIME = 5645.717 SECONDS

COMPARTMENT CONDITIONS AT 5645.717 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	308.1	129.3	0.0399	0.7147	0.1890	0.0563
2	308.2	129.7	0.0401	0.7060	0.1867	0.0671
3	307.6	129.6	0.0397	0.7121	0.1884	0.0598
4	307.4	129.8	0.0394	0.7131	0.1886	0.0588
5	309.4	130.0	0.0409	0.6952	0.1839	0.0801
6	393.4	172.5	0.7602	0.1082	0.0286	0.1029

SPRAYS WILL BE ACTIVATED AT 5765.766 SECONDS DUE TO
TBULK = 364.6 AND PKPA = 141.0 IN COMPARTMENT 5

SPRAYS WILL BE SWITCHED TO RECIRCULATION AT 5765.766 SECONDS
(0.000 SECONDS AFTER BEING ACTIVATED)

BURN INITIATED IN COMPARTMENT 2 AT TIME = 5646.059 SECONDS

COMPARTMENT CONDITIONS AT 5646.059 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	315.8	140.5	0.0400	0.7144	0.1889	0.0567
2	352.3	138.6	0.0450	0.7056	0.1843	0.0652
3	317.0	139.4	0.0400	0.7117	0.1881	0.0602
4	348.1	138.9	0.0440	0.7101	0.1857	0.0601
5	643.9	138.9	0.0830	0.7092	0.1670	0.0408
6	393.4	172.6	0.7602	0.1082	0.0286	0.1029

BURN INITIATED IN COMPARTMENT 4 AT TIME = 5646.059 SECONDS

COMPARTMENT CONDITIONS AT 5646.059 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	315.8	140.5	0.0400	0.7144	0.1889	0.0567
2	352.3	138.6	0.0450	0.7056	0.1843	0.0652
3	317.0	139.4	0.0400	0.7117	0.1881	0.0602
4	348.1	138.9	0.0440	0.7101	0.1857	0.0601
5	643.9	138.9	0.0830	0.7092	0.1670	0.0408
6	393.4	172.6	0.7602	0.1082	0.0286	0.1029

BURN COMPLETED IN COMPARTMENT 5 AT TIME = 5646.400 SECONDS

COMPARTMENT CONDITIONS AT 5646.400 SECONDS ARE:

COMP #	TEMP	PRESSURE	XH2O	XN2	XO2	XH2
1	324.0	150.6	0.0402	0.7142	0.1888	0.0568
2	474.2	149.0	0.0593	0.7098	0.1784	0.0525
3	334.9	149.0	0.0415	0.7116	0.1873	0.0595
4	450.8	148.8	0.0560	0.7134	0.1807	0.0498
5	960.6	148.6	0.1262	0.7239	0.1495	0.0004
6	393.4	173.2	0.7602	0.1082	0.0286	0.1030

(ADDITIONAL BURN INFORMATION NOT SHOWN)

##
################################## END OF HECTR RUN ######################################
##

SUMMARY OF BURNS:

5 BURN(S) OCCURRED IN COMPARTMENT 1
9 BURN(S) OCCURRED IN COMPARTMENT 2
8 BURN(S) OCCURRED IN COMPARTMENT 3
8 BURN(S) OCCURRED IN COMPARTMENT 4
9 BURN(S) OCCURRED IN COMPARTMENT 5

>>> GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS <<<

>>> 5651.823 SECONDS 293.7 KPA <<<
>>> 5772.949 SECONDS 1040.4 K <<<

COMPARTMENT PRESSURE MAXIMUMS (KPA):

1. 292.8 2. 293.4 3. 293.4 4. 293.7 5. 293.5
6. 248.5

COMPARTMENT TEMPERATURE MAXIMUMS (K):

1. 735.7 2. 824.4 3. 739.0 4. 747.4 5. 1040.4
6. 423.4

SURFACE TEMPERATURE MAXIMUMS (K):

1.	339.1	2.	347.5	3.	334.0	4.	309.8	5.	347.5
6.	360.2	7.	352.1	8.	341.4	9.	341.4	10.	350.3
11.	356.2	12.	346.3	13.	346.4	14.	351.0	15.	402.6
16.	368.6	17.	367.7	18.	413.8	19.	351.4	20.	388.6
21.	388.1	22.	418.8	23.	423.2				

TOTAL MASSES	WATER+ICE	STEAM	NITROGEN	OXYGEN	HYDROGEN
INITIAL	5.540E+06	1.010E+03	3.867E+04	1.168E+04	0.000E+00
INJECTED SOURCE	4.832E+04	1.572E+05	0.000E+00	0.000E+00	1.195E+03
INJECTED SPRAY	0.000E+00	0.000E+00	0.000E+00	0.000E+00	0.000E+00
FINAL	5.745E+06	8.835E+03	3.867E+04	5.091E+03	3.612E+02

FINAL SUMP VOLUMES (M**3):

1.	3784.045
2.	1416.000
3.	662.228

NUMBER OF TIME STEPS TAKEN:

HEAT TRANSFER	=	11102
FLOW	=	34090
SUCCESSFUL FLOW	=	30590

NUMBER OF FLOW TIME STEPS REPEATED AND REASON:

1711	FLOW REVERSAL
13	CHOKING
1607	EXCESSIVE PRESSURE CHANGE
0	TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
0	NEGATIVE MOLES
8	TEMPERATURE OFF TABLES
0	TEMPERATURE TOO LOW
86	EXCESSIVE PRESSURE OR TEMPERATURE CHANGE FOR HEAT TRANSFER

FLOW TIME STEP CONTROLLING FACTORS AND TIMES USED:

13879	PRESSURE CHANGE
0	TOTAL FLOW LEAVING COMPARTMENT TOO LARGE
11618	MAXIMUM STRETCH FACTOR
4	MINIMUM STEP SIZE

```
      5003    MAXIMUM STEP SIZE
        86    MATCHING HEAT TRANSFER UPDATING TIME

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

FINAL COMPARTMENT CONDITIONS AT  8000.066 SECONDS ARE:

COMP #  TEMP     PRESSURE     XH2O       XN2        XO2        XH2

 1      336.0      137.8     0.1656     0.7088     0.0793     0.0462
 2      343.0      138.1     0.1966     0.6796     0.0762     0.0476
 3      339.5      138.0     0.1865     0.6899     0.0773     0.0463
 4      340.0      138.2     0.1918     0.6855     0.0768     0.0459
 5      347.8      138.3     0.2016     0.6727     0.0756     0.0501
 6      381.7      159.4     0.4932     0.1847     0.0347     0.2874

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

ACHILES OUTPUT

$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$
$ HECTR VERSION 1.0                                                           $
$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$$

    BWR MARK III SAMPLE PROBLEM$
    ---------------------------------------------------------------------------



8% IGNITION
FANS ON AT 1200 SEC
SPRAYS AUTO, 1 TRAIN
SUPPRESSION COOLING AFTER 1800 SEC
PURGE/VENT SYSTEM - 1 VENT, 2 COMPRESSORS
70/30 SPLIT BETWEEN S/RV'S AND BREAK


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

>>>   6 COMPARTMENT(S)          8 FLOW JUNCTION(S)          23 SURFACE(S) <<<
>>>   1 FAN(S)                  3 SUMP(S)                                 <<<

    SPRAYS WERE AUTO          FANS WERE AUTO


MINIMUM HEAT TRANSFER TIMESTEP       = 1.000E-05 SECONDS
MAXIMUM HEAT TRANSFER TIMESTEP       = 1.000E+00 SECONDS
MINIMUM FLOW TIMESTEP                = 1.000E-06 SECONDS
MAXIMUM FLOW TIMESTEP                = 1.000E+00 SECONDS
MAXIMUM TIMESTEP PRESSURE CHANGE     = 10.1325   KPA
MAXIMUM TIMESTEP TEMPERATURE CHANGE  = 10.0000   K
```

HYDROGEN LIMITS FOR	IGNITION	PROPAGATION UPWARDS	PROPAGATION SIDEWAYS	PROPAGATION DOWNWARDS
COMPARTMENT 1	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 2	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 3	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 4	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 5	8.0%	4.1%	6.0%	9.0%
COMPARTMENT 6	8.0%	4.1%	6.0%	9.0%

FAILURE PRESSURE = 496.0 KPA

COMPARTMENTS:

1. DOME
2. PIE SHAPED SECTION IN ANNULAR REGION
3. ANNULUS BETWEEN 161 AND 209
4. ANNULUS BETWEEN 135 AND 161
5. WETWELL
   (WETWELL)
6. DRYWELL
   (DRYWELL)

SURFACE TYPE KEY:
1. SLAB
2. LUMPED MASS
3. POOL
4. ICE
5. ICE CONDENSER WALL

SURFACES (BY COMPARTMENT NUMBER - SURFACE TYPE -
NUMBER OF LAYERS IF A SLAB) FOLLOWED BY THE SURFACE NUMBER
(AND THE SUMP NUMBER IF A SUMP):

(1-1-1)	1.		CONCRETE FLOOR
(1-1-1)	2.		STEEL POOL WALLS
(1-3)	3.	(3)	UPPER POOL SURFACE (UPPER POOL)
(1-1-1)	4.		CRANE$
(1-1-1)	5.		DOME AND WETWELL WALLS
(2-1-1)	6.		WETWELL WALL - COMP 2
(3-1-1)	7.		WETWELL WALL - COMP 3
(3-1-1)	8.		DRYWELL WALL - COMP 3
(3-1-1)	9.		CONCRETE - COMP 3
(3-2)	10.		MISCELLANEOUS STEEL - COMP 3
(4-1-1)	11.		WETWELL WALL - COMP 4
(4-1-1)	12.		DRYWELL WALL - COMP 4
(4-1-1)	13.		CONCRETE - COMP 4

```
(  4-2)    14.       MISCELLANEOUS STEEL - COMP 4
(  5-1-1)  15.       WETWELL WALL - COMP 5
(  5-1-1)  16.       DRYWELL WALL - COMP 5
(  5-1-1)  17.       CONCRETE - COMP 5
(  5-2)    18.       MISCELLANEOUS STEEL - COMP 5
(  5-3)    19. ( 1) SUPRESSION POOL SURFACE
                    (SUPPRESSION POOL)
                    (SPRAY SOURCE SUMP)
(  6-1-3)  20.       DRYWELL AND REACTOR SHIELD WALLS
(  6-1-1)  21.       REACTOR PEDESTAL MAT AND WEIR WALL
(  6-1-2)  22.       MISC STEEL - DW
(  6-3)    23. ( 2) DRYWELL POOL
                    (DRYWELL SUMP)
```

FLOW JUNCTIONS/COMPARTMENT INTERCONNECTIONS (INTERCONNECTION AREA IN M**2 - FLOW COEFFICIENT):

1.	1	=>	2	2-WAY	DOWNWARDS	(	74.30 -	0.75)
2.	1	=>	3	2-WAY	DOWNWARDS	(	152.10 -	1.50)
3.	2	=>	3	2-WAY	SIDEWAYS	(	135.64 -	1.50)
4.	2	=>	4	2-WAY	SIDEWAYS	(	157.00 -	1.50)
5.	2	=>	5	2-WAY	DOWNWARDS	(	62.40 -	0.75)
6.	3	=>	4	2-WAY	DOWNWARDS	(	228.80 -	1.50)
7.	4	=>	5	2-WAY	DOWNWARDS	(	144.40 -	1.50)
8.	1	=>	6	1-WAY CHECK VALVE	DOWNWARDS	(	0.05 -	1.19)

FAN CONNECTIONS (VOLUMETRIC FLOW RATE IN M**3/S WITH A NEGATIVE NUMBER INDICATING THE USE OF A HEAD CURVE):

1.	1	=>	6	SIDEWAYS	(	-0.6)

*** THIS RUN ENDED AT 8000.066 SECONDS ***

APPROXIMATE GLOBAL PRESSURE AND TEMPERATURE MAXIMUMS

5651.737 SECONDS 292.7 KPA
5772.959 SECONDS 1038.0 K

APPROXIMATE COMPARTMENT PRESSURE AND TEMPERATURE MAXIMUMS

COMPARTMENT	1:	5651.737 SECONDS	292.3 KPA
		5651.887 SECONDS	735.0 K
COMPARTMENT	2:	5651.737 SECONDS	292.6 KPA
		5648.522 SECONDS	823.1 K
COMPARTMENT	3:	5651.737 SECONDS	292.6 KPA
		5650.345 SECONDS	737.5 K
COMPARTMENT	4:	5651.737 SECONDS	292.7 KPA
		5647.896 SECONDS	746.1 K
COMPARTMENT	5:	5651.737 SECONDS	292.5 KPA
		5772.959 SECONDS	1038.0 K
COMPARTMENT	6:	5657.554 SECONDS	248.5 KPA
		1801.625 SECONDS	423.1 K

UOF = 8 UOA = 9

NHT = 3491 NFL = 11400 NAH = 3491

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APPENDIX A

DESCRIPTION OF MODELS

CONTENTS

LIST OF FIGURES

LIST OF TABLES

A. DESCRIPTION OF MODELS

In this section, the details of the methods used in HECTR are described. The code structure and governing equations are discussed first, followed by descriptions of the various physical models that provide terms for the governing equations.

A.1 General Code Structure

A.1.1 Multicompartment Mass, Energy, and Momentum Equations and the Equation of State

The multicompartment gas-transport model is a system of ordinary differential equations expressing conservation of mass, energy, and momentum. The mass conservation equations are formulated for each of four gas species (water vapor, nitrogen, oxygen, and hydrogen) in each compartment on a molar basis. Within each compartment the gases are perfectly mixed. Thus, a single conservation of energy equation is formulated for the total mixture in each compartment. Conservation of momentum is specified at flow junctions, which are the connections between compartments. Gas flow between compartments is caused by pressure differences, gravitational forces, and fans. Compartment interconnections are modeled as orifices with flow resistances. For the equations of state, steam is treated as a real gas, while the other gases are treated as ideal. Figure A-1 presents a simplified flow chart for HECTR. Refer to this figure as necessary during the following discussions.

The independent variable in this model is time, and the governing dependent variables are

$$N_{ij},\ E_i,\ \text{and}\ F_\ell$$

N_{ij} is the number of moles of the j^{th} species of gas in the i^{th} compartment. E_i is the total internal energy in compartment i and can be expressed by

$$E_i = \sum_{j=1}^{N_{gases}} N_{ij} u_{ij} \qquad (N_{gases} = 4) \qquad \text{(A-1)}$$

where u_{ij} is the molar internal energy of the j^{th} gas in the i^{th} compartment. F_ℓ is the volumetric flow rate in the ℓ^{th} junction, defined by $F_\ell = A_\ell v_\ell$ where A_ℓ is the interconnection area and v_ℓ is the gas velocity at the ℓ^{th} junction. The conservation equations define the rate of change of each of these

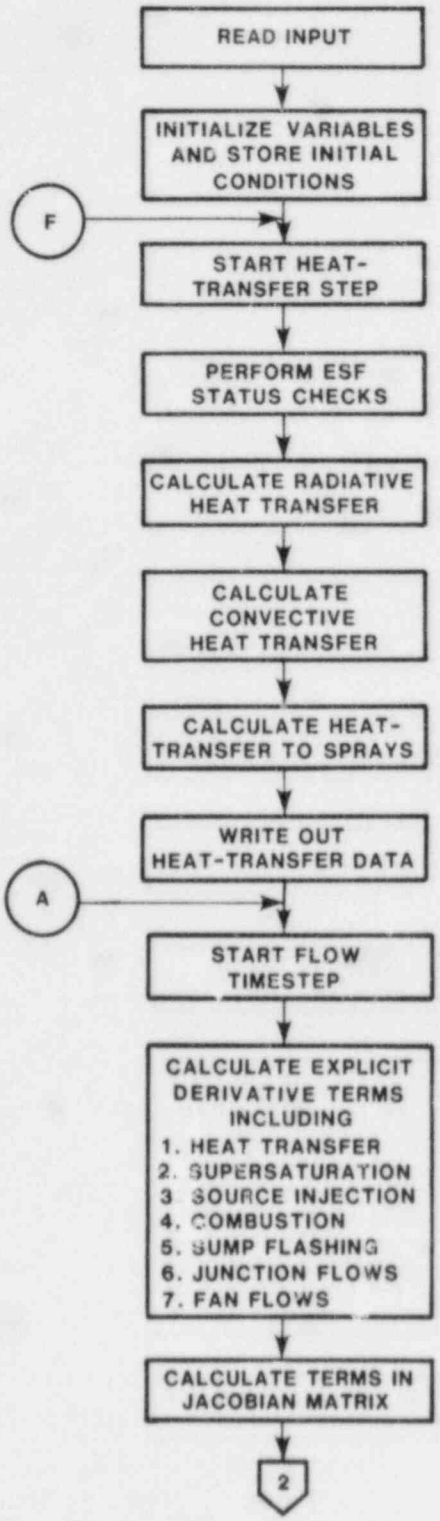


Figure A-1. Simplified Flow Chart for HECTR

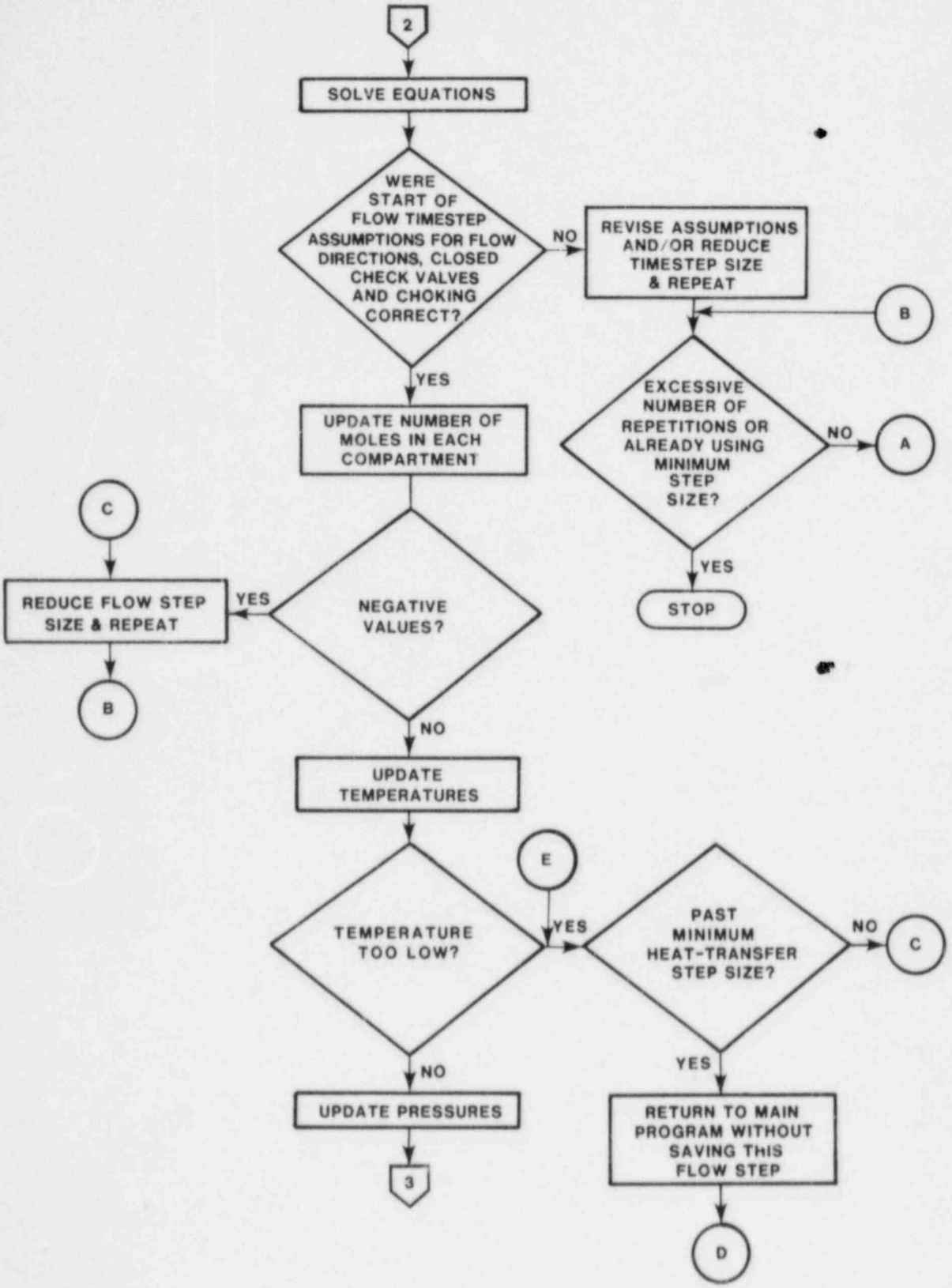


Figure A-1. Simplified Flow Chart for HECTR (Continued)

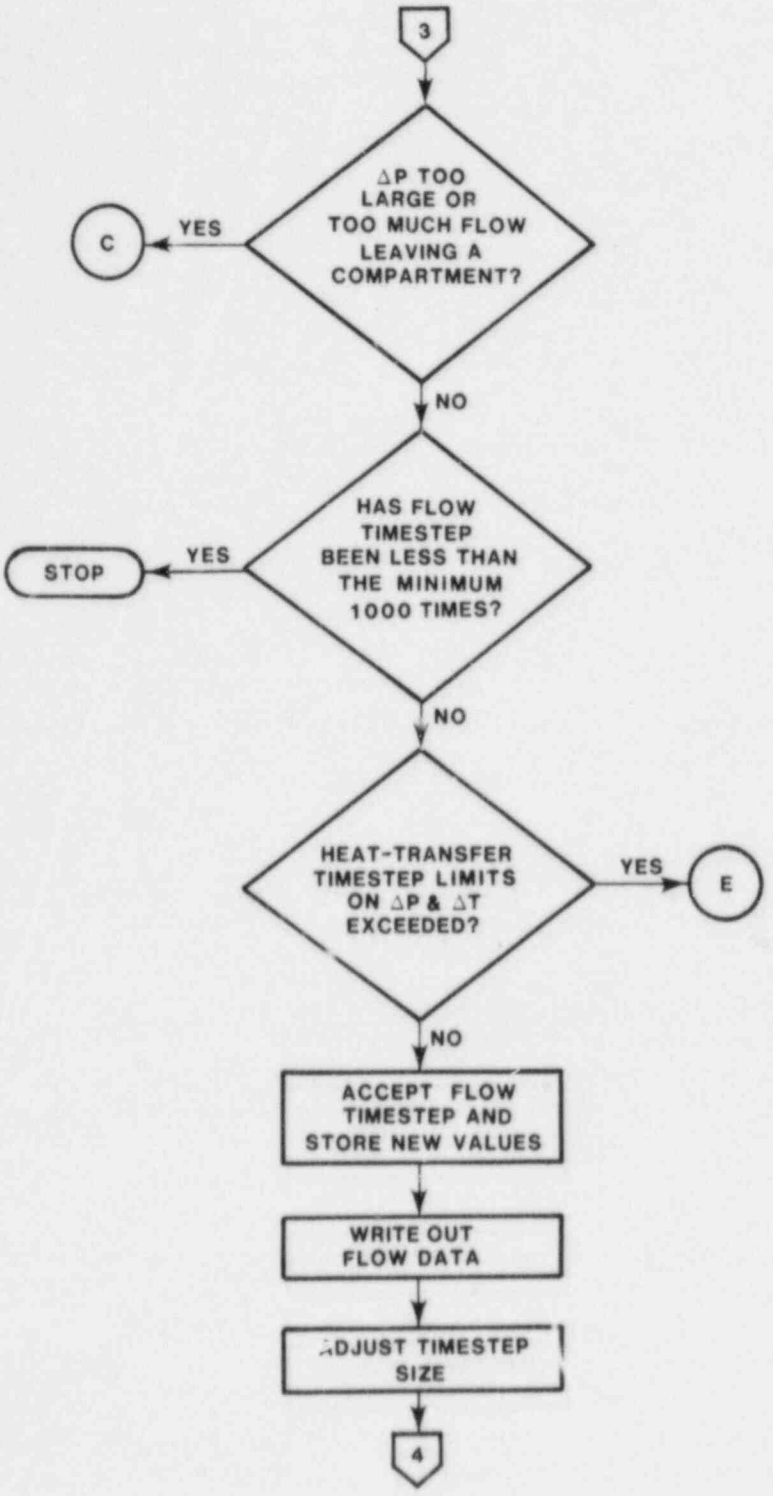


Figure A-1. Simplified Flow Chart for HECTR (Continued)

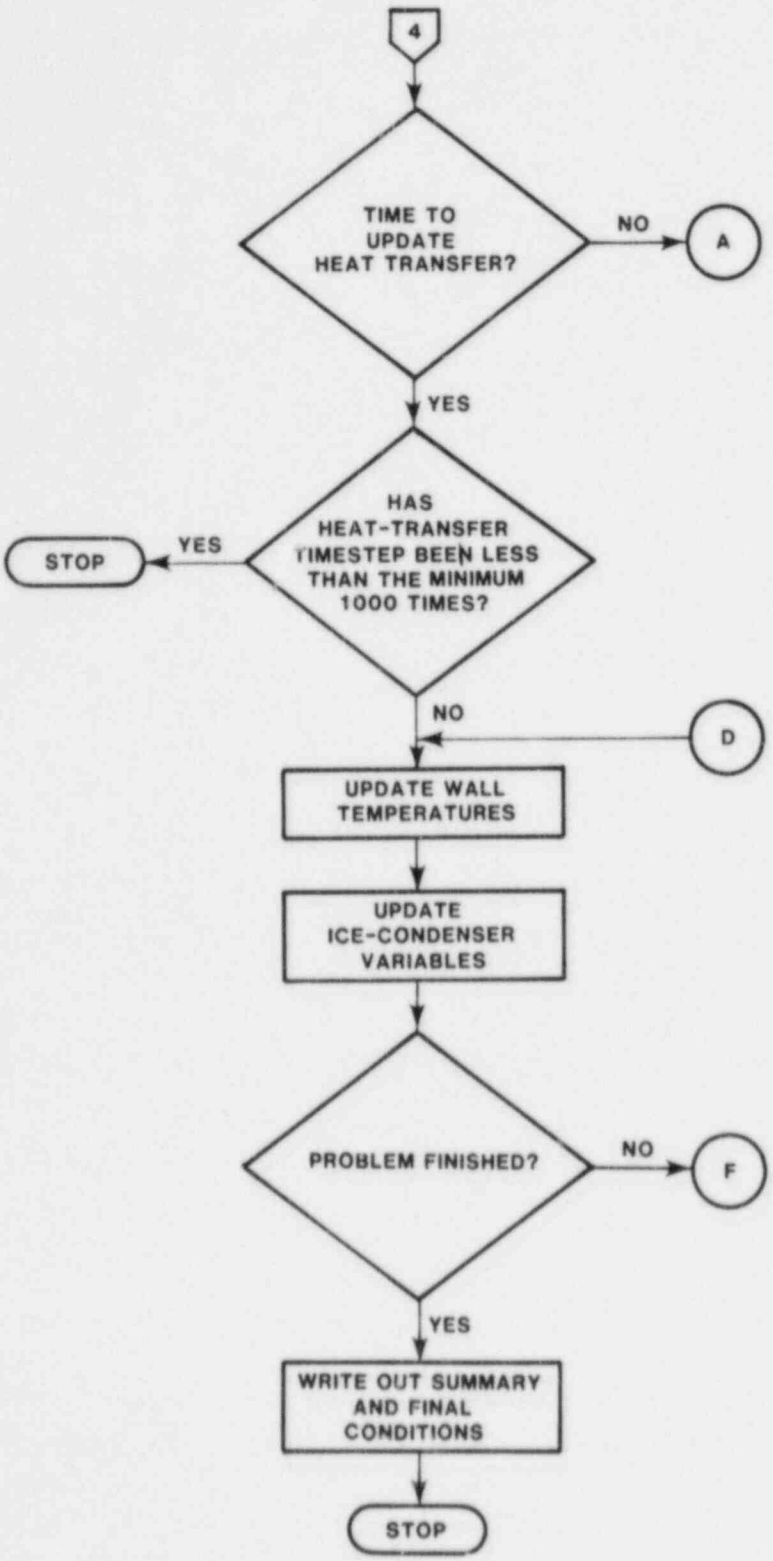


Figure A-1. Simplified Flow Chart for HECTR (Continued)

three types of variables. The total number of equations that are solved simultaneously is

$$N_{eqns} = (N_{gases} + 1)\, N_{comps} + N_{juncs} \qquad (A\text{-}2)$$

where N_{comps} and N_{juncs} are the number of compartments and the number of flow junctions, respectively.

The conservation equations and equation of state are given below with the same subscript convention as used above. The positive flow direction for the ℓ^{th} junction is from compartment i to compartment k (see Figure A-2). Note that the intercompartment fan flows are included separately from the junction flow terms, F_ℓ. A derivation of a momentum equation similar to Eq. A-5 may be found in Reference 1.

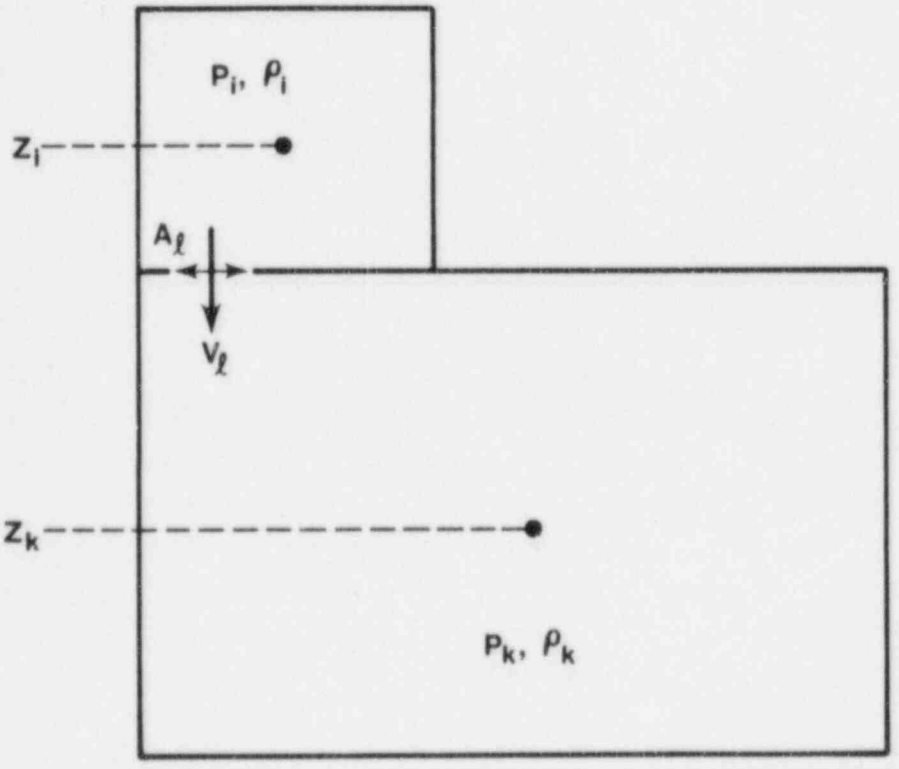


Figure A-2. Flow Junction Parameters

Conservation of Molar Content:

$$\frac{dN_{ij}}{dt} = - \sum_{\substack{\ell \\ (F_\ell>0)}} \frac{F_\ell}{V_i} N_{ij} - \sum_{\substack{\ell \\ (F_\ell<0)}} \frac{F_\ell}{V_k} N_{kj} + \left(\frac{dN_{ij}}{dt}\right)_{\substack{\text{ext.} \\ \text{source}}}$$

$$+ \left(\frac{dN_{ij}}{dt}\right)_{\substack{\text{chem.} \\ \text{source}}} + \left(\frac{dN_{i,H_2O}}{dt}\right)_{\substack{\text{evap.,} \\ \text{cond.}}} + \left(\frac{dN_{ij}}{dt}\right)_{\text{fans}}$$

$$+ \left(\frac{dN_{i,H_2O}}{dt}\right)_{f\ell} + \left(\frac{dN_{ij}}{dt}\right)_{SP} \qquad \text{(A-3)}$$

Conservation of Energy:

$$\frac{dE_i}{dt} = \sum_{j=1}^{N_{gases}} \left[- \sum_{\substack{\ell \\ (F_\ell>0)}} \frac{F_\ell}{V_i} N_{ij} h_{ij} - \sum_{\substack{\ell \\ (F_\ell<0)}} \frac{F_\ell}{V_k} N_{kj} h_{kj} \right.$$

$$\left. + \left(\frac{dN_{ij}}{dt}\right)_{\substack{\text{ext.} \\ \text{source}}} h_{j,source} \right] + \left(\frac{dN_{i,H_2O}}{dt}\right)_{\substack{\text{evap.,} \\ \text{cond.}}} h_{i,H_2O}$$

$$+ \left(\frac{dN_{i,H_2O}}{dt}\right)_{F\ell} h_{i,H_2O} - \left(\frac{dQ}{dt}\right)_{\substack{\text{rad.,} \\ \text{conv.}}} - \left(\frac{dQ}{dt}\right)_{\text{sprays}}$$

$$+ \left(\frac{dE_i}{dt}\right)_{\text{fans}} + \left(\frac{dE_i}{dt}\right)_{SP} \qquad \text{(A-4)}$$

Conservation of Momentum:

$$\frac{dF_\ell}{dt} = \frac{2}{(\rho_i + \rho_k)(L/a)_\ell} \left[(P_i - P_k) + g[\rho_i(z_i - z_\ell) \right.$$

$$\left. + \rho_k(z_\ell - z_K)] - \frac{K_\ell(\rho_i + \rho_k) F_\ell |F_\ell|}{4A_\ell^2} \right] \qquad \text{(A-5)}$$

Equation of State:

$$P_i = \frac{ZN_{i,H_2O}RT_i}{V_i} + \sum_{j=2}^{N_{gases}} \frac{N_{ij}RT_i}{V_i} \qquad \text{(A-6)}$$

where

V_i = volume of Compartment i (m^3)

$\left(\frac{dN_{ij}}{dt}\right)_{\substack{ext.\\source}}$ = rate of addition of species j into compartment i from an external source (moles/s)

$\left(\frac{dN_{ij}}{dt}\right)_{chem.}$ = chemical molar rate of change of species j due to combustion (moles/s)

$\left(\frac{dN_{i,H_2O}}{dt}\right)_{\substack{evap.,\\cond.}}$ = positive or negative rate of change of atmospheric water vapor due to evaporation from or condensation on surfaces and spray droplets (moles/s)

$\left(\frac{dN_{ij}}{dt}\right)_{fans}$ = rate of addition of gas into compartment i due to intercompartment fans (moles/s)

$\left(\frac{dN_{i,H_2O}}{dt}\right)_{F\ell}$ = rate of addition of steam to compartment i due to sump boiling

$\left(\frac{dN_{ij}}{dt}\right)_{SP}$ = rate of addition of gas due to flow through the suppression pool (see Section A.2.10) (moles/s)

h_{ij} = enthalpy of the j^{th} gas evaluated at the temperature in the i^{th} compartment (J/mole)

$h_{j,source}$ = enthalpy of the j^{th} gas evaluated at the source temperature (J/mole)

$\left(\frac{dQ}{dt}\right)_{\substack{rad.,\\conv.}}$ = sum of the rates of radiative and convective heat transfer from the gas (W)

$\left(\frac{dQ}{dt}\right)_{sprays}$ = rate of heat transfer from the gas to the spray droplets (W)

$\left(\frac{dE_i}{dt}\right)_{fans}$ = energy addition to compartment i due to intercompartment fans (see Eq. A-23) (W)

$\left(\frac{dE_i}{dt}\right)_{SP}$ = energy addition to compartment i due to gas flow through the suppression pool (see Section A.2.10) (W)

ρ_i = gas density in compartment i (kg/m^3)

$(L/a)_\ell$ = ratio of effective gas inertial length to effective gas flow area for the ℓ^{th} junction (m^{-1}).

P_i = pressure in compartment i (Pa)

g = acceleration due to gravity (m/s^2)

z_i = elevation of compartment i (m)

z_ℓ = elevation of flow junction ℓ (m)

K_ℓ = loss coefficient due to flow through the ℓth junction

A_ℓ = interconnection area of the ℓth junction (m^2)

Z = compressibility factor for steam (tabular function of temperature and steam partial pressure)

R = universal gas constant (J/mole-K)

T_i = gas temperature in compartment i (K)

Note that there is nothing in the above equations to explicitly prevent unphysical (or at least nonequilibrium) situations from occurring. In particular, subcooled (supersaturated) steam is possible. Therefore, a check is performed whenever new gas pressures and temperatures are calculated, and if the steam is subcooled, excess steam is removed from the atmosphere over the following timestep and placed in a specified liquid sump. For this case, the following terms are added to the right sides of Eqs. A-3 and A-4 during the next timestep:

$$\left(\frac{dN_{i,H_2O}}{dt}\right)_{sc} = -\frac{\Delta N_{sc}}{\Delta t} \tag{A-7}$$

$$\left(\frac{dE_i}{dt}\right)_{sc} = \left(\frac{dN_{i,H_2O}}{dt}\right)_{sc} \left(h_{i,H_2O} - h_{fg}\right) \tag{A-8}$$

where

ΔN_{sc} = Approximate amount of mass of steam condensed to bring the compartment to saturation (moles)

Δt = Timestep size (s)

h_{fg} = Heat of vaporization (J/mole)

A.1.2 Method of Solution

The conservation equations in HECTR are solved using a linearized implicit formulation (backward Euler method). This formulation is derived by writing the conservation equations in the general form

$$\frac{d\bar{y}}{dt} = \bar{f}(\bar{y},t) \tag{A-9}$$

where $\bar{y}$ is a vector of the governing dependent variables ($N_{i,j}$, E_i, and F_ℓ). A Taylor series expansion of $f(\bar{y},t)$ up through first order terms is then performed, producing

$$\frac{d\bar{y}}{dt} = \bar{f}(\bar{y}_0,t_0) + \left(\frac{\partial \bar{f}}{\partial \bar{y}}\right)_{\bar{y}_0,t_0} (\bar{y} - \bar{y}_0) \tag{A-10}$$

where $\bar{y}_0$ is the vector of initial conditions evaluated at t_0 and $\partial\bar{f}/\partial\bar{y}$ is the Jacobian of $\bar{f}$. Finally, applying a finite difference approximation to the left hand side of Eq. A-10 results in the linear system of equations

$$\frac{\bar{y} - \bar{y}_0}{\Delta t} = \bar{f}(\bar{y}_0,t_0) + \left(\frac{\partial \bar{f}}{\partial \bar{y}}\right)_{\bar{y}_0,t_0} (\bar{y} - \bar{y}_0) \tag{A-11}$$

This system of equations can be written more conveniently as

$$A\Delta\bar{y} = \bar{b} \tag{A-12}$$

where

$$A = \frac{1}{\Delta t} I - \left(\frac{\partial \bar{f}}{\partial \bar{y}}\right)_{\bar{y}_0, t_0} \tag{A-13}$$

$$\Delta\bar{y} = \bar{y} - \bar{y}_0 \tag{A-14}$$

$$\bar{b} = \bar{f}(\bar{y}_0, t_0) \tag{A-15}$$

and I is the identity matrix. Solving this system determines the updated values for the dependent variables contained in y after a timestep of length Δt.

In HECTR, only the terms of the Jacobian involving flows are calculated. This reduces the amount of computation required both to create the matrix A and to solve the resulting linear system involving A. The general structure of the Jacobian matrix used is

$$\begin{vmatrix} 0 & 0 & \partial\dot{N}/\partial F \\ 0 & 0 & \partial\dot{E}/\partial F \\ \partial\dot{F}/\partial N & \partial\dot{F}/\partial E & \partial\dot{F}/\partial F \end{vmatrix}$$

Here, the dots indicate differentiation with respect to time. The calculated terms are presumed to dominate the matrix, thus allowing the other terms ($\partial\dot{N}/\partial N$, $\partial\dot{N}/\partial E$, $\partial\dot{E}/\partial N$, and $\partial\dot{E}/\partial E$) to be neglected. The form of the matrix A is also considerably simplified. The linear equation solver used in HECTR for the solution of Eq. A-12 has been modified especially to take advantage of the regular pattern of zeroes found in the A matrix.

Equation A-12 is solved in HECTR by the following sequence of operations. First, the right hand side, b, is calculated, and then the A matrix is calculated. Next, the equations are scaled to reduce the condition number of A. An LU decomposition is then performed on A. Every 1000 timesteps the condition number of A is calculated to check if the matrix is still well conditioned. Finally, the values of Δy are solved through back substitution.

A.1.3 Timestep Control

In HECTR there are two major kinds of timesteps: heat-transfer timesteps (ΔT) and flow timesteps (Δt). Heat-transfer rates are relatively constant over a longer time scale than is required to solve the conservation (flow) equations. Thus, we have decoupled the heat-transfer calculations from the flow calculations. Heat- and mass-transfer rates caused by radiation, convection, condensation, and sprays are computed at the beginning of a heat-transfer timestep. These rates are then held constant while the flow calculations are performed in one or more flow timesteps (so that each heat-transfer timestep contains one or more flow timesteps). During each flow timestep, the conservation equations are integrated over the time interval Δt. Then, new compartment temperatures are determined from the new values for the number of moles and the internal energies; volume changes caused by sumps or melting ice are incorporated; and pressures are updated through the equation of state. Flow timesteps are sometimes repeated. Causes include excessive pressure changes, flow reversals, door closings, choking, too much gas volume flowing out of a compartment, the number of moles of a gas species in a compartment becoming negative, the temperature of a compartment falling below freezing, and an excessive pressure or temperature change occurring during the current heat-transfer timestep. The heat-transfer timestep ends when one of various conditions (discussed below) is met. Surface temperatures are then updated through a heat-conduction or lumped-mass calculation, and the cycle repeats with new heat-transfer rates being calculated based on the new containment conditions.

The HECTR timestep controller automatically chooses both the heat-transfer and the flow timesteps. The lengths of these timesteps are constrained by both user-specified parameters (see Section 4.2.3.6.3) and internal HECTR limits. For flow timesteps HECTR allows a maximum pressure change of 300 Pa per compartment and permits at most 95% of a compartment's gas volume to flow out into other compartments. The heat-transfer timesteps are limited by maximum pressure and temperature changes of 10132.5 Pa and 10 K per compartment during a single heat-transfer timestep. Both kinds of timesteps are further constrained by user-specified minimums and maximums (the default values are $0.000001 < \Delta t < 2$ seconds and $0.00001 < \Delta T < 2$ seconds). It should be noted that HECTR will use a timestep smaller than the minimum if necessary, but HECTR will do this only 1000 times before the calculation will automatically terminate with a message provided. Also, neither timestep is allowed to increase by more than a factor of 1.5 per timestep. Finally, there must be an integral number of flow timesteps per heat-transfer timestep. This sometimes results in cutting the last flow timestep in a heat-transfer timestep shorter than its previously selected length.

There is also a third kind of timestep used in HECTR, which controls the suppression pool motion. Each flow timestep may contain one or more of these suppression pool timesteps. This timestep is discussed in greater detail in Section A.2.10.

A.2 Physical Models

A.2.1 Flow Junctions

Gases can be transferred between compartments because of flow through flow junctions, fans, or suppression pool vents. Fans are discussed in Section A.2.2 and suppression pool vent flows are discussed in Section A.2.10. Four types of flow junctions are included in HECTR:

1. Two-way flow through an orifice
2. One-way flow through an orifice (check valve)
3. One-way flow through a variable area orifice (door)
4. Flow through drains in an ice-condenser containment

Note that two-way flow does not mean that the flow can be going in both directions during the same timestep, but rather that the flow direction can freely change from one timestep to the next. The most common junction is the first type. The flows are determined according to Eq. A-5, with user-specified values for flow area, flow resistance, and the ratio of the inertial length to the flow area (see Section A.1.1). The second type of flow junction is similar to the first, except that flow is allowed in one direction only. The junction is assumed to be fully open as soon as the flow begins and to be closed as soon as the flow attempts to reverse.

The third type of flow junction allows the flow area to vary as a function of the differential pressure between compartments. This type of junction is used for modeling ice-condenser doors. The model was taken with only minor changes from Reference 2. A minimum differential pressure is specified that must be exceeded before the junction area will be allowed to increase beyond its minimum value, A_{min} (usually set to zero). Once the junction is open, the flow area is determined from the following expressions:

$$\frac{A}{A_0} = \frac{1.0 - \cos\theta}{1.0 - \cos\theta_0} \qquad \text{(A-16)}$$

and

$$\frac{\theta}{\theta_0} = \frac{\Delta P \cos\theta}{\Delta P_0 \cos\theta_0} \qquad \text{(A-17)}$$

where

A = flow area (m^2)

A_0 = fully open flow area (m^2)

ΔP = differential pressure across the junction minus the minimum pressure to open (Pa)

ΔP_0 = differential pressure to hold the junction fully open (Pa)

θ = door opening angle (radians)

θ_0 = fully open door angle (radians)

A_0, P_0, θ_0, and the minimum pressure to open the junction are user inputs.

The door flow area is very sensitive to small changes in pressure, and thus, the flows through the doors can vary dramatically from one timestep to the next, causing some numerical problems for HECTR. To alleviate these problems, some artificial smoothing is employed in the door model. The flow area used in the calculation is determined from

$$A_{new} = \begin{cases} 0.8A_{old} + 0.2A \text{ for } A > A_{min} \\ 0.5A_{old} + 0.5A \text{ for } A \leq A_{min} \end{cases} \quad \text{(A-18)}$$

where A_{old} is the area used in the previous timestep, and A is the value determined from Eq. A-16.

HECTR includes a special type of junction for floor drains that exist in ice-condenser containments. These drains allow water from the sprays to drain from the upper compartment to the lower compartment sump. HECTR models the drains as normal two-way flow junctions, but includes logic for closing the drains under certain conditions. HECTR will close the drains whenever the sprays are initiated or the lower compartment sump volume exceeds a user-specified value, such that the bottom of the drains would be covered.

Under certain conditions, the HECTR flow equations must be modified. In particular, if a check valve is closing, then an explicit expression is used for the flow equation to force the flow to zero at the end of the timestep. This is accomplished by setting the terms $\partial \dot{F}_\ell / \partial N$, $\partial \dot{F}_\ell / \partial E$, and $\partial \dot{F}_\ell / \partial F$ in the matrix A to zero and using the following expression for the corresponding term in the vector $\bar{b}$.

$$\frac{dF_\ell}{dt} = \frac{-F_\ell}{\Delta t} \quad \text{(A-19)}$$

Flow junction velocities are not allowed to exceed sonic flow velocities. A basic HECTR assumption is that all flows are of low Mach number. Nevertheless, it is possible for the predicted flow velocities to be equal to or above the speed of sound. In such a case, the timestep is repeated using an explicit formulation similar to that discussed above. However, for this case, the flow is forced to the speed of sound, rather than to zero. The same terms in the A matrix are set to zero for this case, but the flow derivative expression used in the vector $\bar{b}$ is

$$\frac{dF_\ell}{dt} = \frac{F_s - F_\ell}{\Delta t} \text{ , for } F_\ell \geq 0 \qquad \text{(A-20)}$$

$$= \frac{-F_s - F_\ell}{\Delta t} \text{ , for } F_\ell < 0$$

where F_s is the volumetric flow rate through the junction at sonic conditions.

If the flow at a junction reverses direction during a timestep, the mass and energy conservation equations must be modified. This is necessary because HECTR uses a donor formulation for the mass and energy equations (i.e., gases that flow between two compartments are assumed to be at the conditions of the upstream [donor] compartment). If the flow reverses during a timestep, the donor compartment also changes. Because of the implicit formulation that is used in HECTR, conditions of the donor compartment at the end of the timestep can be used during the entire timestep to give results that are equivalent to subdividing the timestep and using the appropriate donor compartment when calculating each part of the timestep. Thus, if the flow reverses during a timestep, HECTR repeats the timestep using the conditions of the new donor compartment when calculating the flow terms in the A matrix and b vector for the mass and energy equations.

A.2.2 Intercompartment Fans

The HECTR fan model can treat flow between any pair of compartments, and any number of different fans can be included. There are three fan model options available in HECTR:

1. Constant flow rate
2. Flow using a built-in head curve
3. Flow using an arbitrary user-input head curve

The rate of change of mass and energy in compartment i due to fan flow is

$$\frac{dN_{ij}}{dt} = \sum_k FN_{ikj} \qquad \text{(A-21)}$$

where

$$FN_{ikj} = \begin{cases} \dfrac{-FR_{ik}}{V_i} N_{ij} & \text{for } FR_{ik} \geq 0 \\ \dfrac{-FR_{ik}}{V_k} N_{kj} & \text{for } FR_{ik} < 0 \end{cases} \qquad \text{(A-22)}$$

and

$$\frac{dE_i}{dt} = \sum_k FE_k \qquad \text{(A-23)}$$

where

$$FE_k = \begin{cases} -\sum_{j=1}^{N_{gases}} \dfrac{FR_{ik}}{V_i} N_{ij} h_{ij} & \text{for } FR_{ik} \geq 0 \\ -\sum_{j=1}^{N_{gases}} \dfrac{FR_{ik}}{V_k} N_{kj} h_{kj} + W_{fan} & \text{for } FR_{ik} < 0 \end{cases} \qquad \text{(A-24)}$$

Here, k = connected compartment

j = gas species

FR = fan volumetric-flow rate (m^3/s)

N = number of moles in a compartment

V = compartment volume (m^3)

h = gas enthalpy (J/mole)

W_{fan} = work done by a fan (W)

The terms resulting from Eqs. A-21 and A-23 are entered into the general mass and energy conservation equations presented in Section A.1.1.

As noted earlier, HECTR contains a built-in pressure head versus fan flow curve. This normalized curve is presented in Table A-1, where P represents the fraction of the specified shutoff head, and F represents the fraction of the maximum flow rate. These values were taken from Reference 3. If the pressure gradient is in the direction of the fan flow, F is set equal to 1.0. Thus, overspeeding a fan is not permitted in HECTR. For P greater than one, F is set to 0.0, and reverse flow through the fans is prohibited.

Table A-1

Pressure Head Versus Fan Flow Values (Normalized)

P	F
<0.0	1.0
0.0	1.0
0.1635	1.0
0.3846	0.9224
0.5769	0.8362
0.7692	0.7241
0.8173	0.6897
0.8654	0.6552
0.9135	0.6031
0.9615	0.5345
1.0	0.4741
>1.0	0.0

A.2.3 Hydrogen Combustion

The combustion model consists of correlations for ignition limits, propagation criteria, combustion completeness, and flame speed. The combustion completeness and flame speed correlations were derived from a variety of experiments that were performed in the VGES and FITS experimental facilities at Sandia, References 4 and 5. All basic parameters of the model may be user-specified on a global or a compartment-by-compartment basis, or default values may be used.

A burn can initiate in a compartment whenever a specified hydrogen concentration is exceeded, provided that the atmosphere in the compartment is not inerted by a shortage of oxygen or an excess of steam. The values of these limiting concentrations are termed the ignition limits. Once a burn has started in a compartment, it can propagate into an adjacent connected compartment if the composition of the gases in this adjacent compartment falls within the propagation

limits. These limits depend on the spatial relationship of the two compartments (i.e., whether the adjacent compartment is located above, below, or on the same level as the burning compartment). The ignition and propagation limits may be user-specified on a global or compartment-by-compartment basis, or the default values may be used. These default values are shown in Table A-2.

Table A-2

Default Hydrogen Ignition and Propagation Limits

Parameter	Mole Fraction		
	H_2	O_2	H_2O
Ignition Limits	$\geq$ 0.08	$\geq$ 0.05	$\leq$ 0.55
Upward Propagation	$\geq$ 0.041	$\geq$ 0.05	$\leq$ [illegible] 5
Horizontal Propagation	$\geq$ 0.06	$\geq$ 0.05	$\leq$ 0.55
Downward Propagation	$\geq$ 0.09	$\geq$ 0.05	$\leq$ 0.55

A burn can propagate through either a flow junction or a fan. Each fan is assumed by default to have a nonreturn damper (or check valve) so that burns will be prevented from propagating in either direction through a fan when the volumetric flow rate is zero. Also, by default, burns are not allowed to propagate upstream through a fan. Either of these defaults can be overridden for all fans or any set of fans. One last important propagation criterion is the fraction of the burn time that must elapse in a burning compartment before propagation into adjacent compartments can be attempted. This number is the propagation factor, k, which is specified for propagation through each flow junction and fan path. "k" must satisfy $0 \leq k \leq 1$. The default value of the propagation factor for all paths is 0.5. Note that all combustion parameters are calculated individually in each compartment into which a burn propagates at the time that the propagation occurs.

Combustion completeness may be user-specified. The default correlation for combustion completeness is:

$$X_f = \text{Max}\ [(1.0 - 12.4375X_i)X_i,\ 0.005\ X_i] \qquad \text{(A-25)}$$

where X_i and X_f are the initial and final mole fractions of hydrogen, respectively. Using this correlation, combustion is assumed to be complete for hydrogen concentrations at or above 8%.

Either the flame speed or the burn time may be user-specified. The default flame speed correlations used in HECTR for various situations are shown below, where X_s is the initial mole fraction of steam and the velocity is given in m/s:

$(0.0 \leq X_i \leq 0.1)$

$$V = (59.2X_i + 1.792)C \tag{A-26}$$

$$C = \begin{cases} 1.0 - 4.53X_s + 5.37X_s^2 & \text{for } X_s \leq 0.4 \\ 0.05 & \text{for } X_s > 0.4 \end{cases} \tag{A-27}$$

$(0.1 < X_i \leq 0.2)$

$$V = (172.88X_i - 9.576)C \tag{A-28}$$

$$C = \begin{cases} 1.0 - 4.53X_s + 5.37X_s^2 & \text{for } X_s \leq 0.4 \\ 0.05 & \text{for } X_s > 0.4 \end{cases} \tag{A-29}$$

$(0.2 < X_i \leq 0.3)$

$$V = (50.0X_i + 15.0)C \tag{A-30}$$

$$C = \begin{cases} (1.0 - 4.53X_s + 5.37X_s^2)\,(3.0 - 10.0X_i) & \\ \quad + (1.0 - 1.29X_s)\,(10.0X_i - 2.0) & \text{for } X_s \leq 0.4 \\ 0.15 - 5.0X_i + (1.0 - 1.29X_s)\,(10.0X_i - 2.0) & \\ \text{for } X_s > 0.4 & \end{cases} \tag{A-31}$$

$(0.3 < X_i \leq 0.4)$

$$V = (-50.0X_i + 45.0)C \tag{A-32}$$

$$C = 1.0 - 1.29X_s \tag{A-33}$$

$(0.4 < X_i \leq 0.6)$

$$V = (-75.0X_i + 55.0)C \tag{A-34}$$

$$C = 1.0 - 1.29X_s \tag{A-35}$$

$(X_i > 0.6)$

$$V = \text{Max}\ [(-64.3X_i + 48.58)C,\ C] \tag{A-36}$$

$$C = 1.0 - 1.29X_s \tag{A-37}$$

Burn times are calculated by dividing a characteristic compartment dimension by the flame speed. Once the burn time has been calculated, it remains fixed during the burn. The chemical reaction rate is adjusted each timestep to account for intercompartment flows and source injection so that the burn finishes at the predetermined time with the correct final mole fraction of hydrogen.

A.2.4 Radiative Heat Transfer

Radiant heat transfer is important during and following combustion events in containment, and to a lesser extent, following blowdown, if relatively high temperatures and steam partial pressures exist. Most of the radiant heat transfer will come from steam, with air generally nonradiating for the temperature regimes of interest. Reflection of radiation by the containment surfaces is important, as is emission from the walls if their temperatures are elevated during the accident. In the discussion below, the emittance model for steam is presented, along with the governing equations for radiant exchange. The interaction of radiation with sprays and aerosols is not treated in HECTR Version 1.0.

Steam emittance is usually determined from either emittance charts or an exponential wide-band molecular radiation model. Originally in HECTR, we had implemented a seven-band exponential model, but found it to be expensive computationally. This model was replaced by a single equivalent band model suggested by Cess and Lian for mixtures of steam and air.[6] In this model data from the Hottel emittance charts[7] have been fitted to an exponential form. This new model produces results very similar to the wide-band exponential model with a considerable reduction in computation time. The Cess-Lian correlations used in HECTR are

$$e_{k-j} = a_0(1 - e^{-a_1\sqrt{y}}) \tag{A-38}$$

$$y = PP_r L_{k-j} \left(\frac{300}{T_r}\right) \frac{P_r + \left(5\sqrt{\frac{300}{T_r}} + 0.5\right) PP_r}{(101325)^2} \tag{A-39}$$

where

e_{k-j} = steam emittance for a path between surfaces k and j,

a_0, a_1 = determined from Table A-3,

PP_r = path steam partial pressure (Pa),

L_{k-j} = beam length for a path between surfaces k and j (m),

T_r = path gas temperature (K), and

P_r = path total gas pressure (Pa).

Here, P_r, PP_r, and T_r are equal to the compartment values if the surfaces k and j both reside in the same compartment. If the two surfaces are in different compartments (for example, n and m) then values for P_r, PP_r, and T_r are found from

$$P_r = \frac{V_n P_n + V_m P_m}{V_n + V_m} \qquad \text{(A-40)}$$

$$PP_r = \frac{V_n PP_n + V_m PP_m}{V_n + V_m} \qquad \text{(A-41)}$$

$$T_r = \left[\frac{V_n T_n^4 + V_m T_m^4}{V_n + V_m}\right]^{1/4} \qquad \text{(A-42)}$$

where V_n is the volume of compartment n. This model is valid only for surfaces in adjacent compartments; even for adjacent compartments the model may be of limited accuracy. More discussion on this subject is provided in Chapter 3.

The first and last values in Table A-3 represent extrapolations of the Cess-Lian data. This is reasonable because radiation is not important below 300 K, and temperatures above 1500 K are usually present for only very short times, if at all. Note that pressure broadening effects are included in the above formulation and also that the relation reduces to the well-known square-root dependence for the limit of nonoverlapping strong absorption lines.

Table A-3

Coefficients for the Cess-Lian Correlation

T (K)	a_0	a_1 ($m^{-1/2}atm^{-1}$)
273.	0.6838	1.16
300.	0.683	1.17
600.	0.674	1.32
900.	0.700	1.27
1200.	0.673	1.21
1500.	0.624	1.15
2500.	0.461	0.95

The radiative exchange package is formulated assuming that the wall temperature and gas environment are fixed during each heat-transfer timestep. Both the walls and the gas are assumed to be "gray". The net radiative heat flux for each surface is calculated from

$$q_j = \frac{e_j}{1 - e_j} (B_j - J_j) \qquad \text{(A-43)}$$

where

j = surface number

q_j = net heat flux from the surface (W/m^2)

e_j = emissivity of the surface

B_j = blackbody flux emitted from the surface = σT_w^4 (W/m^2)

σ = Stefan-Boltzmann constant (W/m^2-K^4)

T_w = wall temperature (K)

J_j = radiosity (W/m^2)

The surface emissivities are user-specified; however, if liquid layers are present on a surface, then the emissivity for this surface is set to 0.94. The radiosities are determined by solving the following system of simultaneous equations:

$$\frac{1}{1 - e_j} J_j \sum_{k=1}^{N} F_{k-j}(1 - e_{k-j})J_k$$

$$= \frac{e_j}{1 - e_j} B_j + \sum_{k=1}^{N} F_{j-k}\, e_{k-j}\, B_{g,k-j} \qquad j = 1,\ldots,N \quad \text{(A-44)}$$

Where,

N = number of surfaces

F_{j-k} = view factor looking from surface j to surface k

$B_{g,k-j}$ = gas Planck blackbody flux = σT^4 (W/m^2)

These equations are solved with a standard linear equation solver using LU decomposition and back substitution.

A.2.5 Convective Heat Transfer

The convective heat-transfer rate is calculated as the sum of two terms: sensible-heat transfer and latent-heat transfer from steam condensation or evaporation. A diffusion model is used to determine the mass-transfer rate for air/steam mixtures. Models are also provided for pure steam atmospheres and the buildup and disappearance (including flashing) of liquid layers. The correlations used in each of these models are described below.

Sensible-Heat-Transfer Models

The sensible-heat transfer is calculated from

$$q_s = h(T_o - T_w) \qquad \text{(A-45)}$$

where

q_s = sensible heat flux to the wall (W/m^2)

h = heat-transfer coefficient = Nu k/L (W/m^2-K)

T_w = surface temperature (K)

T_o = compartment gas temperature (K)

Nu = Nusselt number

k = thermal conductivity (W/m-K)

L = characteristic length (m) (e.g., wall height, pool width, or ice-condenser hydraulic diameter)

Different correlations are used to calculate the Nusselt number for wall surfaces, sump surfaces, and ice-condenser surfaces. Correlations for both free and forced convection are evaluated for wall and sump surfaces, and the maximum value is used to calculate a heat-transfer coefficient. For ice-condenser surfaces, a forced convection correlation is always used. The thermal properties (conductivity, viscosity, and specific heat) for air and steam are evaluated at the compartment temperature for the forced convection correlations and at the average of the wall and compartment temperatures for free convection. The mass averages of the air and steam thermal properties are then used in the correlations. The correlations currently used in HECTR for the Nusselt number are [8 9]

Wall Surface

Forced Convection

$$Nu = 0.037Re^{.8}Pr^{.333} \qquad (A-46)$$

Free Convection

$$Nu = 0.13(GrPr)^{.333} \qquad (A-47)$$

Sump Surface

Forced Convection

$$Nu = 0.037Re^{.8}Pr^{.333} \qquad (A-48)$$

Free Convection

$$Nu = 0.27(Gr\ Pr)^{.25} \qquad (A-49)$$

Ice-Condenser Surface

$$Nu = 0.023\ C\ Re^{.8}Pr^{.3} \qquad (A-50)$$

where

Re = Reynolds number = $\rho_g vL/\mu$

ρ_g = gas density (kg/m^3)

v = forced convection compartment gas velocity (m/s)

μ = gas viscosity (kg/m-s)

Pr = Prandtl number = $C_p\mu/k$

C_p = gas specific heat (J/kg-K)

Gr = Grashoff number = $g\beta(T_w - T_o)L^3\rho_g^2/\mu^2$

g = acceleration of gravity (m/s^2)

β = expansion coefficient = $1/T_o$ (K^{-1})

C = factor to account for basket roughness and liquid layers (default is 5.0)

The forced convection velocity is a user input. For most cases, it is set in the range of 0.3 to 1.0 m/s. The forced convection velocity in the ice condenser is set to the average of the inlet and outlet flow velocities for that compartment. During a hydrogen burn, the forced convection velocities in burning compartments are set equal to the flame speed.

The convection models in HECTR have been developed with flexibility in mind, recognizing the uncertainty in the models and the need to update them as more data become available. The correlations above are located in subroutine CONVCT and can be readily changed, usually by changing the line where the Nusselt Number is calculated. Also, the flow velocity, characteristic length, area, and maximum liquid film depth can be controlled by the user in the input.

Diffusion Model for Condensation or Evaporation in Air/Steam Mixtures

The steam condensation or evaporation rate is calculated from a mass-transfer/heat-transfer analogy using the same Nusselt number that was used for the sensible heat transfer. The following expressions are used to calculate the mass-transfer rate:

$$J_g = k_g \ell n \left(\frac{P - P_{sw}}{P - P_{so}} \right) \qquad \text{(A-51)}$$

where

J_g = molar flux to surface (moles/m^2-s)
k_g = mass-transfer coefficient (moles/m^2-s)
P_{so} = steam partial pressure in bulk gas (Pa)
P_{sw} = steam partial pressure at surface (Pa)
P = compartment pressure (Pa)

The mass-transfer coefficient is calculated from [10]

$$k_g = \frac{Nu(Pr/Sc)^{2/3}PD_v}{RTL} \qquad (A-52)$$

where

Sc = Schmidt number = $\mu/(\rho_g D_v)$

D_v = molecular diffusivity of steam in air (m^2/s)

R = universal gas constant (J/mole-K)

$$T = \begin{cases} T_o & \text{if forced convection} \\ (T_w + T_o)/2 & \text{if free convection} \end{cases} \quad (K)$$

The mass flux condensing on (or evaporating from, if negative) the surface, M_i, is

$$M_i = J_g M_g \qquad (A-53)$$

and the total amount of heat leaving the gas in the compartment due to convection is the sum of the sensible and latent heat:

$$q_t = q_s + M_g J_g h_b \qquad (A-54)$$

where

q_t = total heat flux (W/m^2)
M_g = steam molecular weight (kg/mole)
h_b = enthalpy of steam in the compartment (J/kg)

Pure Steam Models

Pure steam models are used whenever $P_{so} \geq 0.9999\ P$. If $0.95\ P \leq P_{so} < 0.9999\ P$, then both the diffusion models and the steam models are exercised, and the solution is chosen to minimize the absolute value of q_t. An exception to the

above procedure is that, if a surface is dry and superheated, then q_t is set equal to q_s as defined by Eq. A-45, regardless of the steam concentration. For condensation on a vertical surface, a Nusselt model is used with a correction factor for turbulence effects.[11] The heat transfer coefficient is

$$h_{Nu} = 1.13 \left(\frac{\rho_w g K_l^3 (\rho_w - \rho_g) \left[h_{fg} + 3/8 C_l (T_{sat} - T_w) + C_p (T_o - T_{sat}) \right]}{L \mu_w (T_{sat} - T_o)} \right)^{1/4} \quad \text{(A-55)}$$

and the mass flux is

$$M_i = \frac{h_{Nu} (T_{sat} - T_w)}{h_{fg} + C_p (T_o - T_{sat})} \quad \text{(A-56)}$$

where ρ_w = density of liquid water (kg/m^3)

K_l = thermal conductivity of liquid water (W/m-K)

h_{fg} = heat of vaporization (J/kg)

C_l = specific heat of liquid water (J/kg-K)

T_{sat} = saturation temperature corresponding to steam partial pressure (K)

μ_w = viscosity of water (kg/m-s)

For condensation on vertical surfaces in a pure steam environment, q_s is set to zero as it is assumed that some accounting is taken for sensible heat transfer in the formulation of Eqs. A-55 and A-56. The other pure steam models identified below include q_s as in Eq. A-54. The validity of Eq. A-55 is questionable for cases involving highly superheated steam. However, most pure steam cases encountered will involve conditions near saturation where latent heat-transfer should dominate.

The condensation rate on a horizontal pool surface is determined by assuming that there is a heat-transfer boundary layer in the top portion of the pool that controls the heat transfer. This boundary layer thickness has been arbitrarily set to 1 cm. The mass flux is determined from:

$$M_i = \frac{K_l (T_{sat} - T_w)}{BLT (h_b - h_l)} \quad \text{(A-57)}$$

where BLT = boundary layer thickness (0.01 m)

h_l = enthalpy of liquid water (J/kg)

For evaporation of liquid films on vertical surfaces, we calculate an evaporation rate that will tend to bring the film into thermal equilibrium over the next heat-transfer

timestep. Flashing of liquid pools is done in subroutine SUMPUP as discussed in Section A.2.9. For evaporation of liquid films on other surfaces the mass flux is found from

$$M_i = \frac{M_f C_l (T_w - T_{sat})}{h_{fg} A \Delta t} \qquad \text{(A-58)}$$

where M_f = mass of liquid film (kg)

A = surface area (m^2)

Δt = timestep size (S)

The value of $M_i \Delta t$ is not allowed to be larger than M_f and is also checked relative to the amount of steam in the compartment. The value of Δt is not known a priori in subroutine CONVCT. Therefore, the value used is the previous timestep size. Further discussions of numerical considerations will be presented later.

Flashing Model with Air Present

With air present, the same model is used for flashing as for evaporation of liquid films in a pure steam environment. Equation A-58 is used except that T_{sat} is now the saturation temperature at the total pressure and not at the steam partial pressure. Flashing of water pools is done in the subroutine SUMPUP.

In some cases the diffusion model will predict more mass transfer than the flashing model even though P_{sw} is greater than P. This can happen if P_{sw} is only slightly greater than P, and P_{so} is much less than P. For this case we choose the solution that produces the greatest total heat-transfer rate.

Liquid Films

With steam present, liquid films are likely to be present on wall surfaces. HECTR includes a model for these liquid layers to account for changes in the heat-transfer resistance and the distribution of liquid water throughout the containment. Because of the complex geometry and rough surfaces present in containment, a simple model is used, with adjustable parameters that may be different for each surface. The model assumes that the film thickness can build up to a specified value (the default value is 1 mm) and any additional condensate will drain to the specified sump. A laminar film model is also available to determine the drainage rate based on a vertical surface correlation. The maximum film thickness is still used to prevent unrealistic film thicknesses from occurring. The mass flux running off of the wall, M_e (kg/s), is

$$M_e = FA\rho_w^2 g d^3/(3\mu_w L) \qquad (A\text{-}59)$$

where d is the film thickness (m) and F is a user-specified multiplicative factor with a default value of zero (the default value of zero indicates that no drainage will occur until the maximum film thickness is reached). We then calculate the rate of change of film thickness as

$$\frac{dd}{dt} = \frac{M_i}{\rho_w A} - \frac{Me}{\rho_w A} \qquad (A\text{-}60)$$

HECTR also calculates the change in temperature (or energy) of the liquid layer. This is done as part of the wall conduction solution and will be discussed in that section.

Numerical Considerations

With liquid layers present, checks must be made to prevent the film thickness from becoming less than zero or exceeding the maximum value during a timestep. HECTR determines whether it is possible to exceed the desired bounds during the next timestep, then adjusts the mass-transfer rates accordingly to prevent such an occurrence. These checks are made in subroutine CONADJ, which is called from CONTRL during each flow timestep. If the film thickness is going to be negative, then the evaporation rate is reduced accordingly. If the film thickness is going to exceed the maximum value, then the draining rate is increased. All of the heat- and mass-transfer rates are adjusted to be self-consistent. The film thicknesses are updated in CONTRL at the end of each flow timestep.

It is possible to encounter situations where the mass transfer to a surface occurs alternately by condensation and evaporation. While this rarely occurs, it can cause some numerical difficulty if encountered. To alleviate this problem a weighting factor can be used relating the current values of the heat and mass flux to the values from the previous timestep. That is

$$V = WF * Vnew + (1 - WF) * Vold \qquad (A\text{-}61)$$

where V = value to be used in the calculation

WF = weighting factor

Vnew = value calculated based on current conditions

Vold = value from previous timestep

Normally, WF is set equal to 1.0; however, if the mole fraction of steam exceeds 0.7, then WF is set to 0.1. WF is set near the top of subroutine CONVCT.

A.2.6 Surface Conduction

In HECTR, surfaces can be treated either as multilayered slabs or as simple lumped masses. In either case, all surface properties are assumed to be constant.

The temperature, T (K), of a lumped-mass surface is given as a function of time, t (s), by

$$\frac{dT}{dt} = \frac{qA}{mC_p} \qquad \text{(A-62)}$$

where

q = net heat flux to the surface (W/m^2)

A = exposed surface area (m^2)

m = surface mass (kg)

C_p = specific heat of the surface material (J/kg-K)

This equation is integrated by the Euler method at the end of each heat-transfer timestep.

Heat conduction in a multilayered slab is determined by using a finite difference approximation of the heat equation. A slab in HECTR can have one or more layers. HECTR will convert each multilayered slab into a thermally equivalent, homogeneous steel slab of thickness L (m):

$$L = \sum_{i-1}^{N} \left(\frac{a_{ref}}{a_i} \right)^{1/2} L_i \qquad \text{(A-63)}$$

where

N = number of layers in the slab

a_{ref} = reference material (steel) thermal diffusivity (1.25×10^{-5} m^2/s)

a_i = thermal diffusivity of the i^{th} layer (m^2/s)

L_i = thickness of the i^{th} layer (m)

Two basic parameters are used to specify the nodalization of each thermally equivalent steel slab. These are the number of elements to be used in the nodalization, N_e (≤ 100), and the element distribution exponent, e. The k^{th} element of the finite difference nodalization will have a width Δx_k (m) of

$$\Delta x_k = \left[\left(\frac{k}{N_e} \right)^e - \left(\frac{k-1}{N_e} \right)^e \right] L \qquad (1 \leq k \leq N_e) \qquad \text{(A-64)}$$

Here, element 1 is in contact with the back surface of the slab. Typically, e will be less than 1 so that the elements will be decreasing in length as they approach the front side of the slab (where more resolution is normally needed than at the back). For each slab, the user can either specify N_e and e or let HECTR choose appropriate values. If HECTR chooses the values for N_e and e, it will do so in such a way that

$$\Delta x_k \geq \left(a_{ref} \Delta T_{max}\right)^{1/2} \qquad \text{(A-65)}$$

will always be satisfied, where Δx_k is the width of the k^{th} element (m) and ΔT_{max} is the maximum allowed heat-transfer time-step (s). If Eq. A-65 were not satisfied, the element widths would be too small to ensure the stability of the finite difference heat-conduction equation.

The heat-conduction equation in HECTR is written in a Crank-Nicolson finite difference formulation.[12] This results in a linear system of equations that are solved using a tridiagonal equation solver. In particular, to calculate the slab temperatures on the $(n+1)^{st}$ timestep from the values available from the n^{th} timestep, the following equations are used.

$(2 \leq j \leq M - 1)$

$$T_{j-1}^{n+1} - (s_j + 1)(r_j + 1)T_j^{n+1} + r_j T_{j+1}^{n+1}$$

$$= -T_{j-1}^{n} - (s_j - 1)(r_j + 1)T_j^{n} - r_j T_{j+1}^{n} \qquad \text{(A-66)}$$

where

M = number of nodes $(= N_e + 1)$,

T_j^n = temperature at the j^{th} node on the n^{th} timestep (K),

$$r_j = \frac{\Delta x_{j-1}}{\Delta x_j} \quad ,$$

$$s_j = \frac{\Delta x_{j-1}\, \Delta x_j}{a_{ref} \Delta T} \quad , \text{ and}$$

ΔT = length of the heat-transfer timestep over which the equations are integrated (s).

(j = 1 with insulated boundary condition)

$$-\left(\frac{S_1}{r_1}+1\right) T_1^{n+1} + T_2^{n+1} = -\left(\frac{s_1}{r_1}-1\right) T_1^n - T_2^n \qquad \text{(A-67)}$$

(j = 1 with fixed temperature boundary condition)

$$T_1^{n+1} = T_1^n = T \qquad \text{(A-68)}$$

where

T = the given fixed temperature (K).

(j = 1 with convective boundary condition)

$$\left[-\left(\frac{s_1}{r_1}+1\right) - Nu\right] T_1^{n+1} + T_2^{n+1}$$

$$= \left[-\left(\frac{s_1}{r_1}-1\right) + Nu\right] T_1^n - T_2^n - 2NuT_e \qquad \text{(A-69)}$$

where

$$Nu = \frac{h\ \Delta x_1}{K}$$

h = heat-transfer coefficient from back surface of slab (W/m^2-K)

K = equivalent thermal conductivity of the back surface

$$(W/m-K) = \left(\frac{a_{ref}}{a_N}\right)^{1/2} k_N$$

k_i = thermal conductivity of the i^{th} layer ($W/m-K$)

T_e = environmental gas temperature at the slab's back surface (K)

The element at the front surface has two special properties. It receives the incoming (or outgoing) atmospheric heat flux, and it can include a liquid layer. In HECTR, this liquid layer (if it exists) is combined with the front surface element so that the equation for the final node is

$(j = M)$

$$T_{M-1}^{n+1} - [s_M(r_M + 2z) + 1]T_M^{n+1} = - T_{M-1}^{n} - [s_M(r_M + 2z) - 1]T_M^{n} - \frac{2\Delta x_{M-1}}{K'} q \qquad (A-70)$$

where

Δx_M = thickness of the liquid film (m)

$$z = \frac{k_w a_{ref}}{a_w k_{ref}}$$

k_{ref} = reference material (steel) thermal conductivity (W/m-K)

a_w = thermal diffusivity of water (m^2/s)

k_w = thermal conductivity of water (W/m-K)

K' = equivalent thermal conductivity of the front surface

$$(W/m\text{-}K) = \left(\frac{a_{ref}}{a_1}\right)^{1/2} k_1$$

q = heat-flux incident on the front surface (W/m^2)

A.2.7 Containment Sprays

Containment sprays are important in preventing long-term steam overpressurization and in limiting the pressure and temperature effects of combustion. The containment spray model in HECTR is flexible, allowing injection of sprays into any compartment, carryover of sprays into compartments and sumps below, and either injection of water from an outside source or recirculation from a specified sump. HECTR is not limited to a single drop size; a distribution of drop sizes can be specified.

The drops from containment sprays are assumed to be isothermal, spherical, and traveling at the terminal velocity corresponding to their instantaneous size and mass. They are tracked through a compartment to the bottom where their final temperature and mass determine the heat- and mass-transfer rates to the compartment atmosphere. A user-specified fraction of the drops that have reached the bottom of a compartment is allowed to fall into lower compartments. Drops not falling into other compartments can be transferred to a specified sump.

The gas in a compartment is assumed to be homogeneous with none of its properties changing during the fall time of the drops. Therefore, the solutions represent a quasi-steady-state model. The differential equations describing drop behavior (mass, temperature, and distance fallen) are valid for both condensation on and evaporation from the drops and are presented below.[13 14]

$$\frac{dm}{dt} = -2\pi\rho_g D(1 + .25Re^{1/2}Sc^{1/3})D_c \ln(1 + B) \qquad \text{(A-71)}$$

$$\frac{dT_d}{dt} = \frac{1}{mC_{PL}}\left[\frac{C_p(T_d - T_b)}{(1 + B)^{1/Le} - 1}\right] + h_{fg}\frac{dm}{dt} \qquad \text{(A-72)}$$

$$\frac{dz}{dt} = \left[\frac{4}{3}\frac{(\rho_d - \rho_g)gD}{\rho_g C_D}\right]^{1/2} \qquad \text{(A-73)}$$

Here,

m = droplet mass (kg)

T_d, T_b = droplet and bulk gas temperatures (K)

z = droplet fall height (m)

t = time (s)

ρ_g, ρ_d = gas and droplet densities (kg/m^3)

D = droplet diameter (m)

Re = Reynolds number

Sc = Schmidt number

Le = Lewis number

D_c = diffusion coefficient (m^2/s)

B = mass-transfer driving force = $(Y_d - Y_b)/(1 - Y_d)$

Y_d = mass fraction of vapor at drop surface

Y_b = mass fraction of vapor in bulk gas

C_{PL}, C_P = droplet and gas specific heats (J/kg-K)

h_{fg} = heat of vaporization of water (J/kg)

g = acceleration due to gravity (m/s^2)

C_D = drag coefficient

Both the drag coefficient and diffusion coefficient are calculated internally in HECTR.

The three equations above are reduced to the two equations dm/dz and dT_d/dz by dividing Eqs. A-71 and A-72 by Eq. A-73. The equations are then solved using a standard Runge-Kutta

differential equation solver. The spray model has been formulated to maximize computational efficiency. If a drop reaches an equilibrium temperature (determined by setting Eq. A-72 to zero and solving for T_d), then HECTR switches to integrating only the dm/dz equation. When solving the equations, numerical problems may arise if the droplet completely evaporates during its fall. The velocity (and thus the Reynolds number) of the droplet will decrease as its mass decreases. Therefore, for Reynolds numbers below about 78 (which marks the cutoff point for the low velocity Reynolds number correlation used in the spray model), the following variable transformation is used to make the integration smoother:

$$m^* = m^{1.04/0.87} \tag{A-74}$$

The ODE solver determines the final value of m* and then HECTR calculates the final value of m from this value.

Once the mass and temperature of the drops reaching the bottom of a compartment are known, the total mass- and heat-transfer rates to the compartment atmosphere are calculated.

$$m_e = (m_0 - m_f)DFR \tag{A-75}$$

$$\frac{dq}{dt} = -\left[m_0 C_{PL}(T_f - T_0) + (m_0 - m_f)(h_{fg} + C_{PV}[T_g - T_f])\right] DFR \tag{A-76}$$

where m_e = mass evaporated (kg/s)

m_0 = initial droplet mass (kg)

m_f = final droplet mass (kg)

DFR = droplet flow rate (drops/s)

$\frac{dq}{dt}$ = heat transfer to gas (W)

T_0 = initial droplet temperature (K)

T_f = final droplet temperature (K)

T_g = compartment gas temperature (K)

C_{PL} = liquid specific heat (J/kg-K)

C_{PV} = vapor specific heat (J/kg-K)

h_{fg} = heat of vaporization (J/kg)

The above equations are summed over the number of drop sizes. Any number of drop sizes can be treated with HECTR, however treating more than two drop sizes requires changing a PARAMETER statement (see Appendix B). Generally, two drop sizes are sufficient to produce reasonable results.

Because the spray model is a diffusion model for steam in air, it becomes invalid when the steam mole fraction exceeds 0.99. If this situation is encountered, the calculation will terminate with a message. These problems are discussed further in Chapter 3.

A.2.8 Ice-Condenser Model

To model an ice condenser, the ice region is subdivided into a specified number of compartments internally in HECTR. The user must input two more compartments for the lower and upper plenums. The default number of compartments in the ice region is four (see Figure A-3). This relatively large number of compartments is necessary because the steam concentration can vary significantly through the ice condenser. There is no limit on the number of surfaces in the lower and upper plenums, but only two surfaces are used for each compartment in the ice region. One of the two surfaces in each ice-region compartment models the ice, and the other surface models the ice-condenser walls and portions of the metal baskets that are free of ice. Each ice surface is maintained at a constant temperature. Heat transfer to the ice is calculated assuming that the surface temperature is the maximum of 273.15 K and the ice temperature, while the internal energy of the ice is based on a constant input temperature that can be less than 273.15 K. The metal surfaces are treated as lumped masses. The initial temperature of the metal surfaces is set to the maximum of 273.5 K and the ice temperature. The heat- and mass-transfer relations were described previously in Section A.2.5. Models for the ice-condenser doors are discussed in Section A.2.1.

The ice-melting rate is calculated by the following expression:

$$W_{ice} = (q * A_{ice})/(h_{liq} - u_{ice}) \qquad \text{(A-77)}$$

where

W_{ice} = ice-melting rate (kg/s)
q = heat flux to ice (W/m^2)
A_{ice} = ice heat-transfer area (m^2)
h_{liq} = enthalpy of water at 273.15 K (J/kg)
u_{ice} = internal energy of ice at the ice temperature (J/kg)

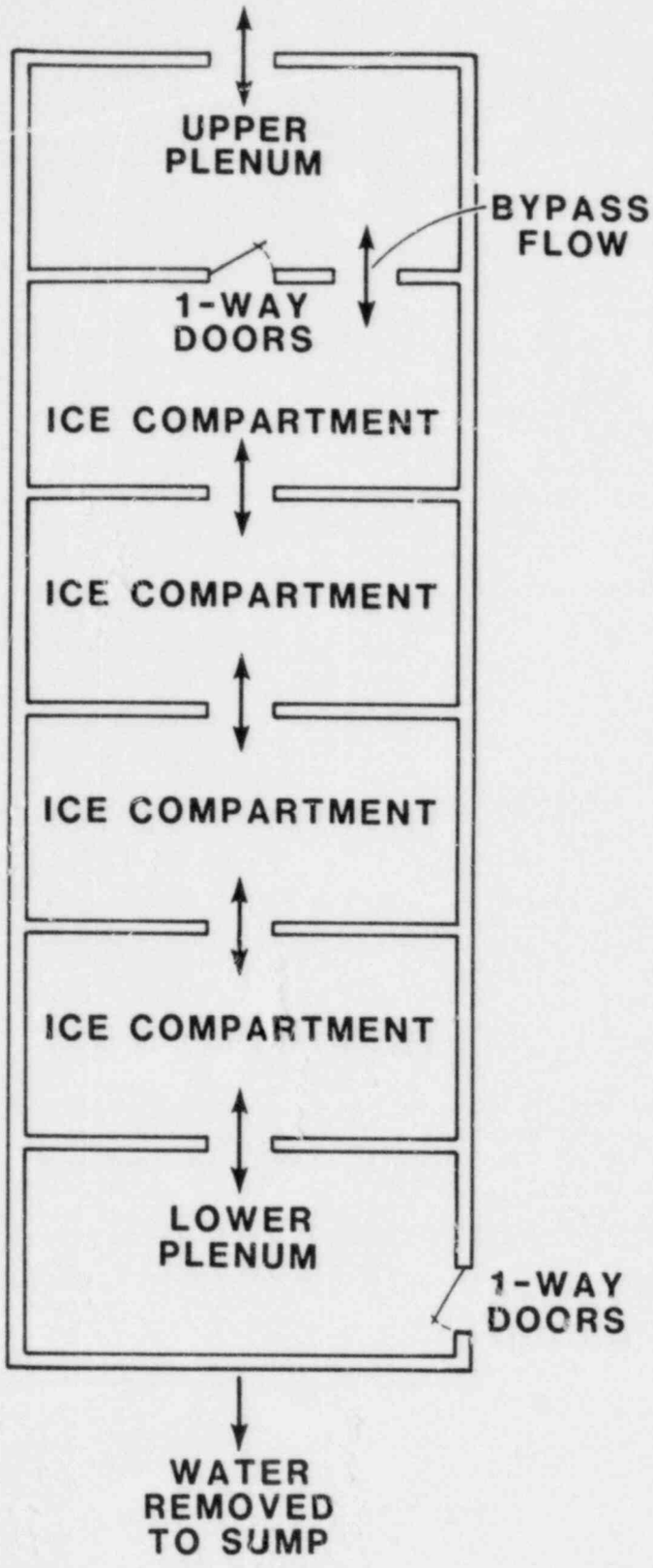


Figure A-3. Ice-Condenser Model

The ice is assumed to melt in a one-dimensional or linear fashion in each compartment. The mass of unmelted ice is calculated by integrating the ice-melting rate during the transient. The corresponding surface area of the ice for heat transfer is calculated using:

$$A_{ice} = (M_{ice,}/M_{ice,o}) * A_{ice,o} \quad \text{(A-78)}$$

where

$A_{ice,o}$ = initial ice heat-transfer area (m^2)
M_{ice} = unmelted ice mass (kg)
$M_{ice,o}$ = initial ice mass (kg)

HECTR does not treat the metal baskets in areas where ice is present. If ice is present, the entire surface area is assumed to be ice. A heat sink is included to treat the walls and baskets that are free of ice. The mass, surface area, and temperature of the metal surface in each ice region are adjusted as the ice melts using the following equations:

$$M_{met} = M_{met,old} + M_{bask} * (M_{ice} - M_{ice,old})/M_{ice,o} \quad \text{(A-79)}$$

$$A_{met} = A_{met,old} + A_{bask} * (M_{ice} - M_{ice,old})/M_{ice,o} \quad \text{(A-80)}$$

$$T_{met} = (M_{met,old} * T_{met,old}) + (M_{met} - M_{met,old}) * T_{ice}/M_{met} \quad \text{(A-81)}$$

where

M_{bask} = mass of baskets (kg)
M_{met} = mass of metal heat-transfer surface (kg)
$M_{met,old}$ = M_{met} from previous timestep (kg)
$M_{ice,old}$ = M_{ice} from previous timestep (kg)
A_{bask} = area of baskets (m^2)
A_{met} = area of metal heat-transfer surface (m^2)
$A_{met,old}$ = A_{met} from previous timestep (m^2)
$A_{ice,old}$ = A_{ice} from previous timestep (m^2)
T_{met} = temperature of metal surface (K)
$T_{met,old}$ = T_{met} from previous timestep (K)

The liquid water formed in the ice regions from ice melting and steam condensation falls down through the ice condenser to the lower plenum. Although this process is too poorly characterized at present to allow analytical modeling, the

heat and mass transfer to the water is significant. Therefore, we have included a simple model for the process in HECTR that can be varied parametrically to bound the phenomena. For this model we assume that the water does not heat up significantly in the ice region. Thus, all of the heat and mass transfer occurs while the water falls through the lower plenum. The controlling parameter is the ice-condenser drain temperature, and the water is assumed to heat up to this temperature, which will be calculated as the minimum of the user-specified drain temperature, the lower plenum gas temperature, and the saturation temperature corresponding to the partial pressure of steam in the lower plenum. Making the assumption that the latent heat transfer dominates the sensible heat transfer, we calculate the condensation rate in the lower plenum from

$$W_{lp} = \sum_{n=1}^{NIC} \left[(W_{mi} + W_{ci})(h_d - h_{li}) + W_{cm}(h_d - h_{lm})\right]_n / (h_s - h_d) \qquad \text{(A-82)}$$

where n = ice compartment

NIC = total number of ice compartments

W_{lp} = condensation rate in the lower plenum (kg/s)

W_{mi} = rate of ice melting in compartment n (kg/s)

W_{ci} = rate of condensation on ice in compartment n (kg/s)

W_{cm} = rate of condensation on metal surface in compartment n (kg/s)

h_d = enthalpy of liquid at drain temperature (J/kg)

h_{li} = enthalpy of liquid at ice-melting temperature (J/kg)

h_{lm} = enthalpy of liquid at metal surface temperature in compartment n (J/kg)

h_s = enthalpy of steam in the lower plenum (J/kg).

The condensation rate calculated in Eq. A-82 may be reduced by HECTR, based on the amount of steam in the lower plenum. With the above expressions we can calculate the total amount of water that drains from the ice condenser into the sump.

$$W_{IC,drn} = W_{lp} + \sum_{n=1}^{NIC} \left(W_{mi} + W_{ci} + W_{cm}\right)_n \qquad \text{(A-83)}$$

This water will be added to the sump with an enthalpy corresponding to the drain temperature.

A.2.9 Sump Model

An arbitrary number of sumps can be specified in each compartment. Mass and energy can be added to or subtracted from each sump by several different processes that will be described in the following paragraphs. A Mark III BWR suppression pool is modeled as a special case of a sump, with additional models included to calculate the pool motion, vent flow, and upper pool dump. These models will be described in Section A.2.10.

Water can be added to the sumps by several processes: condensation on the sump, runoff of condensate from other heat-transfer surfaces, spray droplets, condensation of water from the atmosphere of a compartment if the gas becomes supersaturated, injection of the liquid portion of water sources into a compartment, and drainage of water out of the ice condenser. A different sump can be specified to receive the condensate runoff from each heat-transfer surface. In each compartment, one sump is specified to collect water from sprays and sources, and a different sump can be specified to collect water removed from the atmosphere if it becomes supersaturated. The water draining out of the ice-condenser lower plenum can be deposited only in one sump.

Water can be removed from a sump through actuation of the emergency core coolant systems or containment sprays, overflow from one sump to another, or evaporation. For each sump, the user specifies the capacity of the sump and the receiving sump for the overflow. A sump can be specified to overflow into a second sump, which in turn is specified to overflow back into the first sump. For this case, each sump will fill independently of the other until the capacity of one of the sumps is exceeded. Thereafter, the full sump will overflow into the second sump until it is also full. Both sumps will then continue to fill, exceeding the user-specified capacities. The excess water is divided between the two sumps using the ratio of the surface areas of the two sumps.

Sources, which consist of any of the four gases modeled in HECTR or liquid water, can be injected directly into the sumps. Steam that is injected into a sump is assumed to be condensed in the sump, and the other gases are assumed to be cooled to the sump temperature before entering the compartment connected to the sump.

Sumps can be cooled by heat exchangers, using the model described in Section A.2.11. Convective heat transfer, condensation/evaporation, and radiative heat transfer for the sump surface are calculated using the correlations previously described in Sections A.2.4 and A.2.5.

The maximum temperature of each sump is the saturation temperature corresponding to the pressure of the compartment that the sump is in. Rather than exceed this temperature, enough water is boiled to maintain the sump at saturation. This water is added to the compartment atmospheres as discussed in Section A.1.1.

The mass and energy equations for the sump are listed below:

$$\frac{d}{dt} m_{sump} = W_{cond} + W_{runoff} + W_{spray} + W_{subc} + W_{liq,csrc} + W_{wtr,ssrc} + W_{IC,drn} + W_{spill} - W_{over} - W_{ECC} - W_{spinj} + W_{weir} + W_{vent,stm} + W_{UPdump} \quad \text{(A-84)}$$

$$\frac{d}{dt} (m_{sump} u_{sump}) = W_{cond} h_{stm,cmp} + W_{runoff} h_{runoff} + W_{spray} h_{spray} + W_{subc} h_{subc} + W_{liq,csrc} h_{liq,csrc} + W_{wtr,ssrc} h_{wtr,ssrc} + W_{j,ssrc} (h_{j,ssrc} - h_{j,sout}) + W_{IC,drn} h_{IC,drn} + W_{spill} h_{spill} - W_{over} h_{sump} - W_{ECC} h_{sump} - W_{spinj} h_{sump} + W_{weir} h_{weir} + W_{UPdump} h_{UP} + W_{vent,stm} h_{vent,stm} + W_{vent,j} (h_{vent,j,in} - h_{vent,j,out}) + Q_{conrad} - Q_{htex} \quad \text{(A-85)}$$

where

m_{sump} = mass of water in sump (kg)

u_{sump} = internal energy of sump (J/kg)

Q_{conrad} = convective and radiative heat-transfer rate to sump surface (W)

Q_{htex} = heat-transfer rate from sump due to heat-exchanger cooling (W)

W_i = rate of mass transfer defined by the subscript below (kg/s)

h_i = enthalpy of water defined by the subscript below (J/kg)

subscripts:

cond = condensation on sump surface (negative if evaporation)

runoff = water running off heat-transfer surfaces that is added to this sump

spray = spray water that reaches the bottoms of compartments and is added to this sump

subc = water removed from supersaturated compartments that is added to this sump

liq,csrc = liquid portion of sources injected into compartments that is added to this sump

wtr,ssrc = water sources (steam or liquid water) that are injected directly into this sump

j,ssrc = nitrogen, oxygen, or hydrogen injected directly into this sump

IC,drn = water that drains from lower plenum of ice condenser into this sump

spill = water that spills over from other sumps into this sump

over = water that overflows from this sump

ECC = water removed from this sump to supply ECC

spinj = water removed from this sump to supply spray water

weir = water added to sump due to flow over the weir wall (only for the suppression pool or the drywell sump)

vent,stm = steam added by flow through suppression pool vents (only for the suppression pool)

vent,j = nitrogen, oxygen, or hydrogen flowing through the suppression pool vents

UPdump = water transferred from the upper pool to the suppression pool due to the upper pool dump (added to the suppression pool and subtracted from the upper pool)

sump = sump conditions

stm,cmp = steam in compartment that sump is in

j,ssrc = nitrogen, oxygen, or hydrogen being injected into sump

j,sout = nitrogen, oxygen, or hydrogen injected into sump when it passes from the sump into the compartment the sump is in

UP = upper pool conditions

vent,j,in = nitrogen, oxygen, or hydrogen flowing through the suppression pool vents before flowing into the suppression pool

vent,j,out = nitrogen, oxygen, or hydrogen flowing through the suppression pool vents after passing through the suppression pool

If the sump is subcooled, the new sump mass and internal energy are calculated from

$$m_{sump}^{n+1} = m_{sump}^{n} + \Delta t \frac{dm_{sump}}{dt} \qquad \text{(A-86)}$$

$$u_{sump}^{n+1} = \left(m_{sump}^{n} u_{sump}^{n} + \Delta t \left[\frac{d}{dt} (m_{sump} u_{sump})^{n} \right] \right) / m_{sump}^{n+1} \qquad \text{(A-87)}$$

where

Δt = flow timestep size (s)

n = old time value

n+1 = new time value

The sump temperature is determined by interpolating from a table of temperature versus internal energy.

If the sump is saturated, the new sump mass and temperature are calculated from

$$T_{sump}^{n+1} = T_{sat}(P_{comp}^{n}) \qquad \text{(A-88)}$$

$$m_{sump}^{n+1} = \frac{1}{u_{sat,l}^{n} - u_{stm,c}^{n}} \left\{ m_{sump}^{n} \left(u_{sump}^{n} - u_{stm,c}^{n} \right) \right.$$

$$\left. - \Delta t \left[u_{stm,c} \frac{d}{dt} \left(m_{sump} \right) \right]^{n} + \Delta t \left[\frac{d}{dt} \left(m_{sump} u_{sump} \right) \right]^{n} \right. \tag{A-89}$$

$$\Delta m_{flashed} = m_{sump}^{n} + \Delta t \left(\frac{dm_{sump}}{dt} \right)^{n} - m_{sump}^{n+1} \tag{A-90}$$

where

T_{sump} = sump temperature (K)

$T_{sat}(P_{comp})$ = saturation temperature corresponding to compartment pressure (K)

$u_{sat,l}$ = saturated liquid internal energy at T_{sat} (J/kg)

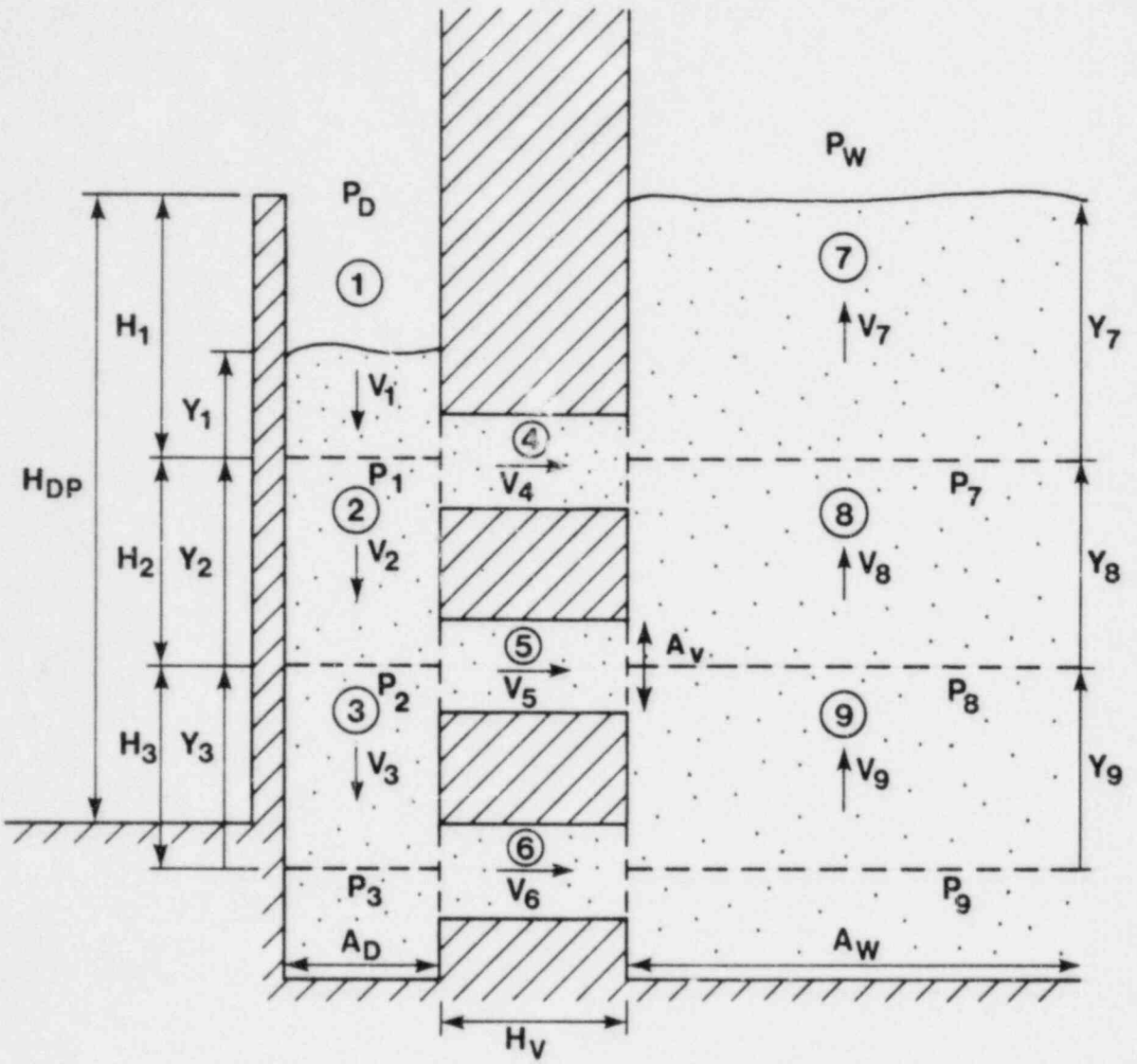
$u_{stm,c}$ = internal energy of steam in compartment that sump is in (J/kg)

$\Delta m_{flashed}$ = mass of water flashed from sump that will be added to compartment as steam (kg)

A.2.10 Suppression Pool Model

The suppression pool model includes all of the effects described previously for the sumps, as well as models for phenomena that are unique to BWR Mark III containments. The additional models calculate the motion of the suppression pool, gas flow rates between the drywell and wetwell (in either direction) if the suppression pool vents are uncovered, draining of water from the upper pool into the suppression pool, flow of water over the weir wall onto the drywell floor, and flow of water back into the suppression pool if the level of the water in the drywell rises above the weir wall. Details of these models are given in the following paragraphs. Pool swell phenomena are not treated by HECTR Version 1.0.

Rather than use detailed two- or three-dimensional formulations (which would require a large amount of computer execution time), the HECTR model for calculating the pool motion uses an approach similar to those used in References 15 and 16. The suppression pool is divided into nine compartments as shown in Figure A-4. The water is assumed to move as a plug through each compartment. Thus, water levels in the



CONCRETE

WATER

A_D = Surface Area of Drywell Side of Suppression Pool

A_W = Surface Area of Wetwell Side of Suppression Pool

A_V = Cross Sectional Area of a Single Row of Vents

ρ = Density of Water in Suppression Pool

Figure A-4. Mark III Suppression Pool Arrangement

compartments would be similar to those shown in Figure A-5 during vent clearing. The water is assumed to be incompressible, and the flow rate is assumed to be uniform within each compartment. The water temperature is assumed to be constant throughout the suppression pool. To calculate the motion of the suppression pool, mass and momentum balances are written for each compartment as shown below (see Figures A-4 and A-5 for definitions of the variables). Note that the pool velocities discussed below are control volume velocities rather than junction velocities.

(A) Compartment on drywell side that is clearing:

(If $i=3$, then V_{i+1} is replaced with 0 in the following equations)

Mass conservation:

$$\frac{d}{dt}(\rho A_D Y_i) + \rho A_v V_{i+3} + \rho A_D V_{i+1} = 0 \qquad \text{(A-91)}$$

Momentum conservation:

$$\frac{d}{dt}(\rho A_D Y_i V_i) + \rho A_v V_{i+3} V_{i+1} + \rho A_D (V_{i+1})^2 = P_D A_D - P_i A_D + \rho g A_D Y_i \qquad \text{(A-92)}$$

(B) Compartments on drywell side that are below (A)

(If $i=3$, then V_{i+1} is replaced with 0 in the following equations)

Mass conservation:

$$-\rho A_D V_i + \rho A_v V_{i+3} + \rho A_D V_{i+1} = 0 \qquad \text{(A-93)}$$

Momentum conservation:

$$\rho A_D H_i \frac{dV_i}{dt} - \rho A_D V_i^2 + \rho A_v V_{i+3} V_{i+1} + \rho A_D (V_{i+1})^2 = P_{i-1} A_D - P_i A_D + \rho g A_D Y_i \qquad \text{(A-94)}$$

(C) Compartment on wetwell side that is clearing:

(If $i=9$, then V_{i+1} is replaced with 0 in the following equations)

Mass conservation:

$$\frac{d}{dt}(\rho A_w Y_i) - \rho A_v V_{i-3} - \rho A_w V_{i+1} = 0 \qquad \text{(A-95)}$$

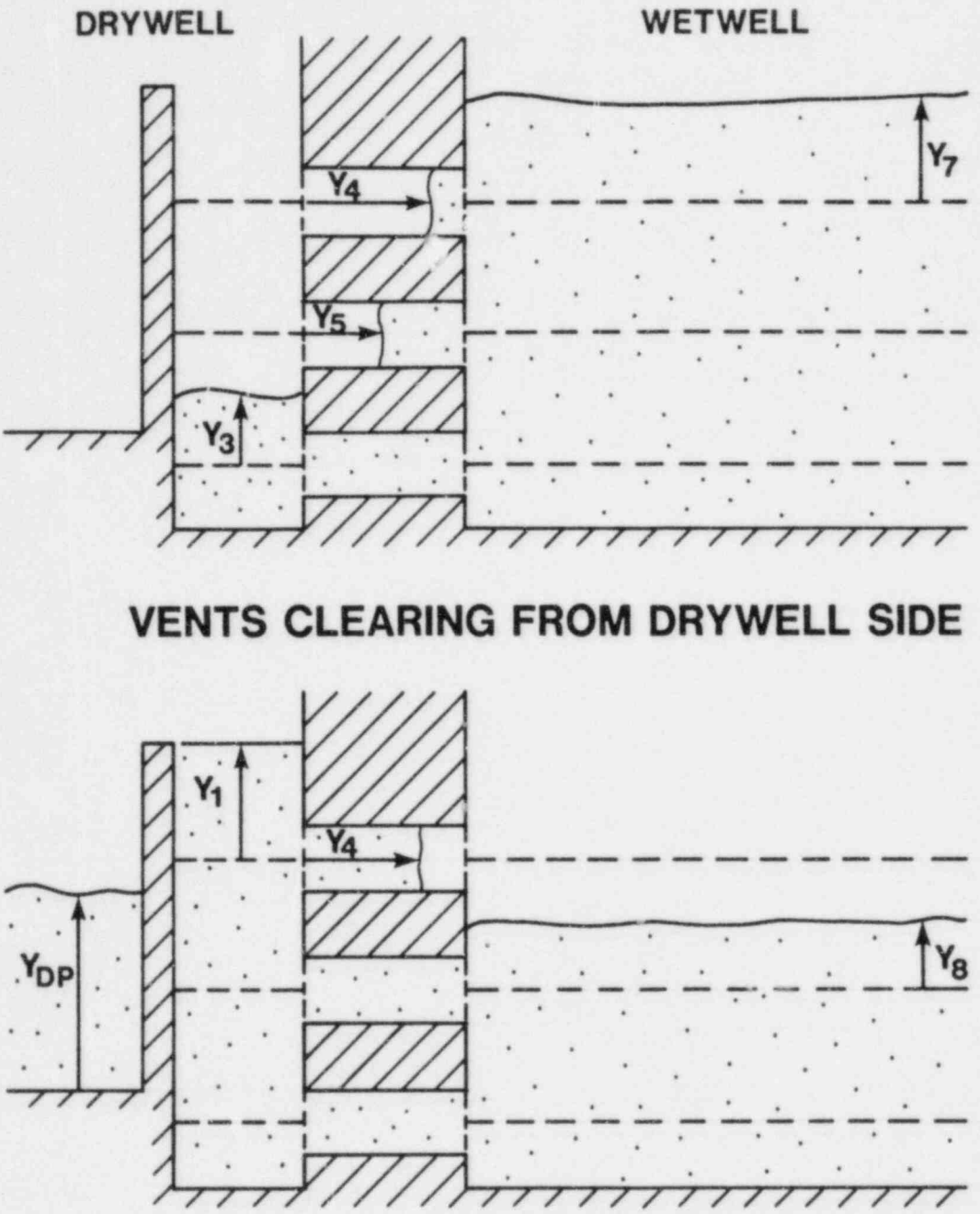


Figure A-5. Suppression Pool Vent Clearing

Momentum conservation:

$$\frac{d}{dt}(\rho A_w Y_i V_i) - \rho A_v V_{i-3} V_{i+1} - \rho A_w (V_{i+1})^2 = P_i A_w - P_w A_w - \rho g A_w Y_i \quad \text{(A-96)}$$

(D) Compartments on wetwell side that are below (C)

(If $i=9$, then V_{i+1} is replaced with 0 in the following equations)

Mass conservation:

$$\rho A_w V_i - \rho A_v V_{i-3} - \rho A_w V_{i+1} = 0 \quad \text{(A-97)}$$

Momentum conservation:

$$\rho A_w H_{i-6} \frac{dV_i}{dt} + \rho A_w V_i^2 - \rho A_v V_{i-3} V_{i+1} - \rho A_w V_{i+1}^2 = P_i A_w - P_{i-1} A_w - \rho g A_w H_{i-6} \quad \text{(A-98)}$$

(E) Vents that are clearing

i) Clearing from the drywell side

Mass conservation:

$$\frac{d}{dt}\left[\rho A_v (H_v - Y_i)\right] + \rho A_v V_i = 0 \quad \text{(A-99)}$$

Momentum conservation:

$$\frac{d}{dt}\left[\rho A_v (H_v + Y_{ad} - Y_i) V_i\right] + \rho A_v V_i^2 = \left[P_D - \left(P_{i+3} + k_{out}\, \rho\, \frac{V_i^2}{2}\right)\right] A_v \quad \text{(A-100)}$$

ii) Clearing from the wetwell side

Mass conservation:

$$\frac{d}{dt}(\rho A_v Y_i) - \rho A_v V_i = 0 \quad \text{(A-101)}$$

Momentum conservation:

$$\frac{d}{dt}\left[\rho A_v \left(Y_i + Y_{ad}\right) V_i\right] - \rho A_v V_i^2$$

$$= \left[\left(P_{i-3} - k_{in}\,\rho\,\frac{V_i^2}{2}\right) - P_w\right] A_v \qquad \text{(A-102)}$$

(F) Vents that are full of water

Mass conservation:

$$\frac{d}{dx}\,(\rho A_v V_i) = 0 \qquad \text{(A-103)}$$

Momentum conservation:

$$\rho A_v (H_v + Y_{ad})\,\frac{dV_i}{dt} = \left[\left(P_{i-3} - k_{in}\,\rho\,\frac{V_i^2}{2}\right) - \left(P_{i+3} + k_{out}\,\rho\,\frac{V_i^2}{2}\right)\right] A_v \qquad \text{(A-104)}$$

These equations can be combined to give a set of differential equations that include only derivatives of the vent velocities. This linear set of equations is solved for the derivatives of the vent velocities at the old time. The vent velocities at the new time are calculated by Euler's method, and the remaining suppression pool velocities are calculated from continuity relations. The equations used are shown below.

For i=4,6

$$V_i^{n+1} = V_i^n + \left(\frac{dV_i}{dt}\right)^n \Delta t_{SP} \qquad \text{(A-105)}$$

For i=1,3

$$V_i^{n+1} = \frac{A_v}{A_D} \sum_{j=i+3}^{6} V_j^{n+1} \qquad \text{(A-106)}$$

For i=7,9

$$V_i^{n+1} = \frac{A_v}{A_w} \sum_{j=i-3}^{6} V_j^{n+1} \qquad \text{(A-107)}$$

If a control volume is above the suppression pool surface or if a vent is cleared, then the velocity shown above for that control volume is not calculated.

The timestep used to calculate the pool motion does not have to be the same as the timestep used to solve the flow junction equations. A smaller value can be used for calculating the suppression pool motion if necessary. The timestep size for suppression pool motion is based on the rate of change of the vent velocity derivatives. The expression used to calculate a timestep size is

$$\Delta t_{SP} = 0.3 \left| \left[\left| \frac{dV}{dt} \right|_{max} / \left(\left| \frac{dV}{dt} \right|_{max} - \left| \frac{dV}{dt} \right|_{max,old} \right) \right] \right| \Delta t_{old} \qquad \text{(A-108)}$$

where

Δt_{SP} = timestep size (s)

Δt_{old} = old timestep size (s)

$\left| \frac{dV}{dt} \right|_{max}$ = maximum absolute value of vent velocity derivatives (m/s^2)

$\left| \frac{dV}{dt} \right|_{max,old}$ = maximum absolute value of vent velocity derivatives from old timestep (m/s^2)

The timestep is not allowed to increase to more than twice the timestep used on the last step and can not be greater than 0.1 seconds. A check is also made so that the suppression pool surface can not cross more than one control volume in a timestep.

The liquid surface positions for each pool control volume are calculated from the following equations (assuming that the control volume is not completely full or empty).

For i=1,3

$$Y_i^{n+1} = Y_i^n - \frac{\Delta t_{SP}}{2} \left(V_i^{n+1} + V_i^n \right) \qquad \text{(A-109)}$$

For i=4,9

$$Y_i^{n+1} = Y_i^n + \frac{\Delta t_{SP}}{2} \left(V_i^{n+1} + V_i^n \right) \qquad \text{(A-110)}$$

Several checks must be made to prevent the water levels in the control volumes from reaching physically unrealistic values. As a vent clears, the level in the vent will usually exceed the vent length slightly, which in turn forces extra water into the control volume into which the water is flowing.

Since the vent level should actually be stopped at the end of the vent, enough water is removed from the downstream control volume to move the vent level back to the end of the vent. If the water level on either the drywell or the wetwell side of the suppression pool rises above a vent that is partially cleared, as shown in Figure A-6a, then the water that is above the vent centerline is moved into the vent and all further upward motion of the pool is stopped until the vent refills. If a vent refills before the pool level reaches the vent, as shown in Figure A-6b, the water flowing out of the vent is transferred to the top of the pool. If the level on the drywell side of the suppression pool rises above the weir wall, the water is transferred to the drywell sump. If the drywell sump level has also reached the weir wall, the levels in the drywell sump and the drywell side of the suppression pool will rise (or fall) together.

If the pool motion model described above predicts that any of the three suppression pool vents is cleared, gases are allowed to flow between the drywell and the wetwell. The flow rate through each cleared vent is calculated from the following equation:

$$\frac{d}{dt} F_{vent,l} = \frac{1}{\rho_g (H_v/A_v)} \left[P_D + \rho_{DW} g z_{DW} - P_w - \rho_{WW} g Z_{WW} + \rho g Y_{sum} - 0.5 k_{vent} \rho_g \frac{F_{vent,l} |F_{vent,l}|}{A_v^2} \right] \quad \text{(A-111)}$$

where

$F_{vent,l}$ = volumetric-flow rate from drywell to wetwell through lth row of vents (m^3/s)

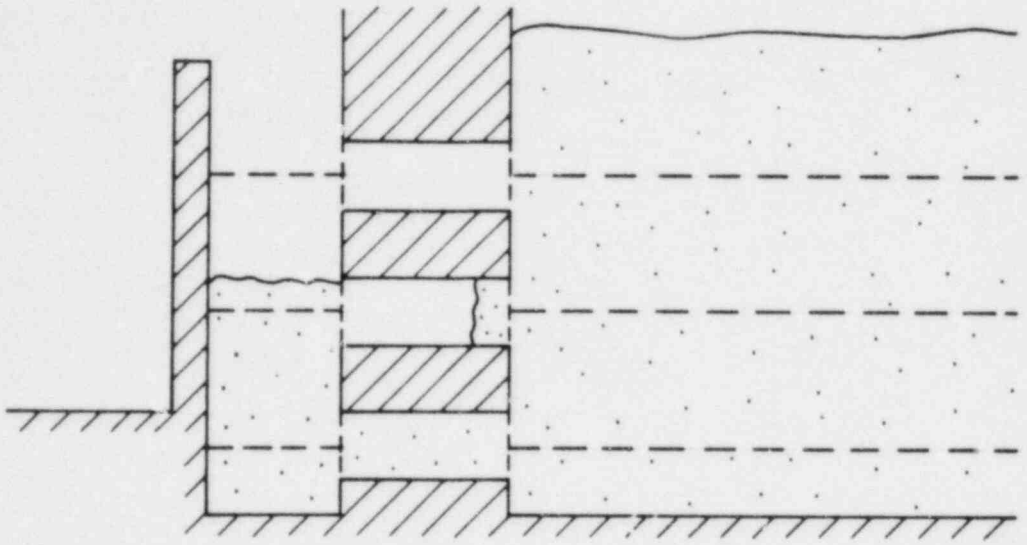
ρ_g = density of gases flowing into suppression pool (drywell density if flowing from drywell; wetwell density if flowing from wetwell) (kg/m^3)

ρ_{DW} = density of gases in drywell (kg/m^3)

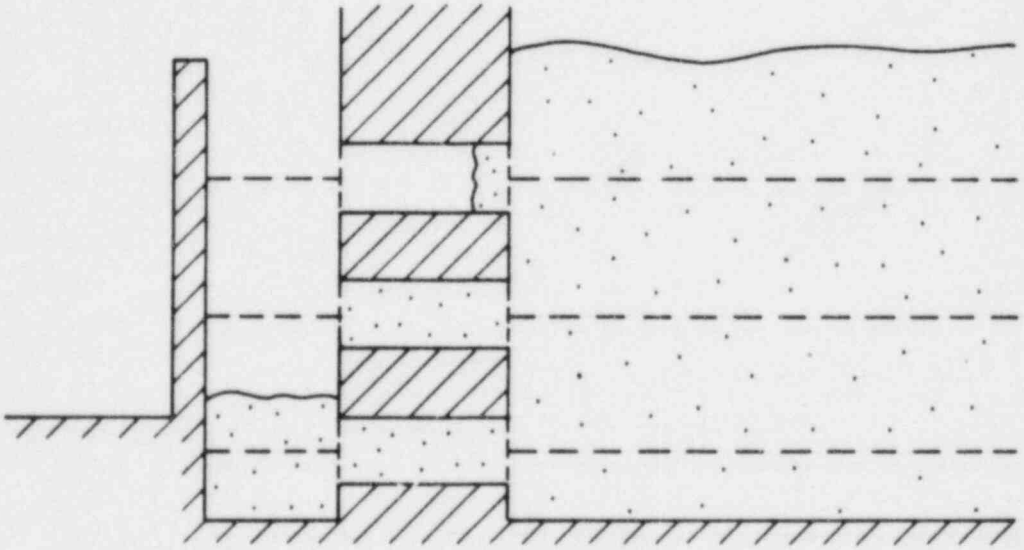
ρ_{WW} = density of gases in wetwell (kg/m^3)

Z_{DW} = drywell elevation (See Section A.1.1) (m)

Z_{WW} = wetwell elevation (See Section A.1.1) (m)



a. **DRYWELL SIDE FILLING ABOVE CLEARED VENT**



b. **VENT REFILLING BEFORE DRYWELL SIDE LEVEL REACHES VENT**

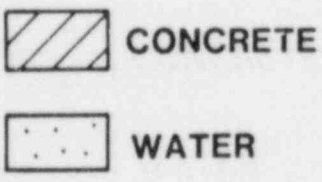


Figure A-6. Special Cases for Suppression Pool Motion

Y_{sum} = - Height of suppression pool surface above vent centerline if flowing from drywell
+ Height of suppression pool surface above vent centerline if flowing from wetwell (m)

k_{vent} = flow loss coefficient for row of vents

This is similar to the momentum equation used for normal HECTR junctions, but the head of water above the suppression pool vent ($\rho g\ Y_{sum}$) is included. The vent flow equations are solved simultaneously with the compartment mass, energy, and flow equations. The three vent flow equations are added to the set of equations already being solved. These equations are treated the same as normal HECTR 2-way junctions when calculating terms for the Jacobian matrix.

All steam that flows through the suppression pool is assumed to condense in the suppression pool, and all gases that flow through the suppression pool are assumed to be cooled to the suppression pool temperature. Since the temperature and composition of gases entering the suppression pool are different from those exiting the suppression pool, the terms in Eqs. A-3 and A-4 due to gas flow through the vents will be different for the wetwell and the drywell. The terms are calculated from

If flow is from drywell to wetwell:

Drywell

$$\left(\frac{dN_{ij}}{dt}\right)_{SP} = \frac{-N_{DW,j}}{Vol_{DW}} \sum_{\ell=1}^{3} F_{vent,\ell} \qquad \text{(A-112)}$$

$$\left(\frac{dE_i}{dt}\right)_{SP} = -\left(\sum_{j=1}^{4} \frac{N_{DW,j}}{Vol_{DW}} h_{DW,j}\right) \left(\sum_{\ell=1}^{3} F_{vent,\ell}\right) \qquad \text{(A-113)}$$

Wetwell

For j=1

$$\left(\frac{dN_{ij}}{dt}\right)_{SP} = 0 \qquad \text{(A-114)}$$

For j=2,4

$$\frac{dN_{ij}}{dt}_{SP} = \frac{N_{DW,j}}{Vol_{DW}} \sum_{\ell=1}^{3} F_{vent,\ell} \qquad \text{(A-115)}$$

For j=1,4

$$\left(\frac{dE_i}{dt}\right)_{SP} = \left(\sum_{j=1}^{4} \frac{N_{DW,j}}{Vol_{DW}} h_{SPout,j}\right)\left(\sum_{\ell=1}^{3} F_{vent,\ell}\right) \quad \text{(A-116)}$$

If flow if from wetwell to drywell:

Drywell

For j=1

$$\left(\frac{dN_{ij}}{dt}\right)_{SP} = 0 \quad \text{(A-117)}$$

$$\left(\frac{dN_{ij}}{dt}\right)_{SP} = \frac{-N_{WW,j}}{Vol_{WW}} \sum_{\ell=1}^{3} F_{vent,\ell} \quad \text{(A-118)}$$

$$\left(\frac{dE_i}{dt}\right)_{SP} = -\left(\sum_{j=2}^{4} \frac{N_{WW,j}}{Vol_{WW}} h_{SPout,j}\right)\left(\sum_{\ell=1}^{3} F_{vent,\ell}\right) \quad \text{(A-119)}$$

Wetwell

$$\left(\frac{dN_{ij}}{dt}\right)_{SP} = \frac{N_{WW,j}}{Vol_{WW}} \sum_{\ell=1}^{3} F_{vent,\ell} \quad \text{(A-120)}$$

$$\left(\frac{dE_i}{dt}\right)_{SP} = \left(\sum_{j=1}^{4} \frac{N_{WW,j}}{Vol_{WW}} h_{WW,j}\right)\left(\sum_{\ell=1}^{3} F_{vent,\ell}\right) \quad \text{(A-121)}$$

where

Vol_{DW} = drywell compartment volume (m^3)
Vol_{WW} = wetwell compartment volume (m^3)
$N_{DW,j}$ = moles of the jth gas in the drywell
$N_{WW,j}$ = moles of the jth gas in the wetwell
$h_{DW,j}$ = enthalpy of jth gas in drywell (J/mole)
$h_{WW,j}$ = enthalpy of jth gas in wetwell (J/mole)
$h_{SPout,j}$ = enthalpy of jth gas evaluated at suppression pool temperature (J/mole)

Water can drain from the upper pool into the suppression pool at a user-specified rate after a specified time in the calculation. This water continues to drain at a constant rate

until the mass of water in the upper pool falls below a user-specified minimum value. Thereafter, water will continue to drain from the upper pool if the water mass rises above the minimum value.

A.2.11 Heat Exchanger Model

The heat exchanger model in HECTR is used for cooling sumps or suppression pools, or for cooling containment sprays when they are in the recirculation mode and are drawing water from a sump. The heat exchanger model in HECTR was taken from the MARCH code.[17] This is a model for a oncethrough counter-current flow heat exchanger. An iterative model is employed that matches the heat-transfer rates to the changes in outlet flow temperature. The user-input parameters are

SPFLOR = Rated mass-flow rate (kg/s)
HAEFFR = Rated effective heat-transfer coefficient times the effective heat-transfer area (W/K)
TS1 = Secondary side inlet temperature (K)
WSR = Secondary side mass-flow rate (kg/s)

HECTR supplies the primary side inlet temperature, TSRC, depending upon which sump the water is being drawn from. The model first guesses a value for Q, the heat-transfer rate from the primary to the secondary side. Usually, the value from the previous timestep is used so that convergence is rapid. The primary and secondary side outlet temperatures, TSPR and TS2, are then calculated from

$$TSPR = TSRC - Q/(SPFL*CP) \tag{A-122}$$

$$TS2 = TS1 + Q/(WSR*CP) \tag{A-123}$$

where CP is the liquid specific heat and SPFL is the actual primary side flow rate. A log-mean temperature difference, DTLN, is then calculated:

$$DTLN = \frac{(TSRC - TS2) - (TSPR - TS1)}{\ell n\left(\frac{TSRC - TS2}{TSPR - TS1}\right)} \tag{A-124}$$

The log-mean temperature difference is then used to calculate a heat-transfer rate based on rated parameters:

$$QP = HAEFF * DTLN \tag{A-125}$$

where

$$HAEFF = HAEFFR(SPFL/SPFLOR)^{0.8} \tag{A-126}$$

Q is then compared against QP, and if the convergence criteria are not met ($|(Q-QP)/Q| < 0.01$), Q is adjusted and the process is repeated.

A.3 References

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APPENDIX B

PROGRAM STRUCTURE

CONTENTS

LIST OF FIGURES

B. PROGRAM STRUCTURE

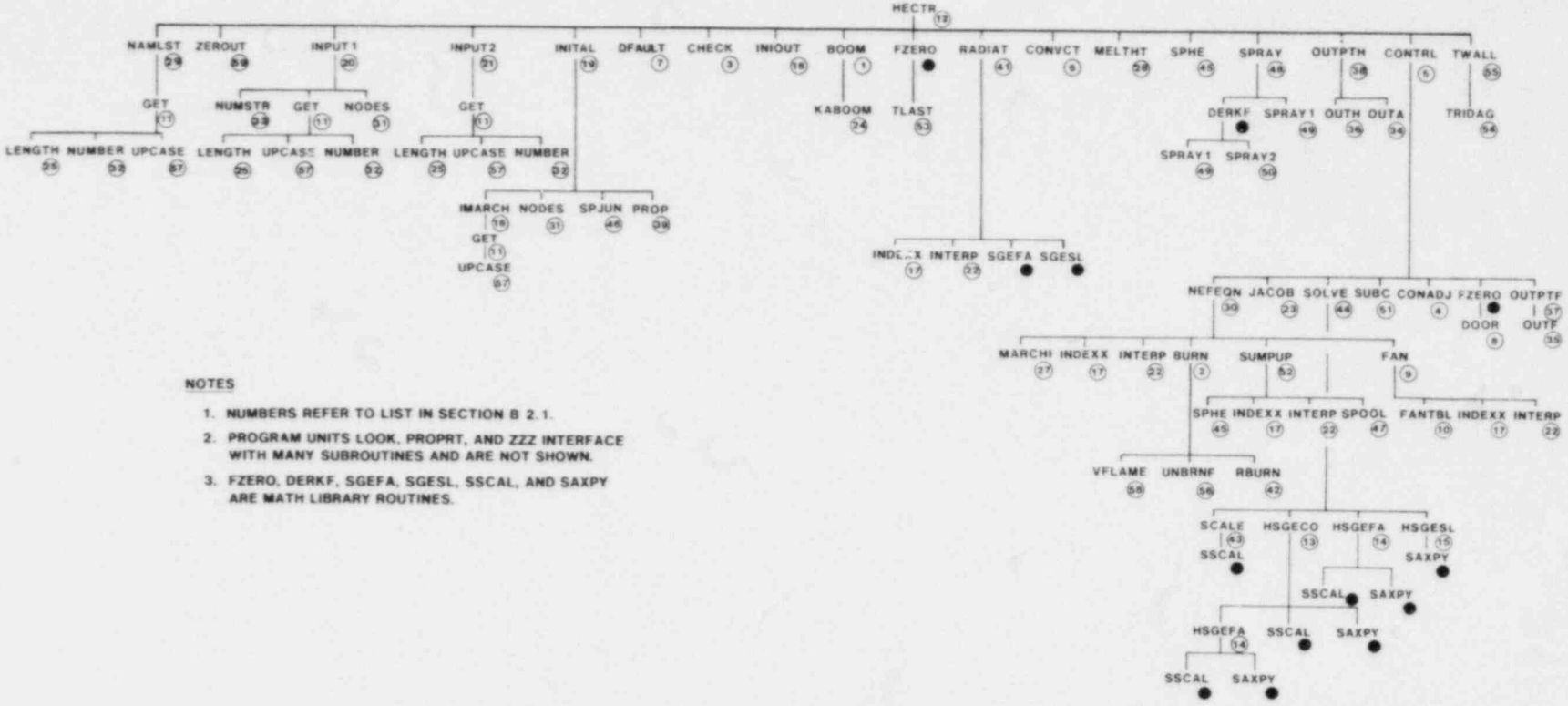
B.1 Introduction

This appendix describes in some detail the program structure of HECTR and ACHILES. These two computer programs are written in ANSI FORTRAN 77 [1]. HECTR and ACHILES are intended to be well-structured, modular, easily modifiable, well-documented (about a third of the lines in HECTR and a fifth of the lines in ACHILES are comments), portable, fast-running, flexible and user-friendly. Nonetheless, the structures of these two programs (especially HECTR) are complex in places. The intent of this chapter is to give the user a general understanding of the structure of HECTR and ACHILES.

Each program consists of a number of program units. A program unit is either a main program or a subprogram. A subprogram can be either block data, a function, or a subroutine. Sections B.2.1 and B.2.2 for HECTR and Sections B.3.1 and B.3.2 for ACHILES list the program units in alphabetical order and by their type (i.e., main program, block data, subroutine, etc.). Most of the data in the two programs are communicated between program units by common blocks. Sections B.2.3 and B.2.4 for HECTR and Sections B.3.3 and B.3.4 for ACHILES list the relationships between program units and common blocks. The organization of the program units in the two programs (the program units called by and calling each program unit) is described in Sections B.2.5 and B.2.6 for HECTR and Sections B.3.5 and B.3.6 for ACHILES. References to SLATEC mathematical library and DISSPLA graphics library routines (see Section C.1) are included in these discussions. Finally, Sections B.2.7 and B.3.7 describe the PARAMETER statements in the two programs. PARAMETER statements are used in HECTR and ACHILES to define constants that set array sizes. The limits of basic problem parameters (such as the maximum number of compartments, flow junctions, surfaces, etc. that are allowed in the input geometry) can be modified by changing the values of the constants in these statements. This allows the user to easily change the amount of computer memory that will be required to run HECTR.

B.2 HECTR

HECTR contains 60 program units and 34 common blocks in about 11400 lines. Figure B-1 presents a chart showing how the program units in HECTR are organized.



NOTES

1. NUMBERS REFER TO LIST IN SECTION B 2.1.
2. PROGRAM UNITS LOOK, PROPRT, AND ZZZ INTERFACE WITH MANY SUBROUTINES AND ARE NOT SHOWN.
3. FZERO, DERKF, SGEFA, SGESL, SSCAL, AND SAXPY ARE MATH LIBRARY ROUTINES.

Figure B-1. Program Organization Chart

B.2.1 Program Units

This section lists the program units in HECTR and gives a short description of each. The character(s) in parentheses before each name identify the program unit type (i.e., main program, block data, subroutine, etc.). The units are listed here alphabetically rather than by the order in which they appear in HECTR.

Key: B - Block Data
CH - Character Function
I - Integer Function
M - Main Program
R - Real Function
S - Subroutine

1. (S) BOOM - Determines if a detonable mixture is present in each compartment. A message is printed if a change in condition occurs.

2. (S) BURN - Hydrogen burn model. Determines if a burn can ignite or propagate into a compartment at the beginning of a flow timestep, and if so, determines the burn time. When burns are occurring, BURN will calculate the molar chemical reaction rates in burning compartments for each timestep.

3. (S) CHECK - Checks the validity of HECTR input. This checking is optional. The primary reason for adding this subroutine was to allow for future expansion of this option.

4. (S) CONADJ - Adjusts surface condensation rates to keep liquid film thicknesses within specified bounds.

5. (S) CONTRL - Controls the numerical solution of the conservation equations. This subroutine integrates these equations over a single heat-transfer timestep.

6. (S) CONVCT - Convective heat-transfer model. Calculates the convective heat flux to a surface, and the condensation or evaporation rate.

7. (B) DFAULT - Contains default values for the variables that can be changed in the NAMELIST-type input.

8. (R) DOOR - Describes door (inertial valve) area as a function of the differential pressure across the door. This is a nonlinear equation that is solved with a root finder (FZERO).

9. (S) FAN - Fan model. Calculates the rate of change of mass and energy in each compartment caused by fan flows. A single call to this subroutine is used to perform the calculations for all fan paths.

10 (B) FANTBL - Contains the default curve that relates the normalized pressure head across a fan to the normalized volumetric flow rate through the fan.

11. (S) GET - Reads a single input record. This record may be either a line of alphanumeric input or one or more lines containing a series of real, integer, and logical values.

12. (M) HECTR - HECTR main program. The major part of the top level HECTR control structure is located here. Also, the final run summaries are printed from this routine.

13. (S) HSGECO - Factors a matrix by Gaussian elimination and estimates the condition number of the matrix. This is a version of the LINPACK routine SGECO that has been modified to take advantage of the special structure used in HECTR for the Jacobian of the conservation equations (see Section A.1.2).

14. (S) HSGEFA - Factors a matrix by Gaussian elimination (does not estimate the condition numbers). This is a version of the LINPACK routine SGEFA that has been modified to take advantage of the special structure used in HECTR for the Jacobian of the conservation equations (see Section A.1.2).

15. (S) HSGESL - Solves the linear system of equations $Ax = b$ using the factorization of A computed by HSGECO or HSGEFA. This is a version of the LINPACK routine SGESL that has been modified to take advantage of the special structure used in HECTR for the Jacobian of the conservation equations (see Section A.1.2).

16. (S) IMARCH - Initializes the external (MARCH) interface.

17. (I) INDEXX - Finds the index I in the array Y such that, for a given number X, $Y(I) \leq X < Y(I+1)$ is satisfied. This locates X in the table Y.

18. (S) INIOUT - Writes initial output to a file. Included in this output are variables detailing the geometry being modeled by HECTR and the accident scenario being considered.

19. (S) INITAL - Initializes HECTR variables and arrays. This is done after all input has been read.

20. (S) INPUT1 - Reads the problem geometry (as described in Section 4.2.2).

21. (S) INPUT2 - Reads the initial conditions and the accident scenario (as described in Section 4.2.3).

22. (R) INTERP - Performs linear interpolation of a table using the location calculated by INDEXX.

23. (S) JACOB - Sets up the matrix A of Eq. A-13 (= I/deltat - J, where I is an identity matrix, deltat is the length of the current flow timestep, and J is the Jacobian matrix of the conservation equations in NEFEQN).

24. (S) KABOOM - Contains the message that is printed when either the failure pressure is exceeded or the gases in any compartment fall within the detonation limits.

25. (I) LENGTH - Finds the length of a character string excluding trailing blanks. This function is part of the input processor.

26. (R) LOOK - Linearly interpolates the property tables contained in the block data PROPRT.

27. (S) MARCHI - External (MARCH) interface. Reads and interprets time histories of source terms from a file created by an external primary system computer code.

28. (S) MELTHT - Calculates ice-melting rates (for an ice condenser) and heat transferred to the melt runoff as it falls through the lower plenum.

29. (S) NAMLST - Simulates a NAMELIST-type input (NAMELIST-input is not part of the ANSI FORTRAN 77 standard, so it is simulated in HECTR).

30. (S) NEFEQN - Calculates the rate of change of the moles of each gas (N) and the total energy (E) in each compartment and also the rate of change of the volumetric flow rate (F) through each flow junction.

31. (S) NODES - Sets up the nodalization to be used for heat conduction calculations for a multi-layered slab. The nodalization is performed after the multilayered slab has been converted into a thermally equivalent homogeneous steel slab.

32. (R) NUMBER - Converts the character string representation of a number into a REAL value. This function is part of the input processor.

33. (CH) NUMSTR - Creates a character string representation of an integer. This function is used to form portions of labels.

34. (S) OUTA - Writes the current values of additional variables defined on heat-transfer timesteps to a file.

35. (S) OUTF - Writes the current values of the main variables defined on flow timesteps to a file.

36. (S) OUTH - Writes the current values of the main variables defined on heat-transfer timesteps to a file.

37. (S) OUTPTF - Determines when to write new values of variables defined on flow timesteps to a file.

38. (S) OUTPTH - Determines when to write new values of variables defined on heat-transfer timesteps to a file.

39. (S) PROP - Determines new gas properties (enthalpies, specific heats, internal energies, and densities) for each compartment. This subroutine is called during each flow timestep after the compartment moles and temperatures are updated.

40. (B) PROPRT - Contains all the liquid and gas property tables used by HECTR.

41. (S) RADIAT - Radiative heat-transfer model. Calculates the net radiative heat flux leaving each surface. The calculations are performed for all surfaces during a single call to the subroutine.

42. (R) RBURN - Calculates the burn rate in a compartment given its current conditions, source terms, the time left until the burn completes, and the final fraction of hydrogen to be left after combustion.

43. (S) SCALE - Scales the linear system of equations $Ax = b$ that it receives from SOLVE so as to reduce the condition number of the matrix A. This improves the stability of the solution technique.

44. (S) SOLVE - Solves the linear system of mass, energy, and momentum conservation equations.

45. (S) SPHE - Calculates the exit temperature for water that is drawn from a sump and passed through a counterflow heat exchanger.

46. (S) SPJUN - Sets up the order for performing spray carryover calculations.

47. (S) SPOOL - Calculates suppression pool motion. In particular, SPOOL determines liquid velocities through the vents, the time that vents clear, and changes in the drywell and wetwell volumes.

48. (S) SPRAY - Spray model. Calculates the rates of heat and mass transfer to the atmosphere caused by a given distribution of spray drops falling through a compartment.

49. (S) SPRAY1 - Calculates the rates of change of the mass of a drop with respect to the distance it has fallen, assuming that the drop has reached its equilibrium temperature. This ordinary differential equation is integrated by SPRAY (using DERKF).

50. (S) SPRAY2 - Calculates the rates of change of the mass and temperature of a drop with respect to the distance it has fallen. This pair of ordinary differential equations is integrated by SPRAY (using DERKF).

51. (S) SUBC - Checks if the atmosphere in any compartment is subcooled (supersaturated). If so, the rate of change of steam mass needed to bring the subcooled atmospheres to saturation over the next flow timestep is calculated. The excess steam will be condensed from the compartment gas and sent to a sump.

52. (S) SUMPUP - Calculates new sump masses and temperatures as well as the rate of change of mass and energy in each compartment due to sump phenomena.

53. (R) TLAST - This is the equation obtained from setting the derivative of the temperature of a drop with respect to the distance it has fallen equal to zero. The root of this equation in a given compartment (determined by FZERO) is the drop equilibrium temperature in that compartment.

54. (S) TRIDAG - Solves the system of equations Ax = b for x where A is a tridiagonal matrix and x and b are vectors.

55. (R) TWALL - Performs a heat conduction calculation for a slab over a heat-transfer timestep, given the radiative and convective heat fluxes to the surface.

56. (R) UNBRNF - Determines the unburned fraction of hydrogen that will be left at the end of a combustion in a compartment given the current (precombustion) hydrogen mole fraction in the compartment. This quantity is 1 minus the combustion completeness.

57. (S) UPCASE - Converts lower case letters in a character string into upper case. This subroutine is part of the input processor.

58. (R) VFLAME - Calculates a flame speed for hydrogen combustion given the current (precombustion) gas mole fractions in a compartment.

59. (S) ZEROUT - Zeroes out HECTR variables and arrays. Also, general constants used throughout the program (molecular weights, pi, etc.) are defined here.

60. (R) ZZZ - Interpolates compressibility tables with respect to both pressure and temperature. Steam is treated as a real gas in HECTR by adding the compressibility factor Z to the ideal gas equation for steam (i.e., PV = ZnRT).

B.2.2 Program Units Identified by Type

This section lists the program units in HECTR categorized by their type.

Block Data:

DFAULT FANTBL PROPRT

Character Function:

NUMSTR

Integer Functions:

INDEXX LENGTH

Main Program:

HECTR

Real Functions:

DOOR INTERP LOOK NUMBER RBURN TLAST TWALL UNBRNF
VFLAME ZZZ

Subroutines:

BOOM	BURN	CHECK	CONADJ	CONTRL	CONVCT	FAN	GET
HSGECO	HSGEFA	HSGESL	IMARCH	INIOUT	INITAL	INPUT1	INPUT2
JACOB	KABOOM	MARCHI	MELTHT	NAMLST	NEFEQN	NODES	OUTA
OUTF	OUTH	OUTPTF	OUTPTH	PROP	RADIAT	SCALE	SOLVE
SPHE	SPJUN	SPOOL	SPRAY	SPRAY1	SPRAY2	SUBC	SUMPUP
TRIDAG	UPCASE	ZEROUT					

B.2.3 Common Blocks Contained by Each Program Unit

This section lists which common blocks, if any, are contained in each HECTR program unit. The character(s) in parentheses before each program unit name identify its type (i.e., main program, block data, subroutine, etc.).

Key: B - Block Data
CH - Character Function
I - Integer Function
M - Main Program
R - Real Function
S - Subroutine

1. (S) BOOM
   DETON8 PROPTY THINGS UNITS
2. (S) BURN
   BURNER FANVAR GEOM STATUS STPSIZ THINGS
3. (S) CHECK
   SUMP THINGS UNITS
4. (S) CONADJ
   CDRYE COMPQJ CONRAD FILM STPSIZ SUMP SURF
   THINGS
5. (S) CONTRL
   BURNER CDRYE COMPQJ CONRAD CONST DOORE FANVAR
   FILM GENCON GEOM ICE MAXIS POOL PROPTY
   SORCES STATUS STPSIZ SUMP SURF THINGS UNITS
6. (S) CONVCT
   CONST FILM GENCON ICE PROPTY SUMP UNITS
7. (B) DFAULT
   ALPHAN BURNER FILM ICE OUTCON STATUS STPSIZ
   THINGS UNITS
8. (R) DOOR
   DOORE
9. (S) FAN
   FANVAR GEOM PROPTY THINGS
10. (B) FANTBL
   FANVAR
11. (S) GET
   UNITS
12. (M) HECTR
   ALPHAN BURNER CDRYE COMPQJ CONRAD CONST FANVAR
   FILM GENCON GEOM ICE MAXIS NODAL POOL
   PROPTY SORCES SP SPRAYE STATUS STPSIZ SUMP
   SURF THINGS TLASTE TOLINT UNITS
13. (S) HSGECO
14. (S) HSGEFA
15. (S) HSGESL
16. (S) IMARCH
   MARCH UNITS
17. (I) INDEXX
18. (S) INOUT
   ALPHAN BURNER FANVAR GEOM ICE NODAL OUTCON
   POOL SPRAYE STPSIZ SUMP SURF THINGS
19. (S) INITAL
   CONST FANVAR GENCON GEOM ICE MAXIS NODAL
   OUTCON POOL PROPTY SORCES SP SPRAYE STATUS
   STPSIZ SUMP SURF THINGS UNITS

```
20. (S ) INPUT1
        ALPHAN BURNER CONRAD DOORE  FANVAR GEOM   ICE
        NODAL  POOL   SPRAYE STATUS SUMP   SURF   THINGS
        UNITS
21. (S ) INPUT2
        CONRAD CONST  GENCON ICE    PROPTY SORCES STATUS
        STPSIZ SURF   THINGS UNITS
22. (R ) INTERP
23. (S ) JACOB
        GEOM   POOL   PROPTY STPSIZ THINGS
24. (S ) KABOOM
        UNITS
25. (I ) LENGTH
26. (R ) LOOK
        UNITS
27. (S ) MARCHI
        MARCH  SORCES UNITS
28. (S ) MELTHT
        COMPQJ CONST  GENCON ICE    PROPTY SUMP   THINGS
        UNITS
29. (S ) NAMLST
        ALPHAN BURNER FILM   ICE    OUTCON STATUS STPSIZ
        THINGS UNITS
30. (S ) NEFEQN
        COMPQJ CONST  GENCON GEOM   ICE    POOL   PROPTY
        SORCES STATUS STPSIZ SUMP   THINGS UNITS
31. (S ) NODES
32. (R ) NUMBER
        UNITS
33. (CH) NUMSTR
        UNITS
34. (S ) OUTA
        COMPQJ CONRAD ICE    OUTCON SPRAYE THINGS
35. (S ) OUTF
        FANVAR OUTCON POOL   THINGS
36. (S ) OUTH
        CDRYE  COMPQJ FILM   ICE    OUTCON PROPTY SORCES
        STATUS SUMP   SURF   THINGS
37. (S ) OUTPTF
        GEOM   OUTCON STPSIZ THINGS
38. (S ) OUTPTH
        FANVAR OUTCON PROPTY SPRAYE STATUS STPSIZ THINGS
39. (S ) PROP
        CONST  GENCON GEOM   THINGS UNITS
40. (B ) PROPRT
        CMP    CONST
41. (S ) RADIAT
        THINGS UNITS
42. (R ) RBURN
43. (S ) SCALE
44. (S ) SOLVE
        STPSIZ UNITS
45. (S ) SPHE
        CONST  SUMP   UNITS
```

```
46. (S ) SPJUN
          SPRAYE
47. (S ) SPOOL
          GENCON GEOM   POOL   PROPTY STPSIZ SUMP   UNITS
48. (S ) SPRAY
          CONST  GENCON SORCES SP     SPRAYE SPRY   SUMP
          TEXPS  THINGS TLIMS  TOLINT UNITS
49. (S ) SPRAY1
          GENCON SP     SPRY   TEXPS  TLIMS
50. (S ) SPRAY2
          CONST  GENCON SP     SPRY   TLIMS  UNITS
51. (S ) SUBC
          COMPQJ CONST  GENCON GEOM   PROPTY STPSIZ THINGS
          UNITS
52. (S ) SUMPUP
          COMPQJ CONST  GENCON GEOM   POOL   PROPTY SORCES
          STATUS SUMP   THINGS UNITS
53. (R ) TLAST
           CONST TLASTE UNITS
54. (S ) TRIDAG
55. (R ) TWALL
56. (R ) UNBRNF
57. (S ) UPCASE
58. (R ) VFLAME
59. (S ) ZEROUT
          CDRYE  COMPQJ CONRAD DETON8 DOORE  FANVAR FILM
          GENCON ICE    NODAL  OUTCON POOL   SORCES SPRAYE
          STATUS STPSIZ SUMP   SURF   THINGS UNITS
60. (R ) ZZZ
          CMP
```

B.2.4 Program Units Containing Each Common Block

This section lists which program units contain each common block in HECTR. This table is the inverse of the previous table.

```
 1. ALPHAN
      DFAULT HECTR  INIOUT INPUT1 NAMLST
 2. BURNER
      BURN   CONTRL DFAULT HECTR  INIOUT INPUT1 NAMLST
 3. CDRYE
      CONADJ CONTRL HECTR  OUTH   ZEROUT
 4. CMP
      PROPRT ZZZ
 5. COMPQJ
      CONADJ CONTRL HECTR  MELTHT NEFEQN OUTA   OUTH   SUBC
      SUMPUP ZEROUT
 6. CONRAD
      CONADJ CONTRL HECTR  INPUT1 INPUT2 OUTA   ZEROUT
```

7. CONST
   CONTRL CONVCT HECTR INITAL INPUT2 MELTHT NEFEQN PROP
   PROPRT SPHE SPRAY SPRAY2 SUBC SUMPUP TLAST
8. DETON8
   BOOM ZEROUT
9. DOORE
   CONTRL DOOR INPUT1 ZEROUT
10. FANVAR
   BURN CONTRL FAN FANTBL HECTR INIOUT INITAL INPUT1
   OUTF OUTPTH ZEROUT
11. FILM
   CONADJ CONTRL CONVCT DFAULT HECTR NAMLST OUTH ZEROUT
12. GENCON
   CONTRL CONVCT HECTR INITAL INPUT2 MELTHT NEFEQN PROP
   SPOOL SPRAY SPRAY1 SPRAY2 SUBC SUMPUP ZEROUT
13. GEOM
   BURN CONTRL FAN HECTR INIOUT INITAL INPUT1 JACOB
   NEFEQN OUTPTF PROP SPOOL SUBC SUMPUP
14. ICE
   CONTRL CONVCT DFAULT HECTR INIOUT INITAL INPUT1 INPUT2
   MELTHT NAMLST NEFEQN OUTA OUTH ZEROUT
15. MARCH
   IMARCH MARCHI
16. MAXIS
   CONTRL HECTR INITAL
17. NODAL
   HECTR INIOUT INITAL INPUT1 ZEROUT
18. OUTCON
   DFAULT INIOUT INITAL NAMLST OUTA OUTF OUTH OUTPTF
   OUTPTH ZEROUT
19. POOL
   CONTRL HECTR INIOUT INITAL INPUT1 JACOB NEFEQN OUTF
   SPOOL SUMPUP ZEROUT
20. PROPTY
   BOOM CONTRL CONVCT FAN HECTR INITAL INPUT2 JACOB
   MELTHT NEFEQN OUTH OUTPTH SPOOL SUBC SUMPUP
21. SORCES
   CONTRL HECTR INITAL INPUT2 MARCHI NEFEQN OUTH SPRAY
   SUMPUP ZEROUT
22. SP
   HECTR INITAL SPRAY SPRAY1 SPRAY2
23. SPRAYE
   HECTR INIOUT INITAL INPUT1 OUTA OUTPTH SPJUN SPRAY
   ZEROUT
24. SPRY
   SPRAY SPRAY1 SPRAY2
25. STATUS
   BURN CONTRL DFAULT HECTR INITAL INPUT1 INPUT2 NAMLST
   NEFEQN OUTH OUTPTH SUMPUP ZEROUT
26. STPSIZ
   BURN CONADJ CONTRL DFAULT HECTR INIOUT INITAL INPUT2
   JACOB NAMLST NEFEQN OUTPTF OUTPTH SOLVE SPOOL SUBC
   ZEROUT

```
27. SUMP
       CHECK  CONADJ CONTRL CONVCT HECTR  INIOUT INITAL INPUT1
       MELTHT NEFEQN OUTH   SPHE   SPOOL  SPRAY  SUMPUP ZEROUT
28. SURF
       CONADJ CONTRL HECTR  INIOUT INITAL INPUT1 INPUT2 OUTH
       ZEROUT
29. TEXPS
       SPRAY  SPRAY1
30. THINGS
       BOOM   BURN   CHECK  CONADJ CONTRL DFAULT FAN    HECTR
       INIOUT INITAL INPUT1 INPUT2 JACOB  MELTHT NAMLST NEFEQN
       OUTA   OUTF   OUTH   OUTPTF OUTPTH PROP   RADIAT SPRAY
       SUBC   SUMPUP ZEROUT
31. TLASTE
       HECTR  TLAST
32. TLIMS
       SPRAY  SPRAY1 SPRAY2
33. TOLINT
       HECTR  SPRAY
34. UNITS
       BOOM   CHECK  CONTRL CONVCT DFAULT GET    HECTR  IMARCH
       INITAL INPUT1 INPUT2 KABOOM LOOK   MARCHI MELTHT NAMLST
       NEFEQN NUMBER NUMSTR PROP   RADIAT SOLVE  SPHE   SPOOL
       SPRAY  SPRAY2 SUBC   SUMPUP TLAST  ZEROUT
```

B.2.5 Subprograms Called by Each Program Unit

This section lists which subprograms (subroutines and functions), if any, are called by each HECTR program unit. Some of the called subprograms are not actually part of HECTR but belong to the SLATEC mathematical library to which HECTR is linked. The character(s) in parentheses before each numbered program unit name identify its type (i.e., main program, block data, subroutine, etc.).

```
Key: B  - Block Data
     CH - Character Function
     I  - Integer Function
     M  - Main Program
     R  - Real Function
     S  - Subroutine

 1. (S ) BOOM
            KABOOM
 2. (S ) BURN
            RBURN  UNBRNF VFLAME
 3. (S ) CHECK
 4. (S ) CONADJ
 5. (S ) CONTRL
            CONADJ FZERO  JACOB  KABOOM NEFEQN OUTPTF PROP
             SOLVE  SUBC  ZZZ
```

```
 6. (S ) CONVCT
            LOOK   ZZZ
 7. (B ) DFAULT
 8. (R ) DOOR
 9. (S ) FAN
            INDEXX INTERP
10. (B ) FANTBL
11. (S ) GET
            LENGTH NUMBER UPCASE
12. (M ) HECTR
            BOOM   CHECK  CONTRL CONVCT FZERO  INIOUT INITAL
            INPUT1 INPUT2 LOOK   MELTHT NAMLST OUTPTH RADIAT
            SPHE   SPRAY  TWALL  ZEROUT
13. (S ) HSGECO
            HSGEFA SASUM  SAXPY  SDOT   SSCAL
14. (S ) HSGEFA
            ISAMAX SAXPY  SSCAL
15. (S ) HSGESL
            SAXPY
16. (S ) IMARCH
            GET
17. (I ) INDEXX
18. (S ) INIOUT
19. (S ) INITAL
            IMARCH LOOK   NODES  PROP   SPJUN  ZZZ
20. (S ) INPUT1
            GET    NUMSTR
21. (S ) INPUT2
            GET    LOOK
22. (R ) INTERP
23. (S ) JACOB
24. (S ) KABOOM
25. (I ) LENGTH
26. (F ) LOOK
27. (S ) MARCHI
28. (S ) MELTHT
            LOOK
29. (S ) NAMLST
            GET    LENGTH NUMBER
30. (S ) NEFEQN
            BURN   FAN    INDEXX INTERP LOOK   MARCHI SUMPUP
31. (S ) NODES
32. (R ) NUMBER
33. (CH) NUMSTR
34. (S ) OUTA
35. (S ) OUTF
36. (S ) OUTH
37. (S ) OUTPTF
            OUTF
38. (S ) OUTPTH
            OUTA   OUTH
39. (S ) PROP
            LOOK
```

```
40. (B ) PROPRT
41. (S ) RADIAT
             INDEXX INTERP SGEFA  SGESL
42. (R ) RBURN
43. (S ) SCALE
             ISAMAX SSCAL
44. (S ) SOLVE
             HSGECO HSGEFA HSGESL SCALE
45. (S ) SPHE
             LOOK
46. (S ) SPJUN
47. (S ) SPOOL
             SGECO  SGESL
48. (S ) SPRAY
             DERKF  LOOK   SPRAY1 ZZZ
49. (S ) SPRAY1
50. (S ) SPRAY2
             LOOK   ZZZ
51. (S ) SUBC
             LOOK   ZZZ
52. (S ) SUMPUP
             INDEXX INTERP LOOK   SPHE   SPOOL
53. (R ) TLAST
             LOOK   ZZZ
54. (S ) TRIDAG
55. (R ) TWALL
             TRIDAG
56. (R ) UNBRNF
57. (S ) UPCASE
58. (R ) VFLAME
59. (S ) ZEROUT
60. (R ) ZZZ
```

B.2.6 Program Units Calling Each Subprogram

This section lists which program units call each subprogram (subroutine or function) in HECTR. This table is the inverse of the previous table. The portion titled "Internal Subprograms" lists which HECTR program units call each HECTR subprogram, while the portion titled "External Subprograms" lists which HECTR program units call each SLATEC mathematical library subprogram. The character(s) in parenthesis before each numbered program unit name identify its type (i.e., main program, block data, subroutine, etc.).

Key: B - Block Data
CH - Character Function
I - Integer Function
M - Main Program
R - Real Function
S - Subroutine

```
*** Internal subprograms ***

 1. (S ) BOOM
            HECTR
 2. (S ) BURN
            NEFEQN
 3  (S ) CHECK
            HECTR
 4. (S ) CONADJ
            CONTRL
 5. (S ) CONTRL
            HECTR
 6. (S ) CONVCT
            HECTR
 7. (B ) DFAULT
 8. (R ) DOOR
            FZERO
 9. (S ) FAN
            NEFEQN
10. (B ) FANTBL
11. (S ) GET
            IMARCH INPUT1 INPUT2 NAMLST
12. (M ) HECTR
13. (S ) HSGECO
            SOLVE
14. (S ) HSGEFA
            HSGECO SOLVE
15. (S ) HSGESL
            SOLVE
16. (S ) IMARCH
            INITAL
17. (I ) INDEXX
            FAN    NEFEQN RADIAT SUMPUP
18. (S ) INIOUT
            HECTR
19. (S ) INITAL
            HECTR
20. (S ) INPUT1
            HECTR
21. (S ) INPUT2
            HECTR
22. (R ) INTERP
            FAN    NEFEQN RADIAT SUMPUP
23. (S ) JACOB
            CONTRL
24. (S ) KABOOM
            BOOM   CONTRL
25. (I ) LENGTH
            GET    NAMLST
26. (R ) LOOK
            CONVCT HECTR  INITAL INPUT2 MELTHT NEFEQN PROP
            SPHE   SPRAY  SPRAY2 SUBC   SUMPUP TLAST
27. (S ) MARCHI
            NEFEQN
```

```
28. (S ) MELTHT
         HECTR
29. (S ) NAMLST
         HECTR
30. (S ) NEFEQN
         CONTRL
31. (S ) NODES
         INITAL
32. (R ) NUMBER
         GET     NAMLST
33. (CH) NUMSTR
         INPUT1
34. (S ) OUTA
         OUTPTH
35. (S ) OUTF
         OUTPTF
36. (S ) OUTH
         OUTPTH
37. (S ) OUTPTF
         CONTRL
38. (S ) OUTPTH
         HECTR
39. (S ) PROP
         CONTRL INITAL
40. (B ) PROPRT
41. (S ) RADIAT
         HECTR
42. (R ) RBURN
         BURN
43. (S ) SCALE
         SOLVE
44. (S ) SOLVE
         CONTRL
45. (S ) SPHE
         HECTR  SUMPUP
46. (S ) SPJUN
         INITAL
47. (S ) SPOOL
         SUMPUP
48. (S ) SPRAY
         HECTR
49. (S ) SPRAY1
         DERKF  SPRAY
50. (S ) SPRAY2
         DERKF
51. (S ) SUBC
         CONTRL
52. (S ) SUMPUP
         NEFEQN
53. (R ) TLAST
         FZERO
54. (S ) TRIDAG
         TWALL
```

```
55. (R ) TWALL
          HECTR
56. (R ) UNBRNF
          BURN
57. (S ) UPCASE
          GET
58. (R ) VFLAME
          BURN
59. (S ) ZEROUT
          HECTR
60. (R ) ZZZ
          CONTRL CONVCT INITAL SPRAY  SPRAY2 SUBC   TLAST

*** External subprograms ***

61. (S ) DERKF
          SPRAY
62. (S ) FZERO
          CONTRL HECTR
63. (I ) ISAMAX
          HSGEFA SCALE
64. (R ) SASUM
          HSGECO
65. (S ) SAXPY
          HSGECO HSGEFA HSGESL
66. (R ) SDOT
          HSGECO
67. (S ) SGECO
          SPOOL
68. (S ) SGEFA
          RADIAT
69. (S ) SGESL
          RADIAT SPOOL
70. (S ) SSCAL
          HSGECO HSGEFA SCALE
```

B.2.7 PARAMETER Statements

PARAMETER statements are used in HECTR primarily to define array sizes. All the arrays in HECTR Version 1.0 have been dimensioned large enough to run the sample problems described in Chapter 6, but have been set small enough so that HECTR will fit in the memory of all the computers mentioned in Appendix C (both the VAX-11 and the CRAY-1 have virtual memory while the CDC CYBER 76 at SNLA has a maximum of 162 K words of small core memory available). To change the size of all the arrays in HECTR that are concerned with a certain item, it is necessary only to modify all the corresponding PARAMETER statements. For example, the maximum number of compartments allowed by HECTR can be increased from 10 to 20 by changing "NC = 10" to "NC = 20" in all the PARAMETER statements in HECTR where NC is set. There is a set of PARAMETER statements near the top of most program units.

Each set is exactly alike, so that this modification can be done simply by a global substitution. (Note: If HECTR is stored using CDC UPDATE or a similar program, then changing values in parameter statements can be accomplished most conveniently when the PARAMETER statements are stored in a COMDECK.)

The symbolic names of constants set in PARAMETER statements in HECTR are listed below, along with the values to which they are set and a short description of what each one represents. All of the symbolic names can be set to any positive value desired by the user (as long as HECTR still fits in the computer's memory) with three exceptions--NG and NNV cannot be changed without also changing other coding in HECTR, and NDE is defined in terms of NC, NG, NJ, and NV and will automatically compensate for changes in any of these values.

NC	=	10	(maximum number of compartments)
ND	=	3	(maximum number of inertial valve flow junctions [doors])
NF	=	3	(maximum number of fan paths)
NG	=	4	(number of gas species: H_2O, N_2, O_2 and H_2)
NJ	=	12	(maximum number of flow junctions)
NS	=	30	(maximum number of surfaces)
NV	=	3	(maximum number of suppression pool vents)
NDR	=	1	(maximum number of drains)
NDS	=	2	(maximum number of spray drop sizes)
NICE	=	4	(maximum number of ice compartments in an ice condenser)
NLAYER	=	5	(maximum number of layers per slab surface)
NNV	=	60	(number of pseudo-NAMELIST variables)
NSC	=	2	(maximum number of compartments in which sprays originate)
NSE	=	50	(maximum number of source-term table entries for each gas)
NSMP	=	3	(maximum number of sumps)
NWN	=	1000	(maximum number of wall nodes = total for all slab surfaces)

NDE	=	(NG+1)*NC+NJ+NV	(maximum number of simultaneous ordinary differential equations to be solved each flow timestep - these are the equations expressing conservation of mass, energy, and momentum)

B.3 ACHILES

ACHILES contains 19 program units and 10 common blocks in about 3500 lines.

B.3.1 Program Units

This section lists the program units in ACHILES and gives a short description of each. The character(s) in parentheses before each name identify the program unit type (i.e., main program, block data, subroutine, etc.).

Key: B - Block Data
CH - Character Function
I - Integer Function
M - Main Program
R - Real Function
S - Subroutine

1. (M) ACHILE - ACHILES main program. Here, the tables are produced, and the data for tables and plots is read.

2. (S) CHEQUE - Checks if the numbers of compartments, surfaces, etc. for a HECTR run fall within the limits set by the PARAMETER statements in ACHILES.

3. (B) DFAULT - Contains default values for the variables that can be changed in the NAMELIST-type input.

4. (S) FETCH - Fetches the basic introductory information about a run from a HECTR generated file.

5. (I) FIND - Finds the position (index) of an integer in a list of integers that has been sorted into ascending numerical order.

6. (S) GET - Reads a single input record. This record may be either a line of alphanumeric input or one or more lines containing a series of real, integer, and logical values.

7. (S) GRAP - Draws the axes for a graph.

8. (S) HEADER - Prints basic introductory information about a HECTR run.

9. (S) INITPL - Initializes plotting with DISSPLA.

10. (S) INTER - Produces the intersection of two integer arrays whose values have been sorted into ascending numerical order. The elements in these arrays are used as pointers.

11. (I) LENGTH - Finds the length of a character string excluding trailing blanks. This function is part of the input processor.

12. (S) NAMLST - Simulates a NAMELIST-type input (NAMELIST input is not part of the ANSI FORTRAN 77 standard, so it is simulated in ACHILES).

13. (R) NUMBER - Converts the character string representation of a number into a REAL value. This function is part of the input processor.

14. (CH) NUMSTR - Creates a character string representation of an integer. This function is used to form portions of plot labels.

15. (S) PLOT - Produces a single graph.

16. (S) SORT - Sorts a list of integers into ascending numerical order.

17. (S) TERMPL - Terminates plotting with DISSPLA.

18. (S) UPCASE - Converts lower case letters in a character string into upper case. This subroutine is part of the input processor.

19. (S) WHICH - Reads the input that defines which compartments, surfaces, etc. are to be included in tables or plots.

B.3.2 Program Units Identified by Type

This section lists the program units in ACHILES categorized by their type.

```
Block Data
   DFAULT
Character Function
   NUMSTR
Integer Functions
   FIND   LENGTH
Main Program
   ACHILE
Real Function
   NUMBER
Subroutines
   CHEQUE FETCH GET GRAP   HEADER INITPL INTER NAMLST
   PLOT   SORT      TERMPL UPCASE WHICH
```

B.3.3 Common Blocks Contained by Each Program Unit

This section lists which common blocks, if any, are contained by each ACHILES program unit. The character(s) in parentheses before each program unit name identify its type (i.e., main program, block data, subroutine, etc.).

Key: B - Block Data
CH - Character Function
I - Integer Function
M - Main Program
R - Real Function
S - Subroutine

```
 1. (M )  ACHILE
             BASICI  BASICN  BATCHM  MAXIS   MISC  UNITS
 2. (S )  CHEQUE
             BASICN  UNITS
 3. (B )  DFAULT
             ALPHAN  BATCHM  KLUDGE  MISC    UNITS
 4. (S )  FETCH
             BASICA  BASICI  BASICN  BASICS  UNITS
 5. (I )  FIND
 6. (S )  GET
             UNITS
 7. (S )  GRAP
 8. (S )  HEADER
             BASICA  BASICI  BASICN  BASICS  MAXIS
 9. (S )  INITPL
10. (S )  INTER
             UNITS
11. (I )  LENGTH
12. (S )  NAMLST
             ALPHAN  BATCHM  KLUDGE  MISC    UNITS
13. (R )  NUMBER
             UNITS
14. (CH)  NUMSTR
             UNITS
15. (S )  PLOT
             ALPHAN  KLUDGE
16. (S )  SORT
17. (S )  TERMPL
18. (S )  UPCASE
19. (S )  WHICH
             UNITS
```

B.3.4 Program Units Containing Each Common Block

This section lists which program units contain each common block in ACHILES. This table is the inverse of the previous table.

```
 1. ALPHAN
       DFAULT NAMLST PLOT
 2. BASICA
       FETCH  HEADER
 3. BASICI
       ACHILE FETCH  HEADER
 4. BASICN
       ACHILE CHEQUE FETCH  HEADER
 5. BASICS
       FETCH  HEADER
 6. BATCHM
       ACHILE DFAULT NAMLST
 7. KLUDGE
       DFAULT NAMLST PLOT
 8. MAXIS
       ACHILE HEADER
 9. MISC
       ACHILE DFAULT NAMLST
10. UNITS
       ACHILE CHEQUE DFAULT FETCH GET INTER NAMLST NUMBER
       NUMSTR WHICH
```

B.3.5 Subprograms Called by Each Program Unit

This section lists which subprograms (subroutines and functions), if any, are called by each ACHILES program unit. Some of the called subprograms are not actually part of ACHILES but belong to the DISSPLA graphics library to which ACHILES is linked. The character(s) in parentheses before each numbered program unit name identify its type (i.e., main program, block data, subroutine, etc.).

```
Key: B  - Block Data
     CH - Character Function
     I  - Integer Function
     M  - Main Program
     R  - Real Function
     S  - Subroutine

 1. (M )  ACHILE
             FETCH  FIND   GET    HEADER INITPL INTER  NAMLST
             NUMSTR PLOT   TERMPL WHICH
 2. (S )  CHEQUE
 3. (B )  DFAULT
 4. (S )  FETCH
             CHEQUE
 5. (I )  FIND
 6. (S )  GET
             LENGTH NUMBER UPCASE
 7. (S )  GRAP
             GRAF   RESET  XGRAXS XNONUM XTICKS YGRAXS YNONUM
             YTICKS
```

```
 8. (S )  HEADER
             LENGTH
 9. (S )  INITPL
             BASALF GRACE  HEIGHT INTAXS MIXALF MX3ALF MX4ALF
             MX5ALF NOBRDR NOCHEK PAGE   TRIPLX VDESCP VSTART
             YAXANG
10. (S )  INTER
11. (I )  LENGTH
12. (S )  NAMLST
             GET    LENGTH NUMBER
13. (R )  NUMBER
14. (CH)  NUMSTR
15. (S )  PLOT
             AREA2D BLNK1  CHNDOT CHNDSH CURVE  DASH   DOT
             ENDPL  FRAME  GRAP   HEADIN LEGEND LEGLIN LINES
             MYLEGN RESET  XLEGND XNAME  YLEGND YNAME
16. (S )  SORT
17. (S )  TERMPL
             DONEPL
18. (S )  UPCASE
19. (S )  WHICH
             SORT   UPCASE
```

B.3.6 Program Units Calling Each Subprogram

This section lists which program units call each subprogram (subroutine or function) in ACHILES. This table is the inverse of the previous table. The portion titled "Internal Subprograms" lists which ACHILES program units call each ACHILES subprogram, while the portion titled "External Subprograms" lists which ACHILES program units call each DISSPLA graphics library subprogram. The character(s) in parentheses before each numbered program unit name identify its type (i.e., main program, block data, subroutine, etc.).

```
Key: B  - Block Data
     CH - Character Function
     I  - Integer Function
     M  - Main Program
     R  - Real Function
     S  - Subroutine

*** Internal subprograms ***

 1. (M )  ACHILE
 2. (S )  CHEQUE
             FETCH
 3. (B )  DFAULT
 4. (S )  FETCH
             ACHILE
 5. (I )  FIND
             ACHILE
```

```
 6. (S )  GET
             ACHILE    NAMLST
 7. (S )  GRAP
             PLOT
 8. (S )  HEADER
             ACHILE
 9. (S )  INITPL
             ACHILE
10. (S )  INTER
             ACHILE
11. (I )  LENGTH
             GET       HEADER    NAMLST
12. (S )  NAMLST
             ACHILE
13. (R )  NUMBER
             GET       NAMLST
14. (CH)  NUMSTR
             ACHILE
15. (S )  PLOT
             ACHILE
16. (S )  SORT
             WHICH
17. (S )  TERMPL
             ACHILE
18. (S )  UPCASE
             GET       WHICH
19. (S )  WHICH
             ACHILE

*** External subprograms ***

20. (S )  AREA2D
             PLOT
21. (S )  BASALF
             INITPL
22. (S )  BLNK1
             PLOT
23. (S )  CHNDOT
             PLOT
24. (S )  CHNDSH
             PLOT
25. (S )  CURVE
             PLOT
26. (S )  DASH
             PLOT
27. (S )  DONEPL
             TERMPL
28. (S )  DOT
             PLOT
29. (S )  ENDPL
             PLOT
30. (S )  FRAME
             PLOT
```

31. (S) GRACE
INITPL
32. (S) GRAF
GRAP
33. (S) HEADIN
PLOT
34. (S) HEIGHT
INITPL
35. (S) INTAXS
INITPL
36. (S) LEGEND
PLOT
37. (S) LEGLIN
PLOT
38. (S) LINES
PLOT
39. (S) MIXALF
INITPL
40. (S) MX3ALF
INITPL
41. (S) MX4ALF
INITPL
42. (S) MX5ALF
INITPL
43. (S) MYLEGN
PLOT
44. (S) NOBRDR
INITPL
45. (S) NOCHEK
INITPL
46. (S) PAGE
INITPL
47. (S) RESET
GRAP PLOT
48. (S) TRIPLX
INITPL
49. (S) VDESCP
INITPL
50. (S) VSTART
INITPL
51. (S) XGRAXS
GRAP
52. (R) XLEGND
PLOT
53. (S) XNAME
PLOT
54. (S) XNONUM
GRAP
55. (S) XTICKS
GRAP
56. (S) YAXANG
INITPL
57. (S) YGRAXS
GRAP

58. (R) YLEGND
PLOT
59. (S) YNAME
PLOT
60. (S) YNONUM
GRAP
61. (S) YTICKS
GRAP

B.3.7 PARAMETER Statements

PARAMETER statements are used in ACHILES to define array sizes. All the arrays in ACHILES have been dimensioned large enough to run the sample problems described in Chapter 6, but have been set small enough so that ACHILES will fit in the memory of all the computers mentioned in Appendix C (both the VAX-11 and the CRAY-1 have virtual memory, while the CDC CYBER 76 at SNLA has a maximum of 162 K words of small core memory available). To change the size of all the arrays in ACHILES that are concerned with a certain item, it is necessary only to modify all the corresponding PARAMETER statements. For example, the maximum number of data points plotted per graph can be increased from 500 to 1000 by changing "NPTS = 500" to "NPTS = 1000" in all the PARAMETER statements in ACHILES where NPTS is set. There is a set of PARAMETER statements near the top of most program units. Each set is exactly alike, so that this modification can be done simply by a global substitution.

The symbolic names of constants set in PARAMETER statements in ACHILES are listed below, along with the values to which they are set and a short description of what each one represents. All of the symbolic constants can be set to any value desired by the user as long as three conditions are met: (1) ACHILES must fit in the computer's memory, (2) the value of the constant must be positive (an array cannot be dimensioned to zero or less), and (3) if the symbolic constant is NC, NF, NG, NJ, NS, NV, NSC, or NSMP, then its value should be greater than or equal to that of the HECTR symbolic constant of the same name. Typically, symbolic constants defined in PARAMETER statements in ACHILES are set to larger values than the corresponding constants in HECTR. This has been done to allow ACHILES to handle changes in HECTR's limits with a minimum of effort, and also because the arrays in ACHILES take up little space when dimensioned by these constants. The symbolic constants in ACHILES have been set to larger values than we have needed to run any problems with HECTR. If the user is running on a computer with virtual memory, we recommend increasing the value of NPTS to at least 1000, as the typical resolution of a good quality plotting device is around this number. Finally, it should be noted that NNV cannot be changed and NCOLS cannot be decreased without also changing other coding in ACHILES.

NC	=	40	(maximum number of compartments)
NF	=	5	(maximum number of fan paths)
NG	=	4	(number of gas species: H_2O, N_2, O_2 and H_2)
NJ	=	80	(maximum number of flow junctions)
NS	=	60	(maximum number of surfaces)
NV	=	3	(maximum number of suppression pool vents)
NICE	=	4	(maximum number of ice compartments in an ice condenser)
NSC	=	2	(maximum number of compartments in which sprays originate)
NSMP	=	10	(maximum number of sumps)
NNV	=	37	(number of pseudo-NAMELIST variables)
NPTS	=	500	(maximum number of data points plotted per graph)
NCOLS	=	7	(maximum number of graphs that can be produced in one pass of data reads)

B.4 Reference

1. American National Standard Programming Language FORTRAN, American National Standards Institute, New York, New York, 1978.

APPENDIX C

CONTROL LANGUAGE

CONTENTS

C. CONTROL LANGUAGE

C.1 Introduction

HECTR and ACHILES have been written to be as portable as possible between computers. HECTR is written in ANSI FORTRAN 77 and should execute properly on any computer that runs the full language.[1] Most of ACHILES, the output processor for HECTR, is also written in ANSI FORTRAN 77. However, as of January 1, 1984, the plot package used by ACHILES, DISSPLA, did not have an ANSI FORTRAN 77 version available.[2] Thus, it is necessary to convert a set of character strings into a set of Hollerith constants in subroutine PLOT so that ACHILES can interface properly with the DISSPLA plot package.

In this appendix, we describe procedures for running HECTR and ACHILES on three different computers at SNLA: (1) a VAX-11 running VMS, (2) a CRAY-1 running COS, and (3) a Control Data Corporation (CDC) CYBER 76 running SCOPE 2. These three systems are the major scientific computer systems used at SNLA. These examples may also provide guidance in setting up the control language for running HECTR and ACHILES at other installations, but some site-specific differences should be expected.

Both HECTR and ACHILES require special libraries. HECTR must be linked with the SLATEC Common Mathematical Subprogram Library so that an equation root finder, a linear system solver, and an ordinary differential equation system solver can be accessed.[3] At SNLA, this library should be available on all scientific systems. For other installations, which may not have this library available, the user can append the source of the SLATEC subprograms required by HECTR onto the end of the HECTR source and then perform a normal compilation and link. ACHILES uses the DISSPLA package to produce graphs. Again, this package should be available on all scientific systems at SNLA. If this package is not available on the user's computer, then ACHILES can still be used to produce tables but will not be able to create any plots. All calls to DISSPLA routines in ACHILES have been localized to four subroutines (INITPL, TERMPL, PLOT, and GRAP). These four subroutines can be easily replaced by dummy subprograms so that ACHILES can be compiled and linked normally if DISSPLA is not available on the user's computer.

C.2 VAX-11 Running VMS

HECTR and ACHILES can be run either interactively or in a background mode on a VAX-11. Since the VAX-11 has a short computer word length (4 bytes), both the number of significant digits available for variables (hence the precision of arithmetic calculations) and the computational speed will be

low relative to computers like the CRAY-1 and the CDC CYBER 76 (which have computer word lengths of 8 and 10 bytes, respectively). HECTR performs all calculations in single precision; therefore, there may be a loss of accuracy on a VAX-11 for calculations requiring large numbers of time-steps. This will be especially true if the sprays are on for some part of the run (see Section 6.1, which discusses the simple two-compartment sample problem). We have typically run short problems interactively on a VAX-11 and used the CRAY-1 and the CDC CYBER 76 for CPU-intensive production runs.

We will now explain exactly how to compile, link, and run HECTR and ACHILES interactively on a VAX-11, assuming that the user has the FORTRAN source files for the two programs and a data file for HECTR. We will show selected portions of a sample interactive session, with the system, HECTR, and ACHILES prompts and responses underlined. Any typing that is not underlined (and is not a part of the description of the prompts) must be entered by the user into the computer. For convenience, assume that the files HECTR.FOR and ACHILES.FOR contain the FORTRAN source of HECTR and ACHILES, respectively. Also, assume that the file SLATEC.FOR contains the FORTRAN source of the routines from the SLATEC library used by HECTR. Finally, assume that the file TC.DAT contains the HECTR input data for the simple two-compartment sample problem presented in Section 6.1.1. This file contains the input for the problem geometry (unit URD) and the initial conditions and the accident scenario (unit UIC) concatenated together (it should NOT contain the initial NAMELIST-type input).

At SNLA, executing the commands

```
$ @sd:[mathlib]mathsysms
$ @sys$psyms:graphsyms
```

defines a series of symbols relating to the math and graphics libraries, respectively. This action needs to be done before attempting to compile and link HECTR and ACHILES. Typically, these commands are placed in the user's LOGIN.COM file so that they will be executed each time the user logs onto the computer. Once the appropriate symbols have been defined by executing the above commands, the user can compile and link HECTR as follows:

```
$ fortran hectr
$ link hectr,'slatec'/library
$ delete hectr.obj;*
```

This procedure creates both an object file (HECTR.OBJ) and an executable file (HECTR.EXE). The object file is no longer necessary after it has been linked, so it can be deleted. A very similar procedure is used to compile and link ACHILES:

```
$ fortran achiles
$ link achiles,'LINK_DISS','LINK_xxx'
$ delete achiles.obj;*
```

Here, xxx is a 3-letter device code that indicates on what kind of device the graphics produced by ACHILES will be plotted. For example, if ACHILES is to produce graphics for a Tektronix terminal, then the device code would be TEK.

If the user does not have the SLATEC library available on his or her computer, an executable HECTR file can still be produced by performing

```
$ append slatec.for hectr.for
$ fortran hectr
$ link hectr
$ delete hectr.obj;*
```

which appends the file containing the SLATEC routines onto the end of the HECTR FORTRAN source. If the user does not have the DISSPLA library available, then two options for ACHILES are possible. The subroutines INITPL, TERMPL, PLOT, and GRAP can be dummied out by deleting all of the executable statements in them; then ACHILES can be compiled and linked without any special libraries attached. This allows ACHILES to produce tables but not plots. The alternative is to rewrite the above subroutines using a graphics package that is available on the user's computer.

Running HECTR and ACHILES on VMS is very simple. For example, to run the simple two-compartment problem of Section 6.1 and produce only tables from ACHILES, the following actions are needed:

```
$ assign tc.dat for004
$ run hectr
$

INITIAL COMPARTMENT CONDITIONS AT      0.000 SECONDS ARE:

COMP #   TEMP    PRESSURE    XH2O          XN2          XO2          XH2

                    . . .

FORTRAN STOP
$ run achiles
$
```

```
------
TABLES
------
all
skip
all
quit
FORTRAN STOP
$
```

Here, the file TC.DAT is assigned to logical unit number 4, which is the default unit in HECTR from which the input about the problem geometry, the initial conditions, and the accident scenario (described in Sections 4.2.2 and 4.2.3) is read. The dollar sign immediately following the line "run hectr" is a required user input that must be typed in at the terminal before HECTR will continue. The dollar sign marks the end of the initial NAMELIST-type input (described in Section 4.2.1), which is always read from unit 5. In this example, there was no such input except for the dollar sign terminator, but this need not be the case. For example, entering the statement "UOM=1" on a separate line before the dollar sign results in redirecting the HECTR output from the terminal into the file FOR001.DAT, which HECTR will create. Other useful options are setting "BATCH=TRUE", which causes HECTR to echo the input data it reads (HECTR defaults to not doing this on a VAX) and specifying "UOA=9", which permits HECTR to write out the values of additional heat-transfer timestep variables (see Section 5.2.3.1) to unit 9 so that ACHILES can later tabulate and plot them (the default is to not write out these values). Running HECTR as shown above creates the binary files FOR007.DAT and FOR008.DAT, which contain a history of the values of the major heat transfer and flow-timestep variables, respectively. Next, ACHILES is run. The user again enters a dollar sign, which signifies the end of the ACHILES NAMELIST-type input. ACHILES then prompts for input for table specifications. In this example, tables of the two compartments' pressures, temperatures, gas densities, and mole fractions versus time and the gas velocity in the flow junction versus time will be produced. These tables, along with header information, will be written to the file FOR010.DAT.

C.3 CRAY-1 Running COS

A sample deck for running HECTR and ACHILES on the CRAY-1 is presented below. The notation {eor} indicates an end-of-record card and <...> indicates that a file is to be included at this point as described by the text within the angle brackets. Underlined text indicates that this data is to be replaced by appropriate information, as described later in this section.

```
jobname,T60,STSCZ,SN.                    user's full name - box number
USER(user number,password)
CHARGE(case number)
SEND,'user's full name',box number.
*.
*. REDEFINE $OUT CHARACTERISTICS
*.
DISPOSE,DN=$OUT,DC=SC.
ASSIGN,DN=$OUT,DC=PR,A=FT06,LM=10000.
DISPOSE,DN=$OUT,SDN=LPOUT,DC=ST,DEFER,TEXT='
    'CTASK. ROUTE,LPOUT,DC=PR,TID=sitecode.'.
*.
*. ACQUIRE EXTERNAL (MARCH) INPUT
*.
ACQUIRE,DN=TAPE1,UQ,TEXT='
    'GET(permanent file name/UN=alternate user number)
    CTASK.'.
DELETE,DN=TAPE1.
ASSIGN,DN=TAPE1,A=FT01.
*.
*. ACQUIRE THE HECTR FORTRAN SOURCE FILE
*.
ACQUIRE,DN=HECTR,UQ,TEXT='
    'ATTACH(HECTR/UN=alternate user number) CTASK.'.
DELETE,DN=HECTR.
*.
*. COMPILE, LINK AND RUN HECTR
*.
ACCESS,DN=SLATEC,ID=MATHCRA.
CFT,I=HECTR,ON=HZ.
LDR,LIB=$SCILIB: SLATEC,SET=INDEF,MAP=PART.
*.
SKIPF.
*.
*. SAVE HECTR RESULTS ON TAPE
*.
REWIND,DN=TAPE7:TAPE8:TAPE9.
COPYD,I=FT07,O=TAPE.
COPYD,I=FT08,O=TAPE.
COPYD,I=FT09,O=TAPE.
DISPOSE,DN=TAPE,DC=ST,DF=TR,TEXT='
    'LABEL,TAPE,VSN=tape number,L=HECTR,D=GE,F=S,W,PO=W.
    CTASK.'.
*.
*. ACQUIRE THE ACHILES FORTRAN SOURCE FILE
*.
ACQUIRE,DN=ACHILES,UQ,TEXT='
    'GET(ACHILES/UN=alternate user number) CTASK.'.
DELETE,DN=ACHILES.
*.
*. COMPILE, LINK AND RUN ACHILES
*.
```

```
ACCESS,DN=PLOTPRC,ID=PLOTCRA.
LIBRARY,DN=*: PLOTPRC.
CFT,I=ACHILES,ON=HZ.
REWIND,DN=$OUT.
COPYD,I=$OUT,O=OUT.
DISS,MET,M=PART,P=INDEF.
*.
COPYD,I=FT10,O=OUT.
*.
*. PRODUCE VERSATEC PLOTS
*.
POST,TAPE55,HC1.
COMQ,TAPE77,HC1,(CS=site code).
REWIND,DN=TAPE55.
*.
*. PRODUCE MICROFICHE PLOTS
*.
POST,TAPE55,24L.
COMQ,TAPE77,DIC,(FICHE),T='HECTR-TEST-CASE'.
*.
*. SEND HECTR AND ACHILES OUTPUT TO MICROFICHE
*.
COMQ,$OUT,DAT,T='HECTR-TEST-CASE'.
*.
*. SEND HECTR OUTPUT AND ACHILES HEADER OUTPUT TO A
LINEPRINTER
*.
REWIND,DN=OUT.
COPYD,I=OUT,O=$OUT.
DISPOSE,DN=$OUT,SDN=LPOUT,DC=ST,DEFER,TEXT=^
   'CTASK. ROUTE,LPOUT,DC=PR,TID=site code.'.
EXIT.
*.
*. ERROR EXIT
*.
DUMPJOB.
DEBUG,BLOCKS.
{eor}
<HECTR initial NAMELIST-type input of Section 4.2.1>
<HECTR problem geometry input of Section 4.2.2>
<HECTR initial conditions and accident scenario input of Sec-
tion 4.2.3>
{eor}
<ACHILES NAMELIST-type input of Section 4.3.1>
<ACHILES table and plot input of Section 4.3.2>
```

A large part of the control language concerns redirecting various portions of the HECTR and ACHILES output to different physical devices. In particular, HECTR binary output is saved on magnetic tape before being processed by ACHILES. The HECTR output and the ACHILES header information are sent both to microfiche and to a lineprinter, while the ACHILES

table output is sent only to microfiche. Graphs produced by ACHILES are plotted on both microfiche and a Versatec plotter. Thus, all output, except the dayfile, will be copied onto microfiche, while all HECTR output and all ACHILES output, except the tables, will be sent either to a lineprinter or to a Versatec plotter. The rest of this section will indicate some specifics to be aware of in the deck presented above.

The first four lines of the control language identify the user to the system. Specifying the SN parameter on the job card is necessary only if a magnetic tape is being used during the job. The first ASSIGN statement sets the size limit of the output dataset $OUT to a large value so that large tables can be produced with ACHILES without causing the job to abort. The second DISPOSE statement causes the contents of the file $OUT to be sent to the site indicated if an abnormal termination of the job occurs. For example, specifying RO as a site code will send the contents of $OUT to one of the RJET lineprinters in building 823 at SNLA. A copy of this statement, located just before the EXIT card, causes the contents of the file $OUT to be sent to the site indicated on normal job termination. The local file TAPE1 contains external (MARCH) source-term input for HECTR (this data will be recognized by HECTR if the initial NAMELIST-type input contains the statement "MRCHSC=n" where n is the number of a compartment in the HECTR input [see Section 4.4.2]). Note that the unit FT01 has been changed to the name TAPE1 (similarly for all the other units referenced in the control language). This has been done to avoid possible problems with the COS interface to FORTRAN 77. TAPE1 (in this example) is an indirect access file that is acquired from the front end machine with a GET command. ACHILES is also saved as an indirect access file. HECTR, however, is sufficiently large so that it is saved as a direct access file and so must be acquired with an ATTACH command. HECTR reads its input from $IN (the standard input) and writes its output to $OUT. The contents of $OUT are copied to the file OUT after executing HECTR; OUT contains the text that is to be sent to the lineprinter at the end of the job. HECTR produces one or more of the binary files TAPE7, TAPE8, and TAPE9 during a run, which contain time histories of variables calculated by HECTR that are to be processed by ACHILES. It is often useful to save these files on magnetic tape (or other offline storage devices) in case of later requests for information from a run.

ACHILES is linked with the DISSPLA graphics library using the DISS procedure. ACHILES reads user input from $IN and writes header information by default to both $OUT and TAPE10. All tables are written only to $OUT, however. The word MET in the line "DISS,MET,..." indicates that ACHILES graphic output will be written to a Basic Graphics Package metafile (TAPE55),

which can then be postprocessed to produce output on any number of devices. Here, the postprocessor (POST), using the Sandia Virtual Device Interface, is run twice on the contents of the metafile. The first time that POST is executed, output is produced for a Versatec plotter; executing POST the second time creates graphics output printed on microfiche. Finally, the last COMQ command near the bottom of the control language sends the nongraphics contents of the file $OUT to microfiche. For both cases, the microfiche is titled "HECTR-TEST-CASE". All blanks in these titles will be eliminated so it is necessary to use some other character as a separator. Also, a period or a dollar sign in a title should never be used, otherwise errors can occur. An end-of-record card separates the control language from the HECTR input, and another end-of-record card delimits the ACHILES input.

Once the HECTR results have been saved on magnetic tape, the files can be retrieved anytime, and ACHILES can be run independently. The previously described control language can be used for this purpose just by replacing the sections marked "ACQUIRE EXTERNAL (MARCH) INPUT" through "SAVE HECTR RESULTS ON TAPE" with the following directives (and deleting the first end-of-record card and the HECTR input that follows):

```
*.
*. GET HECTR RESULTS FROM TAPE
*.
ACQUIRE,DN=TAPE,DF=TR,UQ,TEXT=^
     'LABEL,TAPE,VSN=tape number,L=HECTR,D=GE,F=S,R,PO=R.
     CTASK.'.
DELETE,DN=TAPE.
COPYF,I=TAPE,O=FT07.
COPYF,I=TAPE,O=FT08.
COPYF,I=TAPE,O=FT09.
```

C.4 CDC CYBER 76 Running SCOPE 2

A sample deck for running HECTR and ACHILES on the CDC CYBER 76 is presented below. The notation {eor} indicates an end-of-record card and <...> indicates that a file is to be included at this point as described by the text within the angle brackets. Also, underlined text indicates that this data is to be replaced by appropriate information, as described later in this section.

```
jobname,T60,SN.                    user's full name - box number
USER(user number,password)
CHARGE(case number)
SEND,user's full name,box number.
COMMENT.
```

```
COMMENT. REDEFINE OUTPUT CHARACTERISTICS
COMMENT.
DISPOSE,OUTPUT,*PR,ST=NOSEsite code.
COMMENT.
COMMENT. ACQUIRE EXTERNAL (MARCH) INPUT
COMMENT.
FILE,TAPE1,RT=Z,FL=80
PFGET(TAPE1,permanent file name,AU=alternate user number)
COMMENT.
COMMENT. ACQUIRE THE HECTR FORTRAN SOURCE FILE
COMMENT.
FILE,HECTR,RT=Z,FL=80.
PFGET(HECTR,permanent file name,AU=alternate user number)
COMMENT.
COMMENT. COMPILE, LINK AND RUN HECTR
COMMENT.
COPYS,INPUT,TAPE5.
REWIND,TAPE5.
ATTACH,SLATEC.
FTN5,I=HECTR,ANSI,OPT=0,L=0.
LDSET,LIB=SLATEC,PRESET=NGINF.
LGO,PL=10000.
EXIT(U)
REWIND,LGO.
REWIND,TAPE6.
COPY,TAPE6,OUTPUT.
REWIND,TAPE6.
COPY,TAPE6,FISH.
COMMENT.
COMMENT. SAVE HECTR RESULTS ON TAPE
COMMENT.
STAGE,TAPE,VSN=tape number,GE,POST.
LABEL,TAPE,W,L=HECTR.
REWIND,TAPE7,TAPE8,TAPE9.
COPY,TAPE7,TAPE.
COPY,TAPE8,TAPE.
COPY,TAPE9,TAPE.
RETURN,TAPE.
COMMENT.
COMMENT. ACQUIRE THE ACHILES FORTRAN SOURCE FILE
COMMENT.
FILE,ACHILES,RT=Z,FL=80.
PFGET(ACHILES,permanent file name,AU=alternate user number)
COMMENT.
COMMENT  COMPILE, LINK AND RUN ACHILES
COMMENT.
REWIND,TAPE5,TAPE6.
COPYS,INPUT,TAPE5.
REWIND,TAPE5.
FTN5,I=ACHILES,ANSI,OPT=0,L=0.
PFGET(DISS,AU=PLOTLIB)
BEGIN,DISS,DISS,MET,E=NOGO,P=NGINF.
RETURN,DISS.
```

```
DISSABS,PL=100000.
EXIT(U)
REWIND,TAPE10.
COPY,TAPE10,OUTPUT.
REWIND,TAPE6.
COPY,TAPE6,FISH.
PFGET(POST,AU=PLOTLIB)
COMMENT.
COMMENT. PRODUCE VERSATEC PLOTS
COMMENT.
BEGIN,POST,POST,TAPE55,HC1.
PFGET(RHCNBPC,AU=PLOTLIB)
BEGIN,RHC,RHCNBPC.
RETURN,RHCNBPC.
COMQ,TAPE76,HC1,CS=site code.
RETURN,VDI,POSTM.
COMMENT.
COMMENT. PRODUCE MICROFICHE PLOTS
COMMENT.
BEGIN,POST,POST,TAPE55,24L.
COMQ,TAPE77,DIC,FICHE.                    HECTR TEST CASE
COMMENT.
COMMENT. SEND HECTR AND ACHILES OUTPUT TO MICROFICHE
COMMENT.
CDF,FISH.
FICHE,FISH.                               HECTR TEST CASE
COMMENT.
COMMENT. SEND HECTR OUTPUT AND ACHILES HEADER OUTPUT TO A
COMMENT. LINEPRINTER
COMMENT.
DISPOSE,OUTPUT,*PR,ST=NOSEsite code
EXIT.
{eor}
<HECTR initial NAMELIST-type input of Section 4.2.1>
<HECTR problem geometry input of Section 4.2.2>
<HECTR initial conditions and accident scenario input of Sec-
tion 4.2.3>
{eor}
<ACHILES NAMELIST-type input of Section 4.3.1>
<ACHILES table and plot input of Section 4.3.2>
```

A large part of the control language concerns redirecting various portions of the HECTR and ACHILES output to different physical devices. In particular, HECTR binary output is saved on magnetic tape before being processed by ACHILES. The HECTR output and the ACHILES header information are sent both to microfiche and to a lineprinter, while the ACHILES table output is sent only to microfiche. Graphs produced by ACHILES are plotted on both microfiche and a Versatec plotter. Thus, all output, including the dayfile, will be copied onto microfiche, while all HECTR output and all ACHILES output, except the tables, will be printed on either a lineprinter or

a Versatec plotter. The rest of this section indicates some specifics to be aware of in the deck presented above.

The first four lines of the control language identify the user to the system. Specifying the SN parameter on the job card is necessary only if a magnetic tape is being used during the job. The DISPOSE statement causes the contents of the file OUTPUT to be sent to the site indicated at the termination of the job. For example, specifying RO as a site code will send the contents of OUTPUT to one of the RJET lineprinters in building 823 at SNLA. The local file TAPE1 contains external (MARCH) source-term input for HECTR (this data will be recognized by HECTR if the initial NAMELIST-type input contains the statement "MRCHSC=n" where n is the number of a compartment in the HECTR input [see Section 4.4.2]). TAPE1 (as well as HECTR and ACHILES) has a file record type of Z so that it can be accessed by both the CRAY-1 and the CDC CYBER 76. HECTR reads its input from TAPE5 and writes its output to TAPE6. The contents of TAPE6 are copied to the files OUTPUT and FISH, where FISH will contain the text that is to be sent to microfiche. HECTR produces one or more of the binary files TAPE7, TAPE8, and TAPE9 during a run, which contain time histories of variables calculated by HECTR to be processed by ACHILES. It is often useful to save these files on magnetic tape (or other offline storage devices) in case of later requests for information from a run.

ACHILES is linked with the DISSPLA graphics library using the DISS procedure. ACHILES reads user input from TAPE5 and writes header information by default to both TAPE6 and TAPE10. All tables are written only to TAPE6, however. The word MET in the line "BEGIN,DISS,DISS,MET,..." indicates that ACHILES graphic output will be written to a Basic Graphics Package metafile (TAPE55), which can then be postprocessed to produce output on any number of devices. Here, the postprocessor (POST), using the Sandia Virtual Device Interface is run twice on the contents of the metafile. The first time that POST is executed, output is produced for a Versatec plotter; executing POST the second time creates graphics output that is printed on microfiche. Finally, the FICHE command near the bottom of the control language sends the nongraphics contents of the file FISH to microfiche. For both cases, the microfiche is titled "HECTR TEST CASE". An end-of-record card separates the control language from the HECTR input, and another end-of-record card delimits the ACHILES input.

Once the HECTR results have been saved on magnetic tape, the files can be retrieved anytime, and ACHILES can be run independently. The previously described control language can be used for this purpose by replacing the sections marked "ACQUIRE EXTERNAL (MARCH) INPUT" through "SAVE HECTR RESULTS ON TAPE" with the following directives (and by deleting the first end-of-record card and the HECTR input that follows):

```
COMMENT.
COMMENT. GET HECTR RESULTS FROM TAPE
COMMENT.
STAGE,TAPE,VSN=tape number,GE,PRE.
LABEL,TAPE,R,L=HECTR.
COPYP,TAPE,TAPE7.
COPYP,TAPE,TAPE8.
COPYP,TAPE,TAPE9.
RETURN,TAPE.
```

C.5 References

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2. DISSPLA User's Manual (Version 9.0), Integrated Software Systems Corporation, San Diego, California, 1981.

3. The SLATEC Common Mathematical Subprogram Library: SNLA IMPLEMENTATION, SAND80-2792, Sandia National Laboratories, December 1980.

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REPORT NUMBER (Assigned by TIDC and Vol. No., if any)

NUREG/CR-3913
SAND84-1522

2 TITLE AND SUBTITLE

HECTR Version 1.0 User's Manual

3 LEAVE BLANK

4 DATE REPORT COMPLETED

MONTH	YEAR
January	1985

5 AUTHOR(S)

Allen L. Camp
Michael J. Wester
Susan E. Dingman

6 DATE REPORT ISSUED

MONTH	YEAR
February	1985

7 PERFORMING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)

Severe Accident Containment Response
Division 6427
Sandia National Laboratories
Albuquerque, NM 87185

8 PROJECT TASK WORK UNIT NUMBER

9 FIN OR GRANT NUMBER

A1246

10 SPONSORING ORGANIZATION NAME AND MAILING ADDRESS (Include Zip Code)

Containment Systems Research Branch
Office of Nuclear Regulatory Research
US Nuclear Regulatory Commission
Washington, DC 20555

11a TYPE OF REPORT

Final Report

b PERIOD COVERED (Inclusive dates)

12 SUPPLEMENTARY NOTES

13 ABSTRACT (200 words or less)

This report describes the features and use of HECTR Version 1.0. HECTR is a relatively fast-running, lumped-volume containment analysis computer program that is most useful for performing parametric studies. The main purpose of HECTR is to analyze nuclear reactor accidents involving the transport and combustion of hydrogen, but HECTR can also function as an experiment analysis tool and can solve a limited set of other types of containment problems. HECTR Version 1.0 has been particularly tailored to analyze accidents in ice-condenser PWR and Mark III BWR containments. HECTR is designed for flexibility and provides for user control of many important parameters, particularly those related to hydrogen combustion. Built-in correlations and default values of key parameters are also provided.

14 DOCUMENT ANALYSIS - a KEYWORDS/DESCRIPTORS

b IDENTIFIERS/OPEN-ENDED TERMS

15 AVAILABILITY STATEMENT

Unlimited

16 SECURITY CLASSIFICATION

(This page)
Unclassified

(This report)
Unclassified

17 NUMBER OF PAGES

18 PRICE

☆U.S. GOVERNMENT PRINTING OFFICE 1985—576-051/20,009