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User's Manual for CONTAIN 1.1: A Computer Code for Severe Nuclear Reactor Accident Containment Analysis

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ABSTRACT

The CONTAIN 1.1 computer code is an integrated analysis tool used for predicting the physical, chemical, and radiological conditions inside a containment building following the release of radioactive material from the primary system in a severe reactor accident. It can also predict the source term to the environment. CONTAIN is the U.S. Nuclear Regulatory Commission's principal best-estimate, mechanistic containment analysis code for severe accidents. CONTAIN 1.1 is intended to replace the earlier CONTAIN 1.0, which was released in 1984. The purpose of this User's Manual is to provide a basic understanding of the features and models in CONTAIN 1.1 so that users can prepare reasonable input and understand the output and its significance for particular applications. Besides input instructions, the User's Manual also contains brief descriptions of the models. CONTAIN 1.1 is a highly flexible and modular code that can run problems that are either quite simple or highly complex. An important aspect of CONTAIN is that the interactions among thermal-hydraulic phenomena, aerosol behavior, and fission product behavior are taken into account. Both light water reactors and liquid metal reactors can be modeled with CONTAIN 1.1, though many of the sodium-specific models are not documented in this report (a separate CONTAIN-LMR supplement serves this purpose). The code includes atmospheric models for steam/air thermodynamics, intercell flows, condensation/evaporation on structures and aerosols, aerosol behavior, and gas combustion. It also includes models for reactor cavity phenomena such as core-concrete interactions and coolant pool boiling. Heat conduction in structures, fission product decay and transport, radioactive heating, and the thermal-hydraulic and fission product decontamination aspects of engineered safety features are also modeled. To the extent possible, the best available models for severe accident phenomena have been incorporated into CONTAIN, but it is intrinsic to the nature of severe accident analysis that significant uncertainty exists regarding numerous phenomena. In those cases, sensitivity studies can be performed with CONTAIN by means of user-specified input parameters. Thus, the code can be viewed as a tool designed to assist the knowledgeable reactor safety analyst in evaluating the consequences of specific modeling and parameter assumptions.

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ACKNOWLEDGMENTS

The CONTAIN computer code was developed at Sandia National Laboratories under the auspices of the United States Nuclear Regulatory Commission (USNRC) as part of its Severe Accident Research Program. It is intended to embody research results from many different sources, and it would be impossible to list all of the individuals who have contributed (knowingly or not) to the development of the code. However, several people deserve specific mention as key contributors to this effort. Noteworthy among these are Dr. S. Bradley Burson, Dr. Phillip M. Wood, and Dr. Yi-Shung Chen of NRC's Accident Evaluation Branch, who, as program managers, have helped guide the project through many difficult problems.

A number of individuals at Sandia National Laboratories have made important contributions to the code, or to our understanding of it, and also deserve acknowledgment. M. J. Clauser, B. D. Harrison, F. J. Schelling, P. E. Rexroth, F. W. Sciacca, M. E. Senglaub and W. Trebilcock were part of the team that produced CONTAIN 1.0, the predecessor of the current version.

Such a large, integrated code would not have been possible if there had not been a number of high quality, stand-alone codes from which to draw models. Therefore we also acknowledge our debt to the authors of MAEROS, HECTR, SPARC, ICEDF, CORCON and VANESA, and we also express our gratitude for their assistance in understanding and adapting the models in those codes.

A number of individuals have made valuable contributions to the testing and shakedown of CONTAIN 1.1; these include Albert Gu, David Louie, Nancy Russell, and, especially, Jack Tills.

Special thanks also goes to Marti Morgan for consistently excellent secretarial support.

Finally, we would like to thank the numerous researchers in the U.S. and abroad who have utilized CONTAIN, identified problems, suggested improvements, and in general kept the developers on track and in the real world. We apologize to them for whatever code bugs they were bitten by in the past, and assure them that the current version of the code is now bug-free.

NOMENCLATURE

Symbol	Definition	Units
A	Area	m^2
C_{FC}	Turbulent flow coefficient	none
C_{LFC}	Linear flow coefficient	none
C_p	Specific heat at constant pressure	J/(kg-K)
C_v	Specific heat at constant volume	J/(kg-K)
D_v	Diffusivity of the vapor	m^2/s
F_{ij}	View factor from surface i to surface j	none
g	Acceleration due to gravity	m/s^2
H	Specific enthalpy	J/kg
$H_{\ell g}$	Heat of vaporization	J/kg
$H_{\ell v}$	Difference between the specific enthalpy of the bulk vapor and the specific enthalpy of the liquid at their respective temperatures	J/kg
H_{sl}	Heat of fusion	J/kg
h	Heat transfer coefficient	$W/(m^2-K)$
h_i	Cell or flow path elevation	m
J	Mass flux	$kg/(m^2-s)$
K	Mass transfer coefficient	(kmol-s)/(kg-m)
k	Thermal conductivity	J/(m-K-s)
L	Length	m
M	Molecular weight	kg/(kg-mol)
m	Mass	kg
P	Pressure	Pa
$P_{i,0}$	Debris power in cell i	W
P_{vb}	Partial pressure of vapor in atmosphere	Pa
P_{vw}	Saturation pressure at temperature T_{wall}	Pa
p	Specific power	W/kg

NOMENCLATURE (Continued)

Symbol	Definition	Units
Q	Rate of energy transfer as heat	J/s
q	Heat flux	$J/(m^2\text{-}s)$
R	Universal gas constant	J/(kg-mol-K)
r	Release rate	s^{-1}
T	Temperature	K
t	Time	s
U	Internal energy	J
u	Specific internal energy	J/kg
V	Volume	m^3
v	Velocity	m/s
W	Mass flow rate	kg/s
X	Mole fraction	none
x,y,z	Distance along Cartesian coordinates	m
α_g	Gas absorptivity	none
β_g	Coefficient of gas expansion	K^{-1}
γ	Specific heat ratio	none
δ	Thermal diffusion length	m
ϵ	Emissivity	none
ζ	Laplace constant	m
η	Effective thickness of gas film	m
μ	Viscosity	kg/(m-s)
ν	Kinematic viscosity	m^2/s
ρ	Density	kg/m^3
σ	Stefan-Boltzmann constant	$J/(s\text{-}m^2\text{-}K^4)$

Subscript	Description
a	averaged quantity
c	convection
d	dense spherical particle
dry	drywell
dw	change in quantity between drywell and wetwell
eff	effective
evap	evaporation
g	gas mixture
ℓ	liquid
r	radiation
s	particle or surface
sat	saturation
sup	suppression pool
T	total
u	upstream cell or layer right above
v	vapor
w	wall
wet	wetwell

NOMENCLATURE (Continued)

Dimensionless Parameter	Name
$Gr = \frac{L^3 \rho^2 g \beta_g \Delta T}{\mu^2}$	Grashof number
$Nu = \frac{hL}{k}$	Nusselt number
$Pr = \frac{C_p \mu}{k}$	Prandtl number
$Ra = Gr \cdot Pr$	Rayleigh number
$Re = \frac{\rho v L}{\mu}$	Reynolds number
$Sc = \frac{\mu}{\rho D_v}$	Schmidt number
$Sh = Nu \cdot (Sc/Pr)^{1/3}$	Sherwood number

1. INTRODUCTION

1.1 The Need for Severe Accident Containment Analysis

Since the inception of nuclear power as a commercial energy source, safety has been recognized as a prime consideration in the design, construction, operation, maintenance, and decommissioning of nuclear power plants. The reactor core contains a large inventory of radioactive materials that, if released to the environment, could be hazardous to the local population. Because the reactor, by definition, is also a region of potentially high energy density, consideration must be given to all possible mechanisms by which this energy might disperse any part of the radioactive inventory outside the plant. Such an occurrence is extremely unlikely because there are three sequential barriers to fission product release: the fuel cladding, the reactor vessel and primary system boundaries, and the containment building.

Nevertheless, nuclear reactor systems are so complex that dismissing the possibility that one or more of these barriers might fail would be imprudent. Probabilistic risk assessments have shown that the required multiple system failures are improbable but not negligible. The accident at Three Mile Island Unit 2 (TMI-2) demonstrated that significant core melting could occur in a commercial power reactor and that at least the first of the three barriers can be breached. The reactivity-driven explosion at Chernobyl showed that all three barriers could be breached and the public exposed to radioactivity. Although U.S. power reactors are not vulnerable to the type of energetic event that occurred at Chernobyl, that accident reinforced the perception of safety analysts that highly off-normal system and/or operator behavior, though extremely improbable, may, in fact, occur. Consequently, the United States Nuclear Regulatory Commission (NRC) has an ongoing research program, the purpose of which is to gain an understanding of the worst possible type of hypothetical reactor accidents. These are the core-melt accidents, also called "accidents beyond the design basis," or "severe accidents."

Probabilistic risk assessments have consistently shown that the dominant component of risk from the operation of commercial nuclear power plants results from this low probability, high consequence class of accidents. For this reason, severe accident analysis is an important element in the NRC's research program. However, the extreme nature of these accident sequences presents unique difficulties for the reactor safety analyst. First, unlike many other safety engineering disciplines, virtually no relevant historical record of vessel failure accidents exists from which to learn. Second, the reactor and its containment are extremely complex systems, and their designs vary substantially from one plant to another. Third, the fuel debris and the materials it contacts are expected to be subject to such severe conditions that the behavior of even small subelements of these complex systems is not easy to predict. Laboratory scale experiments improve our understanding, but it is difficult to circumvent the fundamental difficulty in severe accident analysis: extrapolation, both in physical scale and in system complexity.

All these considerations lead to two conclusions concerning research methodology. First, detailed, system-level, phenomenological computer

models are essential tools for helping the analyst understand how the reactor and its containment might respond to severe accident conditions. Second, such computational tools cannot substitute for intelligence, engineering judgement, and experimental research.

The CONTAIN computer code is an integrated analysis tool for predicting the physical, chemical, and radiological conditions inside the containment and connected buildings following the release of radioactive material from the primary system in a severe reactor accident. CONTAIN can also be used to predict release to the environment in the event of containment failure. The code does not calculate conditions inside the primary system, nor does it follow the released radionuclides beyond the containment boundaries. These calculations can be performed by other codes. (CONTAIN is, however, sufficiently flexible to be applicable to a number of nonreactor problems, such as the migration of gaseous radioisotopes in waste repositories or safety analysis of radioactive material processing facilities.)

Thus, the term "integrated analysis" does not refer to an integral treatment of the reactor/containment/environment system; rather it applies to the range of phenomena analyzed for the containment system itself. It is customary for reactor safety codes to be restricted in the type of physical phenomena analyzed. Typically, a code analyzes either thermal-hydraulic phenomena (e.g., CONTEMPT or MARCH), fission product decay (e.g., ORIGEN), or aerosol behavior (e.g., HAARM, NAUA). By contrast, CONTAIN simultaneously treats thermal-hydraulic, aerosol, and fission product behavior. This approach simplifies severe accident analysis, but, more importantly, it can provide more accurate analysis because, as illustrated in Figure 1-1, there exist a number of important closed loop feedbacks among these phenomena. Some of these interactions will be discussed in more detail later, but an example is the transport of mobile heat sources (radioactive aerosols) by pressure-driven gas flow, which occurs simultaneously with deposition of the aerosols onto containment surfaces.

CONTAIN is designed to assist the knowledgeable reactor safety analyst in evaluating the consequences of specific modeling and parameter assumptions. The models currently in the code are intended to embody the key results from severe accident research, so that the code is a vehicle for integrating knowledge gained from many different sources. Because the knowledge base is constantly being upgraded through research, the code is also designed to be modular and adaptable; that is, as improved phenomenological models are developed, tested, and validated, they can be incorporated into the code with a minimum of difficulty.

However, at any given time significant gaps exist in the knowledge base, and significant uncertainties and limitations are present in the modeling. In many cases, the judgement of the model developer is involved in making tradeoff decisions. It is impossible to anticipate all the uses of such a code. Thus, in some instances the judgement may be inapplicable, and the models may be inappropriate. It is therefore important that the analyst running the code have a good basic understanding of the models implemented in the code in order to evaluate their relevance in the specific context of the problem being run.

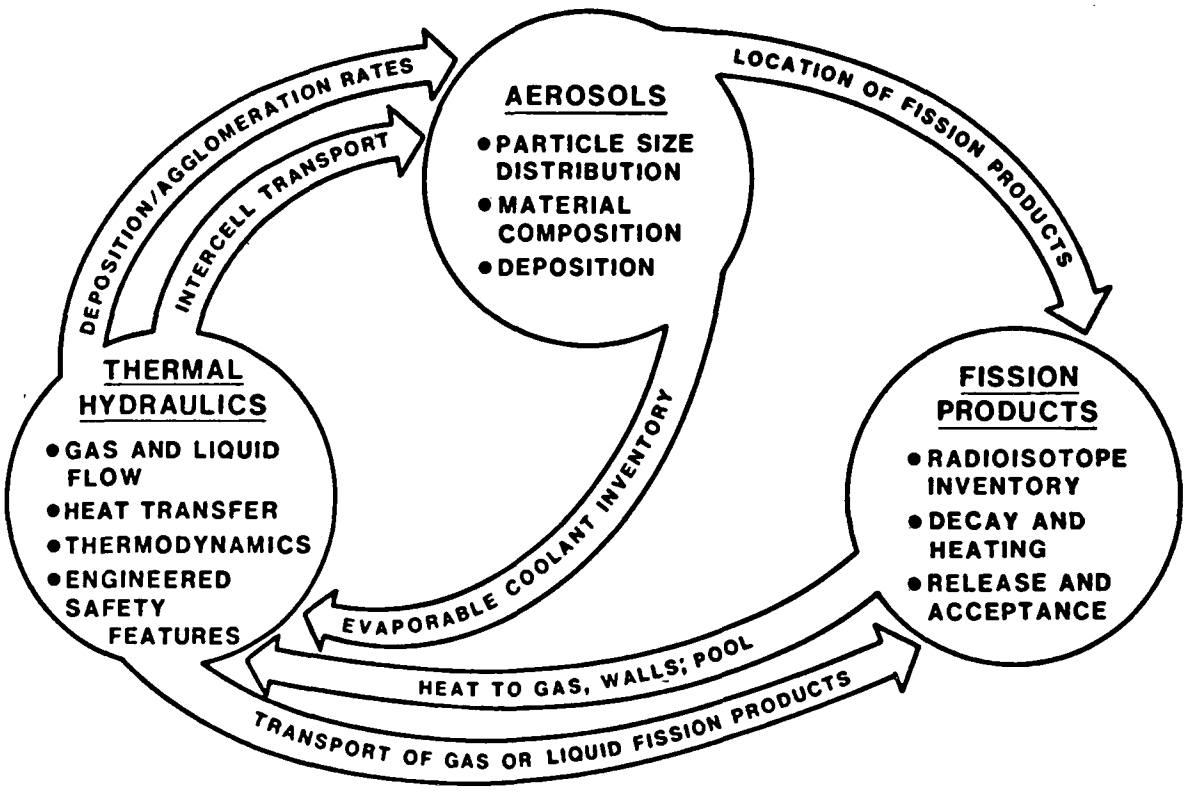

Figure 1-1. Three Basic Phenomenological Areas Treated in CONTAIN and Some Couplings and Feedback Loops Among Them

The purpose of this User's Manual is to provide a basic understanding of the features and models in CONTAIN so that users can prepare reasonable input and understand the output and its significance for particular applications. Thus, besides simple input instructions, the User's Manual also contains brief descriptions of the models. Known limitations in the models are discussed (as well as some suggestions concerning possible ways to overcome the limitations--see Section 5). However, not all modeling and coding details are provided. CONTAIN is a very large code, and a detailed treatment of all the technical features would result in a document too large and complicated to be practical. Many of the models in CONTAIN have been imported directly from other codes which themselves are well documented. In those cases, the detailed documentation sources are cited in the qualitative model descriptions for the analyst who requires more detail. In other cases, when the modeling is original with CONTAIN, the level of mathematical details provided in the User's Manual is greater. However, very little information is provided about code architecture, algorithms, or other programming details, as such descriptions are beyond the scope of the User's Manual.

1.2 Progress in Containment Analysis

The first version of CONTAIN to be documented and widely distributed was released in 1984 as CONTAIN 1.0.[Ber85] Since then, numerous improvements in the code have been made, prompted in part by the rapid expansion in the technical base of knowledge about severe reactor accident phenomena. Many of these improvements have been embodied in interim revisions of the code, which have been periodically released to the user community (revisions 1.01 through 1.06), along with correction pages to the User's Manual. The extent of the revisions reached the point that a new code version, designated 1.1, was prepared and a revised User's Manual was needed. In this section, the principal developments driving the evolution of CONTAIN from Version 1.0 to Version 1.1 are summarized, and the major differences between the two versions are highlighted.

1.2.1 Background

In the past four years, perceptions and knowledge about severe accidents have evolved significantly, and these changes have significantly influenced the development of CONTAIN. There are two categories of sources for the new information: (a) study of the accidents at TMI-2 and at Chernobyl; and (b) products of research in the U.S. and other countries. Of these, the latter has been significantly more directly influential, but the importance of postmortem analysis of the reactor accidents should not be underestimated.

It is now understood that a significant fraction of the core was melted at TMI-2 and that attack of lower head internal structures had commenced at the time the melt progression was arrested. This information is not of direct use for containment analysis except perhaps for the inference that the ability to analyze post-vessel-breach conditions is clearly desirable. More important from the containment analysis viewpoint is the improved information that has emerged about hydrogen combustion and the form of radioactive iodine.

It is known now that there was a hydrogen combustion event in containment at TMI-2. The containment building integrity was certainly not threatened by the burn (it is an exceptionally robust containment), but this new knowledge has heightened the perception of the importance of combustible gas phenomena in containment. A number of improvements to CONTAIN should contribute to better simulation of this aspect of severe accident phenomenology. These include treatment of CO burning, quenching effects of CO_2, improved gas emissivity models, and implementation of a number of options that give the user more control of the ignition criteria.

The issue of the chemical and physical form of radioactive iodine was identified shortly after the TMI-2 accident as an area where previous perceptions would need significant change. More detailed study of conditions inside the debris bed and primary system are now showing that iodine chemistry can be extremely complex and that simplistic treatments may be inadequate. Although CONTAIN 1.1 does not include a complete set of models for iodine chemistry, the treatment of fission product transport has been completely overhauled to allow the user more realistic

options and to accommodate more mechanistic models when they become available.

The Chernobyl accident, in contrast, has not provided much significant technical information of direct applicability to containment analysis. The reactivity excursion that energetically disassembled the containment was so powerful and abrupt that containment phenomena, as usually construed, played no significant role. It is possible, however, that future study of this accident and its consequences may reveal information that will affect the way containment analysis is performed.

In terms of direct impact, it is the research programs in the U.S., Europe, and Japan that have been the stimulus for the evolution of our severe accident models. No attempt will be made here to review these programs. However, it is worth mentioning, if only as an example, one area in which experimental progress has resulted in major changes to CONTAIN. This is the area of molten-core-concrete interactions. Experiments, model development, and analysis in the U.S. and Germany have demonstrated the need for detailed analysis of core-concrete interactions. The importance of aerosol generation due to these processes has also recently been emphasized. Consequently, the incorporation of the CORCON and VANESA codes into CONTAIN has made Version 1.1 significantly more useful than Version 1.0 for analysis of accidents involving molten-core-concrete interactions. Direct incorporation of these models will also allow CONTAIN to evolve in parallel with the stand-alone versions of these codes as further research improves our understanding.

1.2.2 Highlights of Recent CONTAIN Validation and Applications

Another source of improvement for the CONTAIN code is use: first, in code validation exercises, and second, in accident analyses. Analyses of hypothetical accident sequences do not directly contribute to the validation of the code, but sensitivity studies of realistic scenarios can identify critical areas of uncertainty and can also display unexpected interactions among the diverse phenomena. Numerous such studies with CONTAIN have shown the importance of an integrated approach. In many cases, for example, subtle balances may exist between competing processes, and calculational treatments that neglect the key feedback loops may give completely erroneous results even if the constituent stand-alone models are reasonable.

A good example of differences between integrated and nonintegrated calculations is presented in Reference Car87, in which it is shown that the core-concrete interactions predicted by CORCON (operating as a module of CONTAIN) are sensitive to whether the treatment of radiation heat loss to the containment takes into account the containment response. A number of other examples of the importance of integrated analysis are given in Reference Wil87a. For example, it is shown that containment pressures predicted by CONTAIN for a Station Blackout Sequence are sensitive to the treatment of mobile heat sources (e.g., radioactive aerosols and gases). Another example studied in the same paper shows that the rate of depressurization of a failed containment could affect the source term if gravitational settling in the containment during the depressurization

process is enhanced by condensation on aerosols in a saturated atmosphere.

Numerous other calculational studies of accident sequences have been performed with CONTAIN 1.0 (and revisions 1.01-1.06). Appendix A lists a number of reports and papers that discuss these calculations in more detail.

Validation exercises, the comparison of experimental results with both pretest and posttest code calculations, are critically important to the confidence one may have in the results obtained for realistic accident sequences. Because of this importance, validation is a major element of the CONTAIN program. A number of separate-effects codes (CORCON [Col84], VANESA [Pow86], HECTR [Cam86], ICEDF [Owc85a], and SPARC [Owc85b]) are integrated in part or in their entirety into CONTAIN. The validation achieved by these codes is to a large extent carried over to CONTAIN. An independent validation program is also being conducted. Direct comparisons of CONTAIN results with a wide variety of experimental tests have been completed, and CONTAIN is currently involved in a number of ongoing validation programs. Completed validation studies involving CONTAIN include several of the Hanford Engineering and Development Laboratory's ABCOVE tests, the NSPP aerosol experiments at Oak Ridge National Laboratories, the German V44, T31.5, and T31.6 tests at HDR, Pacific Northwest Laboratory's CSE test A-9, the hydrogen burn test series at the Nevada Test Site, and recent LACE tests managed by the Electric Power Research Institute. These studies are described in more detail below.

One of the earliest validation exercises in which CONTAIN participated was the blind test prediction of thermal-hydraulic conditions for a full-scale steam blowdown LOCA simulation, HDR test V44.[Win83a] Temperature and pressures predicted for this design basis accident over a wide range of time scales are in excellent agreement with the experimental data.[Val83] More recently, small break LOCA tests (T31.6) at HDR have been the subject of CONTAIN calculations. Preliminary nonblind posttest results are reported in Reference Lan88, and it is anticipated that additional calculations will be performed in the future.

Many of the other studies were used to validate code predictions of aerosol behavior. The ABCOVE series of experiments generated dry aerosols under conditions simulating LMFBR containments. Close agreement obtained between blind code predictions and experimental test results for AB-5, AB-6, and AB-7 are particularly relevant in demonstrating the effectiveness of CONTAIN's model for aerosols, which uses discrete particle size classes and treats multiple aerosol components.[Hil83, Hil84, Hil85] (Nonblind predictions were made for the earlier tests AB-1 and AB-3.)[Hil79, Mcc79] Further validation of the aerosol model and its coupling to thermal-hydraulics was achieved in the Oak Ridge NSPP test series.[Kre82, Ada82] These tests were conducted in a steam environment more typical of LWR accident conditions, in which condensation and diffusiophoretic effects can strongly influence the observed aerosol behavior. However, the experiments did not present an ideal opportunity for validation of CONTAIN because of some experimental uncertainty in the steam flow rates present. However, as discussed in Reference Mur83, reasonable assumptions about the uncertain experimental parameters led to good agreement between CONTAIN and the measured data. Validation of

CONTAIN's aerosol models is also demonstrated in a report from workers in Japan [Shi87], which makes extensive comparisons between CONTAIN calculations and experiments involving aerosols and sodium combustion. A final example of validation of the aerosol modeling involves the CSE A-9 test, which was designed to assess the radionuclide scrubbing efficiency of containment sprays.[Hil71] Reasonable agreement for both elemental iodine and aerosol depletion due to sprays was obtained.[Mur83]

Validation of the hydrogen burn model in CONTAIN 1.05 against the Nevada Test Site experimental data [Rat85] is the subject of Reference Van86. Again, reasonable agreement was obtained for all important parameters except burn duration in lean mixtures. For these situations, CONTAIN significantly underpredicts burn times, a conclusion that was also reached in an earlier study concerning the HECTR code.[Won86]

The code was used as part of the LACE series of aerosol/thermal-hydraulic tests conducted at Hanford's CSTF in a multinational program coordinated by the Electric Power Research Institute.[Rah88] Blind predictions of aerosol and/or thermal-hydraulic conditions in the LACE series were made not only by Sandia National Laboratories but also by ORNL, UKAEA, JAERI (Japan), CEC (Ispra), and ENEA (Italy).[Sla86, Wil87b] In general, results obtained by all participants are in good agreement with both the aerosol and thermal-hydraulic parts of the exercise.

In addition to studies that are completed, there are several validation programs in which CONTAIN is currently involved. The influence of multiple compartments on aerosol transport and retention is the subject of the DEMONA test series [Hos83]; CONTAIN is being used for this project by CEC and UKAEA. Sandia used CONTAIN for combined hydrogen/steam natural convection experiments (test T31.5) at the HDR facility in Germany in late 1987 and 1988. Finally, a series of Direct Containment Heating (DCH) experiments at the Surtsey facility at Sandia are providing validation for the (unreleased) DCH model.[Tar88]

1.2.3 Differences Between Version 1.1 and Version 1.0

All of the features of CONTAIN 1.1 will be described in several levels of detail in the remainder of this User's Manual. Generally, all of the capabilities of Version 1.0 have been retained, but a variety of new models or options are now available as well. Upward compatibility (the ability to run any deck that ran on previous versions) has been maintained except in a very few cases of unresolvable conflicts between the new models and the old. All of these cases are described in Appendix D, and in all such cases, the code provides diagnostic messages in the error file. The CONTAIN user should develop the habit of scanning the error file for diagnostics whenever the input data set or code version is changed, even if the code appears to have run a problem successfully.

A central difference in capabilities involves the gas flow numerical solution method. In Version 1.0, only an explicit method is available. This limits the usefulness of the code for long problems involving many cells (e.g., greater than six or seven) because of computational cost. It also imposes additional, more subtle limitations. One is the inability to model buoyancy effects because of the difficulty with which

the explicit method treats very small pressure differences. The new implicit method solves all of these problems and is the recommended choice for all multicell problems. The implicit treatment covers not only gas flow but also coolant boiling. Consequently, multicell calculations can now be performed with much longer calculational timesteps than was possible with Version 1.0.

Major new modeling options have also been added. The integration of the CORCON and VANESA models for core-concrete interactions is one of the more important improvements. The addition of the pressure suppression pool vent and safety relief valve (SRV) models make it possible to do complete analyses of boiling water reactors (BWRs). The entire system of radionuclide accounting has also been changed, allowing much more realistic treatment of fission product transport. The handling of radiation transport is better in two ways: first, a new model for emissivity of $H_2O/CO/CO_2$ gas mixtures has been included, and second, the user has the option of using a full net enclosure calculational method for radiative heat transfer if the simpler engineering treatment is deemed insufficient.

Besides these major upgrades, there is a wide range of more minor improvements and/or conveniences. Virtually all deviations from ANSI-standard FORTRAN 77 have been eliminated. The property library has been upgraded and, probably more important, the user can specify thermal properties of any material through input. Carbon monoxide combustion is now modeled, and numerous other user options relating to gas combustion have been implemented. Solution algorithms for condensation of water on or evaporation of water from aerosols have been upgraded, and the lower cell heat conduction routine has been replaced.

In general, the changes from Version 1.0 to 1.1 represent augmentations or additions of capabilities. Therefore, it is expected that input decks successfully run on previous versions of the code will also run on Version 1.1 with few changes in the calculated results. There may be some quantitative changes, however, as in cases that depend on material properties which have been changed. There may also be a few cases in which there is more serious conflict between the old models and the new, and the problem will not give the same results. In such cases, a diagnostic is always written to the error file (see Appendix B). Some of these are also discussed in Chapter 5. In many places, the input format has been changed without any change in the models. However, the old input formats are still supported by the code; the obsolete input formats are documented in Appendix D.

Since code configuration control and quality control are a major goal of the CONTAIN code project, a suite of over thirty standard tests is run on each new revision of the code. Any differences between calculations done with the new version of the code and those done with older versions are scrutinized carefully until the differences are understood and found to be defendable. (However, some new standard tests may not run on old versions of CONTAIN because new features are invoked; downward compatibility is not a goal of the CONTAIN project.)

1.3 Guide to the User's Manual

The unique capabilities of CONTAIN allow the treatment of a large number of disparate phenomenologies (thermal-hydraulic behavior, aerosol and radionuclide behavior, core-concrete interactions, etc.) that can interact in complex ways. Achieving these capabilities has necessarily required complexity in the code and in its input options. Fortunately, the structure of the code is such that this complexity need be considered only insofar as the actual problem at hand demands it; the user can largely ignore information about models that are not needed by the particular problem to be solved.

This guide will assist the new user in efficiently locating and assimilating the information in the Manual that will be required for a specific problem. In developing this guide, it has been assumed that the user is reasonably knowledgeable about containment phenomenology but does not necessarily have prior knowledge about the CONTAIN code. It is also assumed that the user has in mind a well-defined problem and is not interested in spending time studying features that are not needed.

It is strongly recommended that any new user read all of Section 1 with some care in order to obtain an overview of CONTAIN, its capabilities, and its limitations; this much information is required to provide an adequate context for the more detailed information to follow. Section 1.4 includes a discussion of the CONTAIN physical models, which (though much abbreviated) should prove adequate to permit the user to identify the major models or groups of models that will be required for the problem being considered. In general, the discussions in other sections of the Manual presume some familiarity with the information given in Section 1.

Sections 2 and 3 form the heart of the User's Manual. Section 2 provides a description of the various models in greater detail than that given in Section 1.3. However, as discussed above, no effort is made to provide a complete physical and mathematical description; instead, the emphasis is on providing the information required in order to permit intelligent use of the models. Section 3 then gives the detailed description of the input required by the models and their various options.

Sections 2 and 3 are broken down into several levels of subsections, and the subsections are organized along phenomenological lines, with each subsection treating related phenomenologies. Once the user has identified the major models required for the problem under consideration (e.g., from Section 1.4), the Table of Contents may be used to identify the subsections that will provide the more detailed information needed to understand and use these models.

As an additional aid to the user, the organizations of Sections 2 and 3 closely parallel one another. For example, the input required for modeling heat transfer between the atmosphere and the structures within a cell is described in Section 3.3.1.3, while the underlying modeling is discussed in Section 2.3.1.3. The intent has been to keep the actual input specification reasonably concise for the benefit of the experienced user but to make it easy for the new user to find the more detailed information. It is recommended that the new user always read the relevant

portions of Section 2 to better understand what the code actually models in its calculations.

In Section 2, some of the subsections are quite simple and brief, while others are more lengthy and detailed, with descriptions of a number of interrelated models and/or numerous modeling options. The detailed subsections begin with introductory material labeled "Overview," which provides a brief description of what the subsection discusses and indicates when this information is or is not likely to be needed. It also notes some pitfalls that can arise from completely omitting other major groups of models whose relevance to the present group may not be immediately obvious.

Section 4 of the Manual describes the CONTAIN output. Much of the output is optional, i.e., selectable by the user. The user may wish to scan this section in order to form an idea of what output is available. This section also contains information about those features of the output that are not self-explanatory.

Section 5 discusses some of the pitfalls and limitations of the code and its modeling, in order to give a better understanding of the applications to which the code is suited, and also those to which it is not suited. It is recommended that a new user give at least a quick review of this material to note any limitations that may apply to the application being considered. Section 5 also includes some suggestions for extending the code's domain of applicability. For example, there are some processes for which no mechanistic models are provided in CONTAIN, yet there may be ways of simulating the effects of these processes to a degree that is adequate for the user's purposes. It is hoped that the information in Section 5 will assist the user in getting a maximum amount of useful information from the code.

Section 6 of the Manual provides three sample input problems with considerable discussion. All of the major groups of models in CONTAIN are exercised by at least one of these problems. If the user experiences difficulty in applying the input instructions of Section 3 to the problem under consideration, examination of the sample input problems of Section 6 may prove helpful. Instead of attempting to produce entirely new input files, the user may take advantage of existing input files to verify that the code is running properly and then modify them to produce the desired simulation.

Finally, the Manual includes several appendices providing additional information on certain specific aspects of CONTAIN usage and other supplementary information.

1.4 Physical Models

Although some standardization of design for nuclear steam generation systems has occurred, containment designs vary substantially with each power plant. The CONTAIN method of modeling a containment system is generic, allowing the widest possible application. Not all physical models need to be activated; the input for each simulation determines

those physical processes that are to be considered and those to be ignored.

CONTAIN treats a containment system as a network of interconnected compartments or "cells," shown schematically for a typical containment building in Figure 1-2. The cells represent the internal subdivisions of the reactor containment building. The arrows in this figure indicate possible gas flow directions through some of the gas flow paths present in the problem. These cells communicate with each other by means of gas flow, liquid flow, and/or heat flow (i.e., thermal conduction through intervening structures). Because there is considerable flexibility in specifying the properties of each cell and the connections between cells, CONTAIN is able to handle a wide variety of containment types.

For calculational completeness, the environment outside the containment building can be considered as one of the cells present. (It is usually specified to have a very large volume.) A radiological release to the environment then appears in the code as a flow into that cell.

For computational purposes, each cell is divided into two subcells: an upper cell and a lower cell. The upper cell consists of the gaseous atmosphere and the heat transfer structures that are in contact with it. The lower cell can include a coolant pool, layers of fuel debris, molten metal, molten concrete, and the concrete floor. The lower cell models are optional; some cells may consist only of the atmosphere and its associated structures.

The major capabilities of CONTAIN are summarized in the following paragraphs. The summary is organized in the following order:

Cell Atmosphere
Aerosol Behavior
Fission Product Behavior
Intercompartment Flow
Lower Cell Models
Engineered Safety Systems

A more detailed discussion of these capabilities and code features is presented in Section 2.

1.4.1 Cell Atmosphere

The cell atmosphere model in CONTAIN treats the major phenomena expected to play a role in atmosphere behavior during reactor accidents. Some of the phenomena treated are atmosphere thermodynamics, condensation and evaporation, heat transfer to structures, aerosol behavior, chemical reactions (e.g., hydrogen burning), and the intercell flow of gases, fission products, and aerosols. The atmosphere treatment is zero-dimensional, i.e., the atmosphere in each compartment is considered to be thoroughly mixed. In any compartment where a debris pool exists (e.g., the reactor cavity), the pool may be a significant source of the gases, aerosols, and thermal energy injected into the atmosphere in that compartment. The structural members of the compartment itself (floor, walls, roof, etc.), as well as physical objects that occupy the room, may

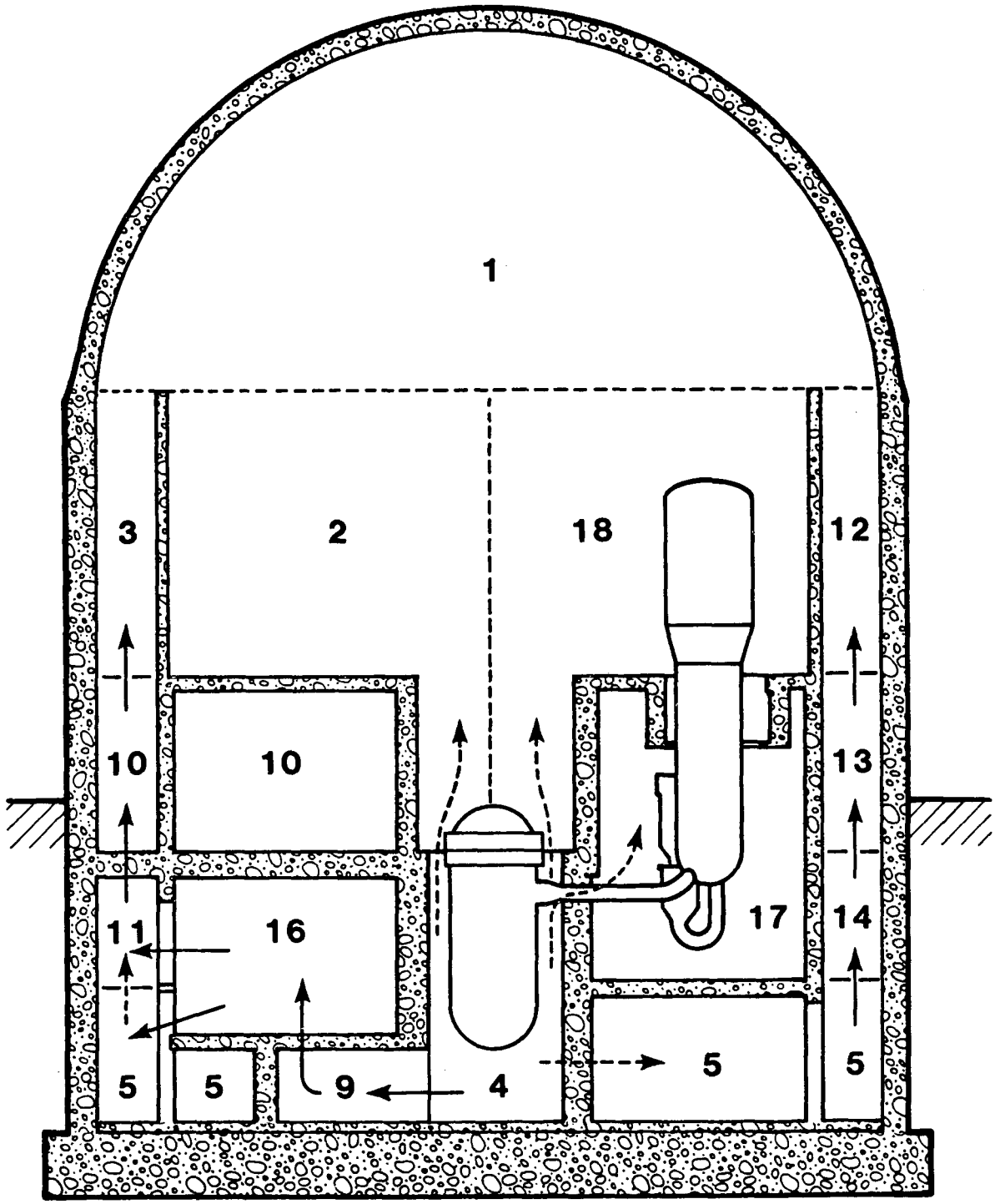

Figure 1-2. Reactor Containment Building Reduced to a Configuration of Eighteen Interconnected Compartments

be treated as thermal sources or sinks. Material can be added to or removed from the cell via the interconnecting flow paths, by lower cell models, or by user-specified source tables.

1.4.1.1 Reactor Types. Both light water reactors (LWRs) and liquid metal reactors (LMRs) can be modeled in CONTAIN. The specification of the reactor type specifies the coolant (water or sodium) and determines the appropriateness of using certain physics models. A number of models specific to sodium-coolant reactors are available (e.g., sodium pool or spray fire models). However, they are not described in this manual, but in a supplement for LMR applications.

1.4.1.2 Atmosphere Thermodynamics. State variables (such as temperature, pressure, and enthalpy) are calculated according to equilibrium thermodynamics. External heat sources and sinks, as well as coolant phase changes, are taken into account. Sources to the atmosphere include heat transfer from structures, heat from the decay of gaseous or aerosol-borne fission products, heat from chemical reactions in the atmosphere, mass and energy from the lower cell, flows into the cell from other cells, and user-defined sources.

1.4.1.3 Surface Heat Transfer. An arbitrary number of structures within each compartment can be treated. The floors, walls, and roof, as well as the surfaces of enclosed objects such as pumps or other machinery, are approximated in the input by choosing shapes that most closely resemble the objects to be modeled. Slabs, hemispheres, and half-cylinders are used as a standard set of shapes from which choices can be made. Each structure can be composed of arbitrary combinations of layers of different materials. Heat entering an object or structural surface may be treated as stored heat, or the surface may represent a heat flow area to another compartment. The heat released by fission products deposited on surfaces by aerosol deposition is taken into account.

1.4.1.4 Surface Condensation. CONTAIN models the condensation onto or evaporation from structure surfaces. The spatial orientation of structures is specified in the input because it can influence the condensation/evaporation rate. The presence of noncondensable gases is also considered because their presence inhibits diffusion of the condensable vapor to the surface. Condensation on, or evaporation from, structures can occur simultaneously with condensation on, or evaporation from, aerosols.

1.4.1.5 Radiative Heat Transfer. Radiative heat transfer is important for many severe accident scenarios. CONTAIN includes a simple model that treats radiation to the structures from the steam, carbon monoxide, and carbon dioxide in the cell atmosphere. This simplified formulation may optionally include radiation from a lower cell to the structures. For problems requiring more detailed analysis, radiative exchange among the surfaces can also be considered by using the more complete net enclosure model. The gas mixture and the surfaces are assumed to be gray.

1.4.1.6 Hydrogen and Carbon Monoxide Combustion. Hydrogen and carbon monoxide combustion is assumed to occur whenever the combustible gas concentration exceeds a specified value and the atmosphere in the cell is not inerted by a shortage of oxygen or an excess of diluents (e.g., CO_2

or steam). If default values are used, an oxygen concentration in excess of 5% and a combustible gas concentration above 7% may induce a burn. Combustion can also propagate to other cells, depending on whether certain criteria are satisfied. Upward, downward, and lateral flame propagation are possible. Models for hydrogen and carbon monoxide burning are taken from the HECTR code.[Cam86] As in HECTR, detonations are not modeled.

1.4.2 Aerosol Behavior (MAEROS)

One of the principal purposes of the CONTAIN code is to characterize the radiological source term in the event of containment failure. Released fission products are most effectively transported throughout the containment and into the environment by gases and airborne aerosols. The MAEROS model in CONTAIN allows for a multisectional, multicomponent treatment of aerosols.[Gel82] A multisectional treatment is one in which the particle size distribution is discrete and can therefore have an arbitrary shape, and a multicomponent treatment is one in which each particle size class can have a different composition with respect to several component materials. These features are important in assessing the radiological consequences of the suspended aerosols. Another important feature of CONTAIN is that condensation on, or evaporation of, water from aerosols is modeled in a manner consistent with the atmosphere thermodynamics calculation.

The CONTAIN aerosol treatment includes models of three agglomeration processes: Brownian, gravitational, and turbulent. In addition, four deposition processes are considered: gravitational settling, diffusiophoresis, thermophoresis, and particle diffusion. In some cases, aerosol deposition by impaction and interception are included in the modeling of engineered safety features (ESFs).

1.4.3 Fission Product Behavior

The composition of the fission product inventory in the reactor core can be determined with considerable accuracy through a knowledge of its power history and the application of any one of several well-documented "burn-up" codes. However, during a core-melt accident, the physical disposition of the radionuclides is highly uncertain. Because CONTAIN does not analyze in-vessel phenomena, it depends on input from the user or other codes to specify the initial locations of the fission product inventory in containment. From that point on, CONTAIN models three aspects of fission product behavior: transport (which determines the locations), decay (which determines inventories of each isotope), and heating (which couples back to the thermal-hydraulic behavior).

1.4.3.1 Fission Product Transport. To determine the location of the radionuclides being studied, CONTAIN tracks them as if they were physically attached to a "host" material. The reason for this fission product host system is that the masses of fission products involved are often very small compared to the masses of the hosts. In these cases, the transport of airborne fission products is controlled by the mechanistic thermal-hydraulic modeling of the movement of the nonradioactive gas

or aerosol host materials. A mechanistic model for iodine removal by sprays and a semimechanistic model for fission product transport in liquid pathways are also available. In addition to the mechanistic models, each fission product can be transferred from one host to another at rates that are specified through the targeted release and acceptance model and can depend on the host temperature. The reason for this flexible system of fission product transport is the high degree of uncertainty involving the physical and chemical forms of fission products and their affinities for the various host materials. The experimental and modeling data base for the release of fission products from fuel and for subsequent chemical changes in the various nuclides is currently inadequate to provide reliable mechanistic models for a code like CONTAIN. The targeted release and acceptance formalism is therefore provided to allow the analyst to evaluate the consequences of different modeling assumptions.

1.4.3.2 Fission Product Decay and Heating. The decay of fission products and the heating of the host materials are modeled in CONTAIN according to the half-lives and power coefficients of fission chain elements. Fission product parent-daughter relationships are defined in the input by specifying the decay chain structure as a series of linear chains. Likewise, the fission product half-lives and power coefficients are also specified in the input. The fission product heating couples back to the thermal-hydraulics since the decay heat of each radionuclide is deposited into its respective host material. However, despite the flexibility inherent in being able to specify each of the power coefficients, it is usually difficult to specify in detail all of the radionuclides that would contribute to decay heating, as this would require a large amount of input. Normally, only a selected subset of radionuclides is of interest for health physics or transport reasons, and it is these radionuclides that are typically specified explicitly. The remaining decay heat from the reactor fuel can be handled in a more generic way: a standard decay power curve is used to calculate total decay power as a function of time since shutdown. The power associated with the explicitly specified radionuclides is subtracted from this total power, and the remaining power is then deposited in a number of locations (coolant pool, atmosphere, etc.) as specified by the user. The use of a standard decay power curve greatly simplifies many calculations.

1.4.4 Intercompartment Flow

Atmosphere flow between cells is modeled as user-specified or pressure-driven orifice flow. The user specifies either the flow rate or the geometry of the flow paths between interconnected pairs of cells. The time at which any flow path is opened or closed may be given, or the paths may be allowed to remain open during the entire run. A flow path may also be opened by specifying a threshold pressure difference between two connected compartments; such a trigger might represent the opening of a rupture disk or the failure of a structural barrier between two compartments. In addition, time-dependent and pressure-dependent flow path characteristics (e.g., area) may be specified, allowing realistic modeling of containment failure and of one-way flow.

The material transferred through the path is a portion of the atmosphere of the upstream compartment. Gaseous fission products move through the flow path at the same velocity as the bulk gases. At the user's option, aerosols may be transported either according to the gas velocity alone or according to the sum of the gas velocity and the component of the aerosol terminal settling velocity parallel to the flow path axis.

Two types of solution methods are available to solve for the flow rates: an explicit Runge-Kutta method and an implicit method. For the explicit method, one may select either a model that includes the effects of inertia on the flow rate or a model that neglects the effects of inertia. For the implicit method, the model including the effects of inertia is primarily the one used, although in some special cases the inertia is neglected.

The implicit method is the one of preference for most problems because of its calculational efficiency. For a variety of reasons certain features are available only with the implicit method. These are (1) gravity-driven gas flow, (2) the instantaneous liquid DROPOUT model for water condensing in the bulk gas, (3) critical, or choked flow, (4) aerosol settling through flow paths, (5) an implicit model for pool boiling that is solved simultaneously with the flow equations, (6) the engineered vent option, and (7) the suppression pool vent system of a BWR.

The engineered vent, which is specified under the ENGVENT input block, is a gas flow path similar in most respects to the regular flow paths specified in the FLOWS input block. The modeling options for the flow through an engineered vent include all of the options available for the regular flow path and some others that are specific to the engineered vent. Unlike the regular flow path, more than one engineered vent may connect any given pair of cells. The modeling options used for each one may also be chosen independently.

Flow of gases, aerosols, and fission products through the suppression pool vent system of a BWR is modeled through a special flow path between cells representing the wetwell and drywell of a BWR. If the vent is covered by the suppression pool, the aerosols and fission products attached to the aerosols are scrubbed in the pool before being introduced into the downstream cell.

1.4.5 Lower Cell Models

Core-melt accident scenarios may lead to a predicted breaching of the primary system and the development of some kind of bed or pool of core debris and coolant in the bottom of the reactor cavity. Ablation of the concrete floor presents the threat of basemat penetration while simultaneously producing water vapor, noncondensable gases (some of which may be combustible), and aerosols, all of which carry fission products, heat, and reaction products into the upper containment atmosphere. The lower cell model deals with these phenomena. These processes may not all occur in all cells; for example, in some cells, the lower cell system may serve simply as a sump for collecting coolant. In others, a lower cell may not be required.

1.4.5.1 Multiple Layer Heat Transfer System. The lower cell model features a system of material layers that corresponds to the physical system anticipated should a core-melt accident occur. The lower cell may include a concrete layer, intermediate layers, and a coolant pool layer. The feature of multiple intermediate layers allows for layers of distinctly different materials such as molten metal and oxide by-products of core-concrete interactions. Because a high level of phenomenological uncertainty prevails concerning the configuration of debris, coolant, and other materials, CONTAIN allows the user to specify the configuration of layers.

For lower cells in which core-concrete interactions are not explicitly modeled through the CORCON model discussed in the next section, the lower cell is treated as a coupled thermal system, with heat transfer coefficients between layers selected from a variety of correlations. The concrete layer is nodalized for improved resolution and accuracy, and the heat transfer is solved one dimensionally. Special provisions are made for the coolant pool layer since the coolant can boil if its temperature exceeds the pressure-dependent saturation temperature. Coolant can also condense onto or evaporate from the pool surface. If CORCON is invoked, the transfer of heat and temperature predictions in the core debris are handled by CORCON.

1.4.5.2 Core-Concrete Interactions. As heat flows from the core debris into the concrete, temperatures rise and the concrete undergoes thermal ablation. The concrete becomes molten and begins to decompose. Vaporized and liquefied ablation products mix with the core debris. Further chemical reactions take place in the core debris, generating hydrogen, carbon monoxide, and other products. The CORCON code, a detailed mechanistic code, models these processes.[Mui81, Col84] CONTAIN features a full integration of the CORCON MOD-2 model. The concrete and intermediate layer architecture in CONTAIN is used to specify the problem to CORCON and to report CORCON results in the context of CONTAIN output. The CORCON model furnishes two types of input to CONTAIN: gas species produced by the core-concrete interactions and the thermal load represented by the hot upper surface of the core debris. Both the coolant pool layer and the upper cell system can interact with this upper surface.

In addition to the CORCON model, the VANESA model has been included in CONTAIN as an option.[Pow86] This model treats aerosol production and fission product evolution from the core debris due to gas from the core-concrete interactions sparging through the molten materials. The aerosols and radionuclides so produced may be incorporated into CONTAIN models.

The modified Fuchs model included in the VANESA code is one of two models available to model the scrubbing of aerosols passing through a coolant pool layer. (The pool is also assumed to scrub any fission products in aerosol form.) Gaseous materials introduced into the pool will be equilibrated at the pool temperature before being passed to the cell atmosphere.

1.4.6 Engineered Safety Systems

Virtually all nuclear power plants include engineered safety features (ESFs) designed to reduce pressure, temperature, and fission product concentrations. They thus reduce the threat to containment integrity and limit fission product release should leakage occur. CONTAIN has detailed models for three major ESFs: containment sprays, fan coolers, and ice condensers. Associated with these models is a framework for the construction of liquid coolant transport systems that provide sources and sinks for the ESFs and control the transfer of coolant between lower cell pools. The components available for such systems include tanks, pumps, orifices, pipes, valves, and heat exchangers, as well as user-specified external sources of coolant. In addition, overflow of coolant liquid from the pool of one cell to that of another can be modeled.

The ESF models are generally mechanistic in nature, so that their range of applicability is greater than would be possible with more empirical models. Because of the integrated treatment of fission products, aerosols, and thermal hydraulics, it is possible to analyze the redistribution of fission products and aerosols due to the operation of the ESFs.

1.4.6.1 Containment Spray. The containment spray system is a nearly universal safety feature in LWR plants. This system provides a high pressure, finely divided water spray to the containment atmosphere. Heat transfer to the droplets and subsequent condensation of atmospheric steam can produce rapid reductions in temperature, pressure, and fission product concentrations. The spray droplets, as well as much of the condensate, collect in a sump at the bottom of the containment. Generally, the initial spray source is from the refueling water storage tank. When this source is exhausted, water is pumped from the sump, through a heat exchanger, and to the spray nozzles. A model has been developed for CONTAIN that determines the heat transfer between the droplets and atmosphere and the associated condensation onto or evaporation from the droplets.

The containment spray model allows for the removal of aerosols, fission products hosted to aerosols, elemental iodine, and less reactive organic iodine compounds from the containment atmosphere. Aerosols and fission products removed from the atmosphere by the sprays can be diverted to the pool of any compartment.

1.4.6.2 Fan Cooler. Fan coolers are included in many containments both to provide nonemergency cooling and to augment the heat removal capabilities of the water sprays. These coolers consist of banks of finned, service-water-cooled coils across which large capacity fans pull the containment atmosphere.

CONTAIN has two fan cooler models. These models provide reasonably mechanistic treatments of fan cooler performance. The first model, similar to that developed for the MARCH code [Woo83], is simple, fast, and adequately reproduces the cooling capacity of actual plant equipment under saturated conditions. It can be used whenever the effects of superheated conditions are expected to be relatively minor.

A second, more mechanistic, fan cooler model is based on forced convective heat transfer correlations similar to those used throughout CONTAIN. The model calculates mass and heat transfer coefficients based on the cell atmospheric conditions. This model can treat superheated conditions. However, it requires a more detailed knowledge of fan cooler characteristics than the simpler model described above.

Because of the relatively cool surfaces and high condensation rates provided by fan coolers, substantial scrubbing of aerosols is expected. The aerosol removal resulting from diffusiophoresis is calculated if the condensation fan cooler model is active.

1.4.6.3 Ice Condenser. Ice condensers are used in some PWR containment systems primarily to limit containment overpressure in the event of a LOCA by condensing steam released from the primary system in a large ice chest. In addition to reducing peak pressures and temperatures, ice condenser systems can be effective in reducing containment aerosol loadings.

The CONTAIN ice condenser model uses the cell atmosphere model to determine the thermodynamic conditions of the air/steam mixture in the ice compartment. Flow through the ice condenser can be initiated by pressure difference criteria specified by the user. Heat transfer to and condensation on the ice structures is treated by the forced convection model that is used throughout CONTAIN. Aerosol removal by the ice and supporting structure is also modeled.

1.4.6.4 Engineered Safety System Individual Components. Modeling of the ESFs includes several components that might typically be used in a reactor safety system. The components modeled include a liquid storage tank, a pump, an orifice, a pipe, a valve, and a heat exchanger. These components can be combined in various ways to model the performance of coolant storage and transfer systems, and auxiliary cooling systems. They can also be used to model the transfer of coolant from one location in containment to another.

1.4.7 Safety Relief Valve Discharge Model

The discharge of gases, aerosols, and fission products from the primary system through a pool is modeled through the safety relief valve (SRV) discharge model. Although intended primarily to describe the SRV discharge through lines leading to the bottom of the suppression pool in a BWR, the model may also be used in other situations where the discharged materials are scrubbed by a pool before being introduced into the atmosphere. The suppression pool vent model for gas flow from the drywell to the wetwell is modeled through a special flow path as discussed in Section 1.4.4.

1.5 Code Structure and Calculational Sequence

The main aspect of code structure of importance to the user is the organization of the phenomenological models into two basic types: cell level models and global models. While the distinction between these two

types is based principally on the manner in which time-dependent calculations are performed with respect to these models, this distinction is reflected not only in the internal code architecture but also in the organization of the input data set and in the manner in which the user specifies storage for arrays. It also determines which of the various timesteps specified by the user are used by a model in the time-dependent calculations. Thus, it is an important distinction for the user to be aware of.

The CONTAIN code is designed to accommodate simultaneously the many different models needed to describe the processes that could occur within each cell. It does so through the "reference cell" concept. Within this concept, any cell in the system being modeled may incorporate or participate in any or all of the phenomenological models available in CONTAIN. The potentially large number of degrees of freedom within each cell are handled through the bilevel cell and global structure of the time-dependent processing. This structure is based on the observation that of the potentially many degrees of freedom within each cell, only relatively few will be coupled strongly to degrees of freedom outside of the cell. Thus, it makes sense to calculate the processes that are not strongly coupled outside of one cell separately from the processes that are strongly coupled.

The time-dependent calculations for processes that are not strongly coupled outside of one cell typically occur in the cell loop shown in the program flow chart of Figure 1-3, and the models so processed are called cell level models. An example of a cell level model is the conduction model for heat transfer structures. As indicated in Figure 1-3, only one cell (the "reference cell") is processed at a time at the cell level. When one cell is being processed, it does not, in general, have direct read or write access to the variables of another cell, although special provisions can be made to obtain values of variables from other cells that are needed by the cell being processed. Thus, strong coupling to degrees of freedom outside of the cell cannot be accommodated efficiently in the cell level processing. However, relatively strong coupling between the cell level processes within a cell may be accommodated because the models are all advanced together in time at the cell timestep, which can be a small fraction of the system, or largest calculational, timestep. (These timesteps are discussed more completely below.)

In contrast, time-dependent calculations for processes that are strongly coupled between cells occur in the global loop shown in Figure 1-3. The principal global model is the intercell gas flow model, which requires simultaneous access to the temperatures, pressures, and atmosphere compositions of all cells.

There is in some cases a degree of arbitrariness in the placement of a model at the cell or global level if the processes described are not strongly coupled to ones outside of the model or the cell, e.g., the fission product decay model. Such models may be processed at the global level for reasons of efficiency if the necessary array access is already present for other reasons--that access is typically required by the intercell gas flow model to calculate the transport resulting from intercell gas flow.

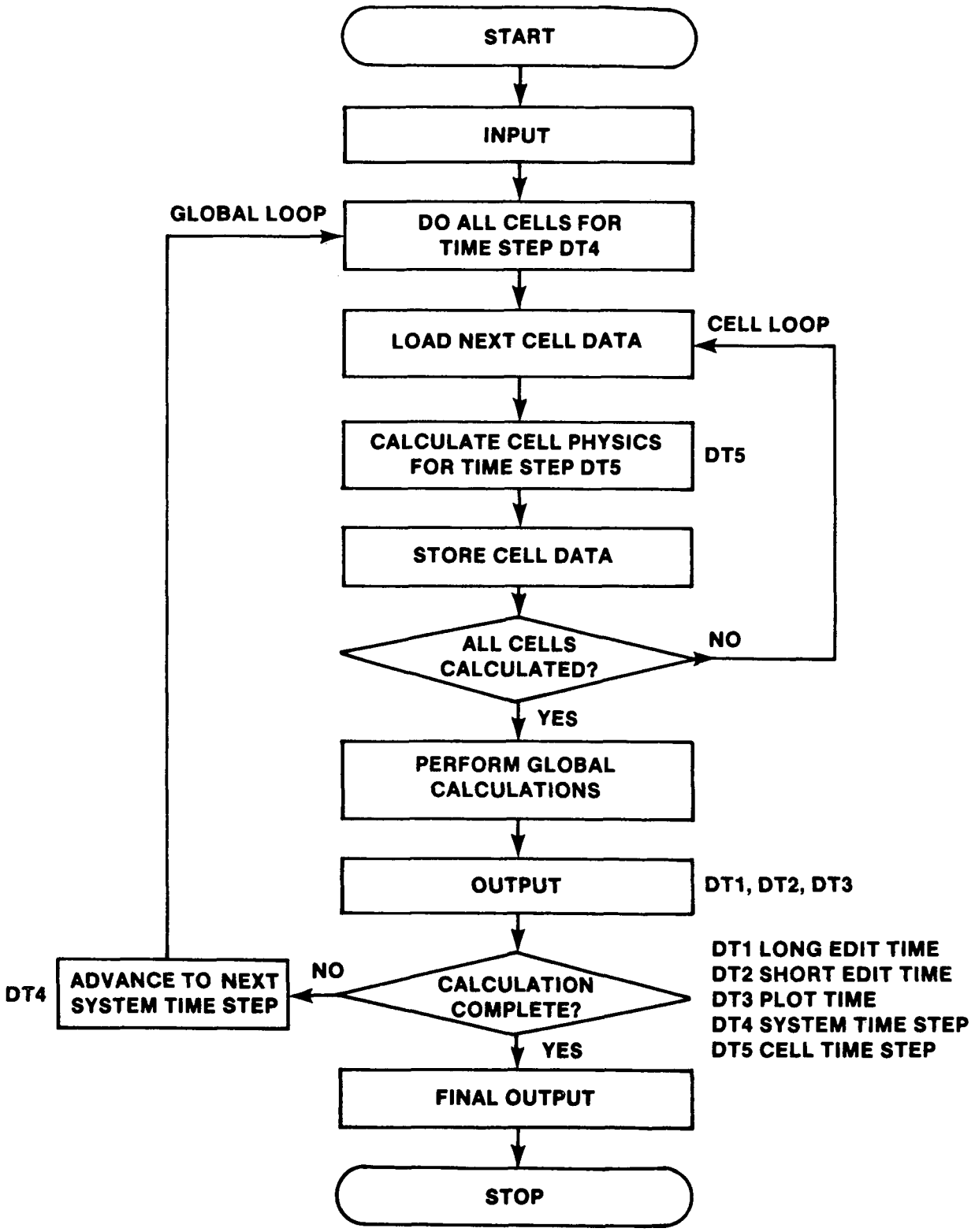

Figure 1-3. Overall Flow Diagram of CONTAIN

In the program flow chart shown in Figure 1-3, several different timesteps are identified, including the ones that control the global and cell level processing. The user has control over five different timesteps, while others are calculated internally. For completeness, all five user-specified timesteps are described below.

(1) Long edit timestep. This is the interval after which detailed output is written to the main output file in printer carriage control format. This interval is typically some multiple of the plot, or edit, timestep discussed below.

(2) Short edit time timestep. This is the interval after which summaries consisting of one line of output per cell are written to the main output file. The short edit interval may be as often as every system timestep (which is described below) or as infrequent as the user desires.

(3) Plot, or edit, timestep. The plot timestep is the interval after which all available plot information for that point in time is written to the plot tape(s). Since it is the basic interval for detailed output, the plot timestep is also referred to as the edit timestep.

(4) System timestep. The system timestep is the largest timestep in the calculational timestep hierarchy. It is defined as the interval after which variables in all models are updated and made available to other models. For example, the cell pressure and temperature are updated in the intercell gas flow model for use by other models once every system timestep.

(5) Cell timestep. Each cell level model is integrated over a system timestep by using a number of cell timesteps. The variables in cell level models are updated and made available to other cell level models within the same cell at the end of every cell timestep. For example, the temperature profile in heat transfer structures is updated every cell timestep. This freedom to subcycle at the cell level within a system timestep can increase computational speed under some circumstances.

The system and edit timesteps may be specified by the user in each of a number of time zones to accommodate varying timescales in the course of a calculation. Except during gas combustion events, the system and edit timesteps used are those directly specified by the user. The other timesteps above are defined in terms of a user-specified multiple or fraction of the system or edit timestep, with the default multiple or fraction being equal to 1. For a complex problem, several iterations may be required before a user finds a timestep sequence that provides the required accuracy, stability, and speed. Sections 2 and 5 furnish some guidance in this respect.

In addition to the user-specified timesteps, there are several "physics" timesteps, which are internally calculated. These are the timesteps chosen by the numerical solvers of individual models for the actual integration of the differential equations. They may be associated with

either global models (e.g., intercell flow and thermodynamics) or cell level models.

The cell and global storage scheme includes execution time dynamic storage allocation and variable array dimensioning. Also, one consequence of "reference cell" processing is that the cell level information for only one cell at a time needs to be present in central memory. These features together could greatly reduce memory requirements. They may allow small memory computers to run realistic problems that would otherwise not fit in memory. The storage scheme also facilitates the ability to restart problems for better computer turnaround on shorter jobs or to recover from interrupted runs. One further potential advantage of "reference cell" processing is that it should make conversion of CONTAIN to parallel processing at the cell level relatively straightforward.

1.6 Overview and Sample of Input

Preparation of input for running a problem with CONTAIN need not be overly complicated. As a result of the modular use of physics routines, certain problems can be formulated rather simply. For more complex and detailed problems, however, the input becomes correspondingly more complicated. To simplify the task, the input has been designed with several key features, including

- A generally free-field, keyword-driven format. Physical models are activated only by the presence of associated keywords in the input stream and are otherwise inactive.

- Default values for input variables. Most models allow the user to specify individual physical parameters. In many cases, however, default values (described in Section 3) will prove satisfactory.

- Separately specified global input and cell level input. Global input (for processes common to more than one cell) and each of the individual cell input sections are grouped separately to allow the user further flexibility in setting up a problem. For example, one cell may require detailed modeling, while others may simply be gas reservoirs.

As an aid to understanding references to input features in Section 2, Table 1-1 presents a representative example of an input file for a relatively uncomplicated problem. Section 3 provides a complete specification of the options activated in this input file, but a brief description of this data set is also given below. In scanning this simple input deck, the reader should note that on each line all information following the symbol && are comments.

The input data shown in Table 1-1 are for a two-cell problem, for which several of the physics models have been activated and a number of default values used. The problem models a single compartment as one cell, with a small flow path to a second cell, which is used to represent the environment. In the first cell, a source of steam reaches a maximum after about

Table 1-1

Sample CONTAIN Input

```
CRAY                                                                  &&   1
&& --------------GLOBAL INPUT------------------------------------    &&   2
CONTROL NCELLS=2 NTITL=1 NAC=1 NSECTN=20  NTZONE=1 EOI                &&   3
MATERIAL                                                              &&   4
    COMPOUND H2 O2 N2  H2OL H2OV FE CONC                              &&   5
TIMES 800.  1400.   50.    100.     3600. 1. 1.                       &&   6
AEROSOL H2OV 0. 0.                                                    &&   7
FLOWS   AREA(1,2)=7.E-5 AVL(1,2)=10. CFC(1,2)=1. QUASI                &&   8
TITLE                                                                 &&   9
           TWO-CELL SAMPLE PROBLEM                                    &&  10
&& --------------CELL 1 INPUT-------------------------------------    &&  11
CELL=1                                                                &&  12
CONTROL NHTM=1 MXSLAB=3 NSOATM=2 NSPATM=4 EOI                         &&  13
GEOMETRY 7.689E4   53.39                                              &&  14
CONDENSE                                                              &&  15
H-BURN                                                                &&  16
AEROSOL=1  H2OV=.1                                                    &&  17
ATMOS=4 1.E5 316.5 H2OV=.001 H2=0.  O2=.2 N2=.75                      &&  18
&& ----------- STEAM-BLOWDOWN-SOURCE-TABLE-----------------           &&  19
    SOURCE=2                                                          &&  20
    H2OV=4  IFLAG=2                                                   &&  21
    T=       0. 3353.    7337.    9011.                               &&  22
    MASS=    0.  16.1     87.7       0.                               &&  23
    ENTH=    0. 1.68E6  1.74E6       0.                               &&  24
    EOI                                                               &&  25
&& ----------- HYDROGEN-SOURCE-TABLE----------------------           &&  26
    H2=4      IFLAG=1                                                 &&  27
    T=       1.45E3  1.51E3 4.51E3  4.69E3                            &&  28
    MASS=     .0132   .00346  .005   .00514                           &&  29
    TEMP=    1800.   1800.   1800.  1800.                             &&  30
    EOI                                                               &&  31
STRUC                                                                 &&  32
    NAME = STEEL   TYPE = WALL   SHAPE = SLAB                         &&  33
    NSLAB=3  IOUTER=1  TUNIF=316.5  CHRLEN=10.                        &&  34
    SLAREA=6.13E3                                                     &&  35
    X = 0.   1.52E-3    3.04E-3     6.35E-3                          &&  36
    COMPOUND = FE  FE  FE                                             &&  37
    EOI                                                               &&  38
&& --------------CELL 2 INPUT-------------------------------------    &&  39
CELL=2                                                                &&  40
CONTROL   EOI                                                         &&  41
GEOMETRY 1.E8 1.E3                                                    &&  42
ATMOS=4   1.E5   300.   N2=.75  O2=.2   H2=0.   H2OV=.001             &&  43
EOF                                                                   &&  44
```

2 hours and ends at about 2.5 hours. Hydrogen is introduced at various times beginning at about 0.4 hours.

The first line of input specifies the machine on which the problem is to run and is used internally in setting machine-dependent options. Following this, lines 3-10 contain the global input, lines 12-38 are for the first cell, and lines 39-43 are for a very simple second cell. The end of the input is signaled by the keyword EOF on line 44.

At the beginning of each major section of input (i.e., the global input or the input for each cell) is the keyword CONTROL, followed possibly by other keywords and then the terminating keyword EOI. These other keywords are used for allocating array space. Line 3, for example, sets the numbers of cells, title lines, aerosol components, aerosol size classes, and time zones; line 13 sets the number of heat transfer structures, the maximum number of thermal nodes for any structure, the number of atmospheric sources, and the maximum number of tabulated source table values for the first cell; line 41 selects only default values for the second cell.

The remainder of the global input (lines 4-10) gives the names of materials required, timing information for the problem, and activating keywords for the global aerosol and flow models. A title has also been included to be used as a heading for each long edit and for the plot files. A number of defaults have been invoked in this section, including the choice of a thermal reactor, omission of certain output options, and values of many aerosol parameters. Other capabilities, such as the modeling of fission product decay heat, engineered systems, and reactor cavity phenomena, are not used in this problem.

Cell input for the first cell (lines 12-38) includes the keywords CONDENSE, H-BURN, AEROSOL, SOURCE, and STRUC, each of which activates separate physics models. Following the required CONTROL and GEOMETRY information on lines 13-14 are lines specifying that heat transfer to and condensation on structures is to be treated and that the gas combustion model is to be activated, with default values of parameters used throughout. Next, initial aerosol and atmospheric conditions for this cell are specified, followed by source tables (lines 20-31) for steam and hydrogen. Lines 32-38 complete the input for the first cell by describing one heat transfer structure within the cell, with such information as the geometry, composition, and initial conditions.

Only essential information has been included in the cell level input for the second cell, which is simply a large atmospheric reservoir representing the environment. A control keyword is again required, although no cell level array space is requested. The volume and characteristic length of the cell must also be specified as part of the GEOMETRY input. The input for this cell is completed by a specification of initial pressure, temperature, and atmospheric composition. No other physical models have been included for this cell.

2. PHYSICAL MODELS AND CODE FEATURES

CONTAIN is a computational implementation of an integrated system of physical models designed to predict the thermal-hydraulic conditions and the aerosol and fission product loadings in containment that may result from a reactor accident. This section describes the major physical models that make up CONTAIN and presents some of the key features of the code.

This section does not go into extensive mathematical detail about the physical models, and detailed discussion of code structure is not included. Nonetheless, the following discussions are intended to give the CONTAIN user a basic understanding of the content of the code and advice on how to use it effectively. Each of the major models and features is discussed separately. The discussions state in general terms what each model does and how the models interact with each other. The broad range of user options are explained, and default values of important parameters are specified.

In the following sections, the words printed in upper case letters are (in most cases) either keywords or character constants (i.e., names) used in the input for CONTAIN, and lower case alphanumeric groups enclosed in quotation marks are variable names used in the input description. These keywords and variable names are used in the following discussions to aid in the transition from the equations that model physical processes to the code input. The keywords, variable names, and the code input requirements are discussed in greater detail in Section 3.

A close correspondence has been maintained between the structures of Section 2, which discusses models, and Section 3, which discusses input. Thus, while reading Section 2, a user needing a more precise specification of the input structure can turn to the corresponding subsection in Section 3. Similarly, uncertainties in the meaning of variables or options mentioned in Section 3 may be resolved by referring to the related model descriptions in the corresponding subsection of Section 2.

2.1 The Bilevel Modeling Approach in CONTAIN

As indicated by the two loops in Figure 1-3 and explained in Section 1.5, CONTAIN has a bilevel structure for model implementation that distinguishes between cell level models and global models. Cell level models, as a rule, describe processes within a cell that are not strongly coupled to processes outside the cell. Global models, on the other hand, typically describe processes that are strongly coupled between cells.

The results of the cell level processing indicated in Figure 1-3 are cast in the form of sources and sinks of mass, energy, fission products, and aerosols for the global models. In the global loop, these sources and sinks are processed by the global level models to generate updated conditions in all cells for the start of the next system timestep. (See Section 1.5 for a discussion of the system timestep.)

The most important global process is the intercell flow of gases. For an arbitrary system of cells and interconnections, an accurate calculation of the flow rate through each flow path must be self-consistent; that is to say, the flow through any one must reflect changes in pressure in the upstream and downstream cells that arise from flows through all other paths. Thus, a global analysis of intercell flows is required.

Most other phenomena treated at the global level in CONTAIN are coupled to or affected by intercell flow. Atmosphere thermodynamics defines the equation of state for the gas, and since the coupling of pressure with intercell flow is strong, for numerical stability the thermodynamics is done simultaneously with the flow calculation. The aerosol and fission product behavior models deal with substances that flow with the gas. Since intercell transfers of these materials should be made at the same time the gas intercell transfer is calculated, it is convenient to place the aerosol and fission product models at the global level.

The intercell flow of liquids (e.g., through drainage systems) is not calculated at the global level. The transfer of liquids is generally not coupled strongly to conditions in more than one cell, so a sequential,

cell-by-cell calculation is feasible. These processes are modeled at the cell level, within the engineered system models (see Section 2.3.3).

2.2 Global Level Models

In addition to the specification of reactor type (Section 2.2.2), four modeling areas are treated at the global level: (1) the specifications of material names and properties; (2) intercell gas flow and atmosphere thermodynamics; (3) aerosol behavior; and (4) fission product decay, heating, and transport. These are discussed in Sections 2.2.2, 2.2.3, 2.2.4, and 2.2.5, respectively. All other modeling areas are treated at the cell level and are discussed in Section 2.3.

2.2.1 Material, Fission Product, and Aerosol Names

CONTAIN provides a library of physical properties for 50 standard materials that can be used in the modeling of containment systems. This library provides temperature-dependent enthalpies, specific heats, densities, viscosities, and thermal conductivities for a variety of materials commonly found in reactor and containment systems. Table 2-1 lists the standard materials available in CONTAIN and the name of each material as used in the code.

In addition to this library of material properties, the user may define new materials and their properties by means of tabular input. These tables are temperature-based and must be given in standard CONTAIN units. It is also possible to redefine the properties of the standard CONTAIN materials through tabular input. A variable, "nwdudm", is included in the global CONTROL block to allow the user to expand the amount of memory reserved for the user-defined tables beyond the default amount of 1000 words.

Great care must be used with user-defined materials, since the range of the user-specified tables may be exceeded and spurious values for properties may result. Only the enthalpy tables are linearly extrapolated

Table 2-1

Materials Available in CONTAIN 1.1

Material	Name Used in CONTAIN	Material	Name Used in CONTAIN
aluminum oxide	AL2O3	plutonium oxide vapor	PUO2V
argon	AR	plutonium vapor	PUV
boron carbide	B4C	potassium oxide	K2O
calcium oxide	CAO	silicon dioxide	SIO2
carbon dioxide	CO2	silicon trioxide	SIO3
carbon monoxide	CO	sodium carbonate	NA2CO3
chromium sesquioxide	CR2O3	sodium hydroxide	NAOH
concrete	CONC	sodium monoxide	NA2O
ferrous oxide	FEO	sodium peroxide	NA2O2
graphite	GRAPH	sodium silicate	NA2SIO3
helium	HE	sodium vapor	NAV
hydrogen	H2	solid iron	FE
ice	H2O	solid plutonium	PU
iron vapor	FEV	solid plutonium oxide	PUO2
liquid iron	FEL	solid sodium	NA
liquid plutonium	PUL	solid uranium	U
liquid plutonium oxide	PUO2L	solid uranium oxide	UO2
liquid sodium	NAL	stainless steel	SS
liquid uranium	UL	stainless steel oxide	SSOX
liquid uranium oxide	UO2L	titanium dioxide	TIO2
liquid water	H2OL	uranium oxide vapor	UO2V
magnesium oxide	MGO	uranium vapor	UV
manganese oxide	MNO	water vapor	H2OV
nitrogen	N2	zirconium	ZR
oxygen	O2	zirconium oxide	ZRO2

beyond their limits. All other properties are simply extrapolated by assuming their values remain constant at the endpoint values. The user must ensure that the tables cover the entire range of temperatures that will be encountered in a given problem.

Most of the materials available in CONTAIN do not undergo phase changes. The exceptions to this are the designated reactor coolants (water and sodium). The coolant can undergo phase changes between liquid and vapor

states. For both water and sodium, the boiling points are treated as pressure-dependent.

The names of materials used in a given run must be specified in the MATERIAL block. The names of standard materials, which are given in Table 2-1, must follow the COMPOUND keyword. (The COMPOUND keyword must immediately follow the MATERIAL keyword.) The names of user-defined materials must follow the USERDEF keyword. These names should be alphanumeric strings of eight or fewer characters that begin with a letter and should not correspond to a CONTAIN keyword or the word GAS. They may be standard CONTAIN names from Table 2-1. The declaration of names after USERDEF implies the presence of a corresponding block of input associated with the USERDAT keyword (see Section 3.2.1.1).

In order to use the CORCON model, it is <u>not</u> necessary to specify any names of CORCON melt species. The dummy material names used to represent CORCON materials in the lower cell intermediate layer are included by default. These names are LCCHOX, LCCMET, and LCCLOX.

The names of fission products used in a run must be specified following the keyword FP-NAMES. FP-NAMES, if used, may follow either the COMPOUND or the USERDEF block. Unlike the material names in the COMPOUND block, which must be chosen from Table 2-1, arbitrarily chosen names can be used for fission products. Nuclide names such as I133, or general names such as DUM1, can be used.

Names of aerosol components may be taken from the COMPOUND block. They may also be defined by specifying the keyword AERNAMES and then the desired names. These names may be chosen arbitrarily.

2.2.2 Reactor Types

CONTAIN is designed for accident analyses of two types of reactors, the LWR and the LMR. The models that deal specifically with LWRs include certain ESFs such as fan coolers, ice condensers, and containment sprays.

The models in CONTAIN that deal specifically with LMRs address sodium pool fires, sodium spray fires, and the combustion of sodium vapor.

Much of the coding in CONTAIN is independent of reactor type. The models that treat phenomena such as aerosol behavior and transport, intercell flow of gases and coolant, fission product behavior, and core-concrete interactions can be applied to essentially any reactor type.

To specify the reactor type, the code user can specify either FAST (for an LMR) or THERMAL (for an LWR). This information sets flags within the code defining the reactor coolant type. Water is the coolant if THERMAL is specified; sodium is the coolant if FAST is specified. These keywords also enable or prevent the activation of certain reactor-specific subroutines, such as POOLFIRE, in a calculation. The default reactor type is THERMAL.

2.2.3 Atmosphere Thermodynamics and Intercell Flow

Overview

Section 2.2.3.1 describes the atmosphere thermodynamics calculations; these will be required for almost any realistic problem. Section 2.2.3.2 discusses the three models available for intercell flow (the inertial flow model, the quasi-steady flow model, and the user-specified flow rate model). Flow path configurations and the flow control options are described in Section 2.2.3.3. Both implicit and explicit integration methods are available. For most multicell calculations, the implicit method will be the more suitable.

If conditions entailing a steam quality less than one can arise in an LWR problem, a mechanistic treatment of the liquid water fraction will require the specification of aerosols with water as an aerosol component (Section 2.2.4). Liquid water removed from the atmosphere (e.g., by condensation) can be lost from the problem unless a lower cell model including a pool is specified (Sections 2.3.2, 2.3.2.5). Modeling the effect of decay heating upon thermal-hydraulic processes generally requires fission product modeling (Section 2.2.5), although an immobile lower cell heat

source based on the ANSI-standard [Ame79] decay power can also be used (see Section 2.3.2.2).

The BWR suppression pool vent flow path model is described in Section 2.2.3.4. The suppression pool vent flow path model treats thermal-hydraulic processes and aerosol and fission product scrubbing processes that take place as the flowing gas passes through the water pool covering the vent exit.

As discussed in Section 2.1, the modeling requirements for intercell flow constitute the principal reason for the existence of the global level of modeling. This is because all mass and energy transfers between cells must be consistent with each other and with cell pressures.

Prior to the intercell flow calculation, cell level models and source tables are used to provide sources of mass, energy, aerosols, and fission products to the global level calculations. For each quantity, an effective source rate for the system timestep is calculated. The intercell flow equations are then integrated over the system timestep, with the assumption that these source rates are constant.

The constituents of the atmosphere may include noncondensable gases, coolant vapor and liquid, aerosols, fission products, and other dispersed solids or liquids. (The distinction between "dispersed" solids or liquids and aerosols will be made clear in Section 2.3.1.2.) During the flow process, the noncondensable gases and the coolant vapor and suspended liquid within each cell are assumed to be in thermodynamic equilibrium. A two-phase thermodynamic state is considered if the conditions warrant. In the thermodynamic calculation, constituents other than noncondensable gases and coolant in the atmosphere are assumed to have negligible specific heat, although they may add heat to the atmosphere.

The flow paths connecting the atmospheres of various cells provide the means by which the atmosphere masses and the aerosol and fission product masses move from cell to cell. The flow path modeling treats both the case where an actual restrictive orifice or flow channel exists between the cells and the case where the flow path is used to model flow

resistance in a lumped parameter sense (i.e., for cells nodalizing an open volume). It is important to understand the difference between a flow path and a cell: a cell is a repository for conserved quantities; a flow path is simply a transfer mechanism between cells. At any particular time, no mass or energy is considered to be in a flow path, and no losses of mass or energy (e.g., aerosol deposition or heat transfer) occur in flow paths.

The integration method employed for flows is either a first-order implicit method or a fourth-order Runge-Kutta method. The implicit method will typically be the method of preference for multicell problems that cover the long times characteristic of severe accidents. The Runge-Kutta method should be reserved for special calculations of transient behavior such as ones undertaken to assess integration errors. In either method, the integration timestep, or flow timestep, is selected automatically. The timestep in the implicit method is selected to ensure that the inventory in a cell does not change (through flow or sources) by more than 20% in total mass during the timestep. Although one would expect the integration error in most cases to be reasonable at the timestep allowed in the implicit method, there is no integration error check. The timestep in the Runge-Kutta method is selected to limit the relative integration error to 0.001 per timestep.

The user may encounter stiffness when using the Runge-Kutta method. For the reader unfamiliar with the concept of stiffness, a set of differential equations is said to be stiff when the maximum allowable timestep for numerical stability in an explicit (e.g., Runge-Kutta) method is very short compared to the time scales of physical interest. Thus, stiffness can result in a very slow code and in expensive calculations. Unless the Runge-Kutta method is specifically required, in the event that stiffness is encountered, the user should switch to the implicit solution method. The implicit method has been found to be comparable in efficiency to the Runge-Kutta method in problems without stiffness and much more efficient in problems with stiffness. If the Runge-Kutta method is specifically required, Appendix C provides information that may allow the user to cope with stiffness.

A variety of features are available only in conjunction with the implicit method. These are (1) gravity-driven gas flow, (2) the instantaneous liquid DROPOUT model for water condensing in the bulk gas, (3) critical or choked flow, (4) aerosol transport between cells through settling, (5) an implicit model for pool boiling that is solved simultaneously with the flow equations, (6) the engineered vent model, and (7) the suppression pool vent model for a BWR.

Flow paths may be defined in the FLOWS input block, the ENGVENT engineered vent input block, and the SPVENT suppression pool vent input block. The regular flow paths (those originally present in CONTAIN 1.0) are defined in the FLOWS block. These flow paths are restricted by code architecture so that at most one such path can be specified between a given pair of cells. In a variety of cases, this architecture may be too restrictive. In these cases, the engineered vent flow path is available as an alternative.

The modeling options for the engineered vent include all of the modeling options available for the regular flow paths and others that are specific to engineered vents. The engineered vent is designed to overcome the restriction on regular flow paths that only one regular flow path may connect a given pair of cells. Unlike the regular paths, any number of engineered vents may connect a given pair of cells. In addition, the modeling options for each engineered vent connecting the two cells may be chosen completely independently.

The flow of gases, aerosols, and fission products through the suppression pool vent system of a BWR is modeled through a special flow path between cells representing the drywell and wetwell. If the vent exit is covered by the suppression pool, the flow is scrubbed in the pool before being introduced into the downstream cell. For an LMR, the suppression pool vent model is available and uses sodium rather than water pools. However, because the suppression pool vent model was developed specifically for water pools, not all modeling options are available.

The available models and options will be described in detail in the following subsections. First, Section 2.2.3.1 describes the atmosphere

thermodynamics calculation. Section 2.2.3.2 describes the three different models available for the flow rate. Section 2.2.3.3 then explains the various options at the user's disposal for controlling the flow path characteristics as functions of time.

Section 2.2.3.4 describes the BWR suppression pool vent model. The vent model consists of three parts: (1) a liquid flow model, (2) a gas flow and condensation model, and (3) two aerosol scrubbing models. The liquid and gas flow models are discussed in Section 2.2.3.4.1. The aerosol scrubbing models are discussed in Section 2.2.3.4.2.

2.2.3.1 The Thermodynamic State Calculation. From the component masses and the total internal energy U_i of the atmosphere, the thermodynamic state calculation determines the temperature T_i, pressure, enthalpy, and saturation condition of the atmosphere in cell i. The pressure P_i and the specific enthalpy H_i for the cell are given as sums over the thermodynamically active components in the atmosphere. These components include all noncondensable gases and the one condensable material appropriate to the reactor type. The material that is treated as being condensable in the atmosphere is the material H2OV for an LWR and the material NAV for an LMR. All other materials specified as gases in the CONTAIN 1.1 material tables and those user-defined materials specified to be gas phase are treated as noncondensables.

The pressure of the noncondensable gases, or of a condensable vapor under superheated conditions, is given by the ideal gas relation. Under saturated conditions, the pressure of the condensable gas is equal to the saturation vapor pressure $P_{sat}(T_i)$. Standard CONTAIN materials use analytic expressions for the saturation vapor pressure, and for the specific enthalpies of the noncondensable and condensable gases. These analytic expressions are contained within the code. For the properties of user-defined materials, the tables specified in the USERDAT input are used. Should the user choose to select the vapor phase of the reactor coolant as a user-defined material, the tabular enthalpy will be used, but CONTAIN's saturation vapor pressure calculation will still be employed. For a noncondensable gas, the specific enthalpy is taken from the analytic expression or the appropriate user-defined table. For the

condensable material, the specific enthalpy is given by a weighted sum over the vapor and liquid specific enthalpies.

The noncondensable gas enthalpies and the liquid and vapor enthalpies are assumed to be functions of temperature only and are the enthalpies under standard pressure (one atmosphere). The enthalpy is arbitrary to one additive constant; in CONTAIN 1.1 that constant is set by defining the enthalpy at 273.15 K to be zero for the noncondensable gases and the liquid fraction of the condensable material, and equal to the heat of vaporization for the condensable vapor. This convention should be observed in constructing the enthalpy tables for user-specified atmosphere sources and for user-defined materials.

Note that the above convention for the enthalpy gives slightly negative internal energies at low temperatures for the noncondensable gases because $U_i = H_i m_i - P_i V_i < 0$ near 273 K, where V_i is the cell volume and m_i is the cell atmosphere mass. Such negative energies are the result of the convention defining the arbitrary additive constant for the enthalpy or energy and are not the result of a problem with the code.

From the internal energy and the component masses it is necessary to invert the internal energy function to obtain the temperature. This is done iteratively. An initial guess for two temperatures close to the expected temperature is made. In practice, these first estimates are chosen to be close to the last known cell temperature. The internal energies for these temperatures are then calculated and compared to the total energy that should be in the cell. If no comparison is acceptable, a new temperature is selected, and the iterative process is continued until acceptable convergence occurs. In the implicit method, if more than 50 iterations are required, the calculation simply will abort. In the explicit method, if more than 30 iterations are required, a message warning of nonconvergence is given, and the calculation proceeds. The reason for proceeding is that a nonconverging thermodynamic calculation usually means that the integrator is trying to take too large a timestep. The Runge-Kutta integrator in that case will reject all values calculated for that timestep and start over with a smaller one. One should note that the inversion routines are extremely robust. Nonconvergence that is

not the result of too large a timestep is usually a symptom of a calculational fault outside the solver, such as a negative mass for the condensable gas. The code does check for negative masses, but intermediate calculations are sometimes performed prior to this check. Another potential cause of nonconvergence may be the use of user-defined materials as gas phase components of the atmosphere, particularly if coarse tables or data violating thermodynamic laws are specified.

It is important to have equilibrium between the liquid and vapor phases of the condensable material in the atmosphere. One storage location (i.e., that of H2OV or NAV) per cell is used to store the total mass of thermodynamically active condensable material. The fractions of liquid and vapor associated with the total mass are determined as required from the equations of state.

Two simple treatments of the liquid portion of the atmosphere condensable material inventory are available: the default treatment leaves the liquid in the atmosphere (e.g., as wet steam) to flow with the gas and contribute to its heat capacity; the alternative (provided the user has specified the implicit method) is to specify the DROPOUT keyword, which causes any such liquid to be instantaneously removed from the atmosphere of a cell and placed in the pool of that cell, if present.

Of course, the most accurate treatment lies intermediate between these extremes. For LWRs, specifying H2OL as the last aerosol component will have the effect of removing the condensable liquid from the atmosphere inventory by placing it on the aerosols through condensation. The result will be a continuous removal of suspended water from the atmosphere through aerosol deposition. In the absence of this option (e.g., for a FAST reactor or to save running time), it is up to the user to choose between the default and DROPOUT options on the basis of which would more realistically model the problem being considered. The DROPOUT feature is enabled only if aerosols are not specified in the problem.

2.2.3.2 Flow Models. Three different ways are available to calculate the flow in a flow path:

- The flow may be calculated from the pressure difference across the flow path in a manner that considers the inertia of the material in the flow path as well as the frictional flow resistance of the flow path itself. This is the inertial flow model available with either the implicit or Runge-Kutta integration method. With the implicit method, this model is used for most flow paths in which the flow is dynamically calculated. (Some special flow paths may use a quasi-steady flow model.) With the Runge-Kutta method, the user has the option of selecting the inertial model for all dynamically calculated flows. The flow is modeled as turbulent with critical flow limits on the flow rate when this model is used with the implicit method. The flow is modeled as turbulent and noncritical when this model is used with the Runge-Kutta method. The inertial flow model is described in Section 2.2.3.2.1.

- The flow may also be calculated from the pressure difference across the flow path by neglecting the inertia of the material in the flow path. The flow rate is assumed to come instantly to the steady state value appropriate to the pressure difference existing across the flow path. This is the quasi-steady flow model. The user has the option with the Runge-Kutta method to use the quasi-steady flow model for all dynamically calculated flows. In general, the user does not have the option to select the quasi-steady flow model for all flow paths with the implicit method. However, for some special flow paths, the implicit method may use a quasi-steady flow model. This model is discussed in Section 2.2.3.2.2.

- Finally, the flow may be set to a user-specified mass flow rate or a volumetric flow rate independent of the pressure difference. Section 2.2.3.2.3 describes the user-specified flow rate model.

Note that the suboptions and flow regimes within the Runge-Kutta method are rather complicated. To assist the reader these are illustrated in Figure 2-1. The various logic branches shown in Figure 2-1 will be discussed in the following sections, except for the REDUCE option for removing stiffness, which is discussed in Appendix C. In general, the implicit method, not the Runge-Kutta method, is recommended on the basis of more complete models and greater computational efficiency.

The flow equations will be discussed in terms of the flow between two cells: i and j. In the discussion below, W_{ij} is the total noncondensable gas and condensable material mass flow rate from i to j, and Q_{ij} is the convective energy transfer rate from i to j. (For the flow in the suppression pool vent, W_{ij} and Q_{ij} should be interpreted as the flow

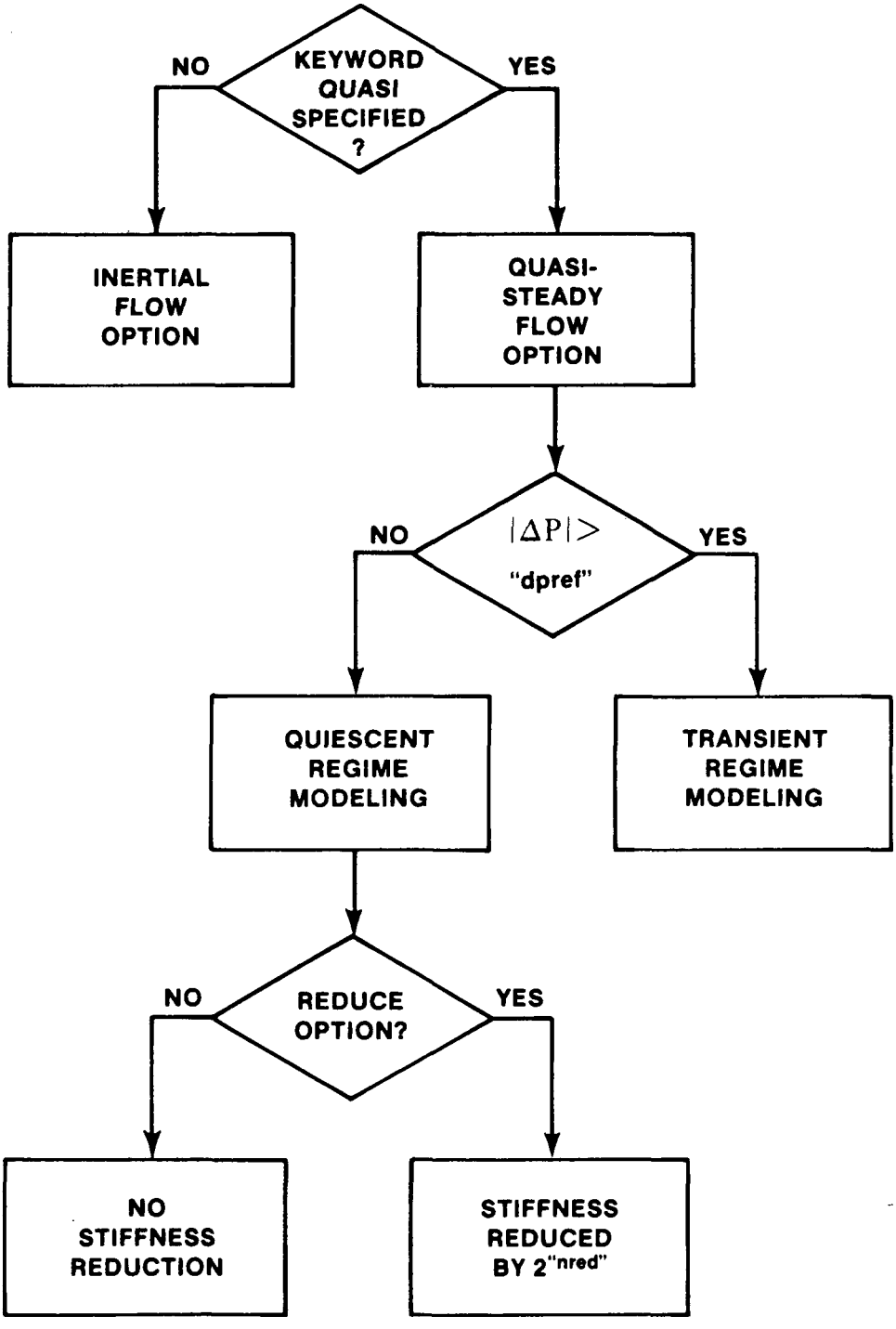

Figure 2-1. Explicit Flow Modeling Options in CONTAIN 1.1

entering the pool.) For all flow models, the mass flow rate for any component k of the atmosphere except possibly for aerosols is given by

$$W_{k,ij} = m_{k,u} W_{ij} / m_u \tag{2-1a}$$

and

$$Q_{ij} = H_u W_{ij} \tag{2-1b}$$

where u is the upstream cell (u = i if the flow is from i to j and u = j if the flow is from j to i), $m_{k,u}$ is the mass of component k in the upstream cell, m_u is the total mass of the gases and the condensable material (H2OV or NAV) in the upstream cell, and H is the cell specific enthalpy. In particular, the component k may be a dispersed, nonaerosol liquid or solid in the atmosphere (see Section 2.3.1.2).

The rate of change of the total internal energy in a cell due to flow includes both convective and gravitational contributions. The rate of change of the internal energy in the upstream cell is given by $-|Q_{ij}|$, whereas the rate of change of the energy in the downstream cell is $|Q_{ij}|+|W_{ij}|g(h_u - h_d)$, where h_u and h_d denote the cell center elevations of the upstream cell and downstream cell, respectively.

For aerosols within the implicit method a gravitational settling term may be present in addition to the convective term represented by Equation (2-1). In this case

$$W_{k,n,ij} = m_{k,u} W_{ij} / m_u + \rho_{k,n,u} v_{g,n,ij} A_{ij} \tag{2-2}$$

where $\rho_{k,n,u}$ is the aerosol component mass concentration in size class n in the upstream cell, $v_{g,n,ij}$ is the component of the gravitational

settling velocity along the flow path axis from i to j, and A_{ij} is the flow area.

2.2.3.2.1 The Inertial Flow Model. The inertial flow model takes into account the inertia of the gas in the flow path, as well as the lumped parameter frictional resistance. If a flow path is opened suddenly at a fixed pressure difference, the inertia delays the buildup of the flow rate to the steady-state value. If two cells are close to pressure equilibrium, the inertia manifests itself in a different manner. At the point at which the pressure difference becomes zero, the flow rate is generally finite because of the inertia of the flowing material. A finite flow rate will tend to reverse the direction of the pressure difference across the flow path. The reversal in the pressure difference will eventually reverse the direction of the flow. Under these conditions, damped oscillatory flow will occur.

For the inertial flow model, the flow equation is a simple acceleration equation:

$$dW_{ij}/dt = (\Delta P_{ij} - C_{FC}\left|W_{ij}\right|W_{ij}/\rho_{ij}A_{ij}^2)A_{ij}/L_{ij} \qquad (2\text{-}3)$$

The A_{ij} is the flow path area, L_{ij} is its effective length, C_{FC} is the turbulent flow coefficient, ρ_{ij} is the gas flow density, and ΔP_{ij} is the driving pressure difference. The last three quantities will be discussed in detail.

The turbulent flow coefficient C_{FC} is a dimensionless number, on the order of unity, that is typically determined empirically. C_{FC} as used here is related to discharge coefficients in conventional engineering references as follows:

$$C_{FC} = \frac{1}{2K^2} \qquad (2\text{-}4)$$

where K is equal to the discharge coefficient K defined in Reference Bau78 or the quantity C in Reference Flo79. In the notation of Chapter 4 of Reference Ide60, the CONTAIN C_{FC} corresponds to the quantity $g\Delta H/(\gamma\omega_o^2)$. In most cases discussed there, this quantity is equal to $\zeta/2$. However, one must be careful since Reference Ide60 is not consistent in the definition of ζ. In some cases, ζ is based on the upstream velocity and not the velocity ω_o in the flow constriction.

In the Runge-Kutta method, the gas flow density ρ_{ij} is taken to be the simple average $(\rho_i + \rho_j)/2$ of the total gas and condensable material density in cells i and j. In the implicit method, it is taken to be the upstream density (ρ_i or ρ_j). The use of the average density is appropriate for a lumped parameter flow path, whereas the upstream density is more appropriate for a physical flow orifice or flow channel. The difference resulting from using one density over the other is not expected to be great.

The definition of the pressure difference ΔP_{ij} depends on user options. For the Runge-Kutta method, ΔP_{ij} is simply the difference in the cell pressures $P_i - P_j$. (The cell pressure is interpreted as the mean pressure in the cell or the pressure at its center of mass.) With the implicit method, the user may specify elevations for the cell center and the ends of the flow paths, and therefore ΔP_{ij} can be more precisely calculated as the pressure difference across the two ends of the flow path. When gas gravitational head corrections between elevations are considered, the more complicated expression given in Equation (2-8) below results.

Critical, or choked flow effects are not considered in Equation (2-3). With the Runge-Kutta method, critical flow is not taken into account at all. With the implicit method, however, critical flow is taken into account in a simplified manner for all flow paths except the special one representing the BWR suppression pool vent. The method used is to limit the flow velocity to the sound velocity in the direction of the pressure drop. For the case that $P_i > P_j$, this is equivalent to setting

$$W_{ij} = \text{Min} \left(W_{ij} , W_{ij}^{c} \right) \tag{2-5}$$

where the critical flow is given by the standard expression [Bir60]

$$W_{ij}^{c} = A_{ij} v_{ij} \left[\gamma_i P_i \rho_i f_i \right]^{1/2} \tag{2-6}$$

where

$$f_i = \left[\frac{2}{1 + \gamma_i} \right]^{(\gamma_i + 1)/(\gamma_i - 1)} \tag{2-7}$$

and where γ_i is the specific heat ratio in cell i and $v_{ij} < 1$ is the vena contracta factor, the ratio of the minimum area intersected by the flow streamlines to the geometric cross-sectional area A_{ij} of the flow path.[Lam45]

If the implicit integration method is selected, the user may also model the effects of gas gravitational heads on the flow. For the regular flow paths, as shown in Figure 2-2, the keywords ELEVCL and ELEVFP are used to enter the elevation information; ELEVCL is used for the cell center elevation, and ELEVFP is used to specify the elevation of each end of the flow path. Note that the elevation of each end must, in general, be entered separately. For engineered vents, ELEVCL in the FLOWS block is still used. However, VELEVB and VELEVF are used to specify the elevations of the two ends of a vent. If the elevation of either end of a flow path or vent is not specified, that elevation by default is set to the cell center elevation. Cell pressures in CONTAIN are assumed to coincide with the pressures at the cell centers or centers of mass of the cells. The user interested in using the ELEVFP, VELEVB, and VELEVF keywords should read the cautionary note at the end of this section.

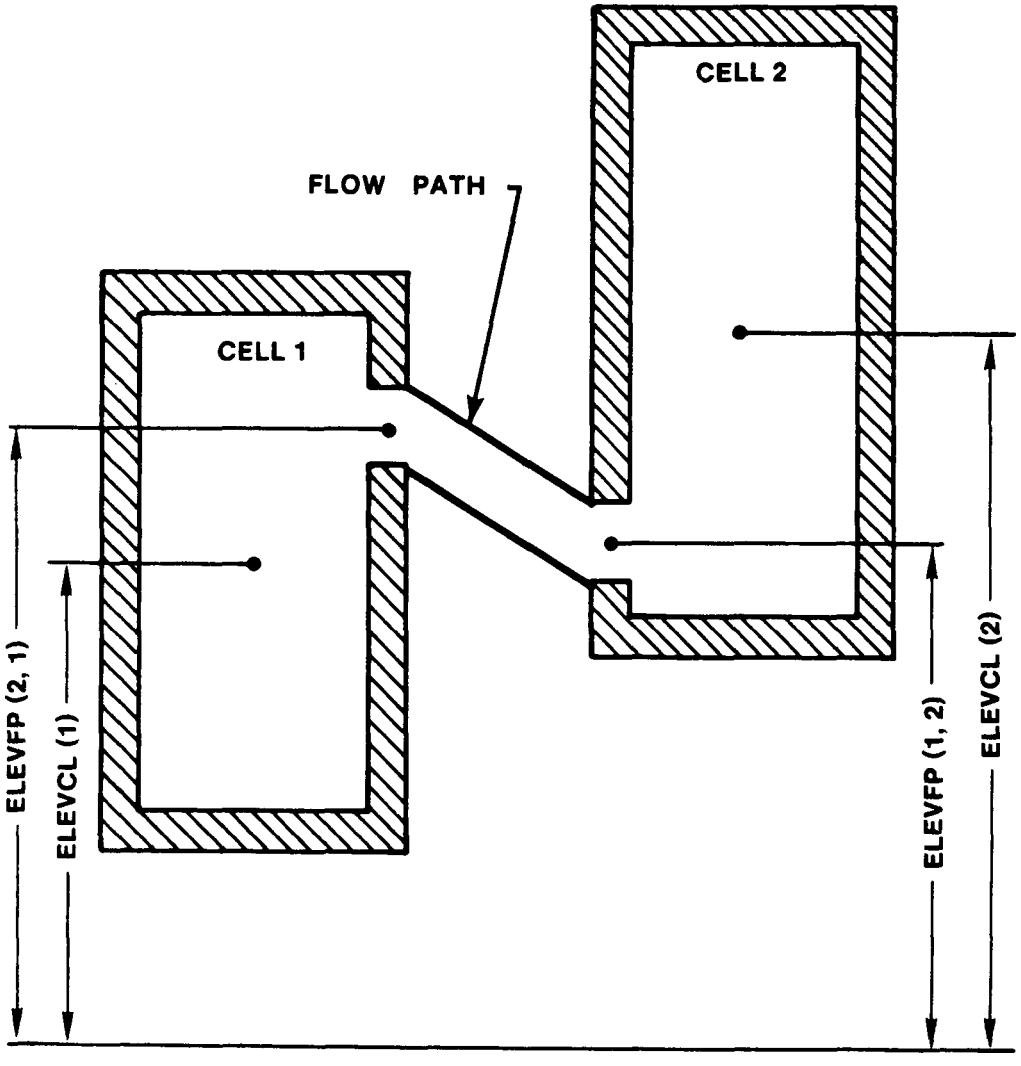

Figure 2-2. The Elevations of Cells and Flow Path Ends Used to Calculate Gas Gravitational Head Corrections

Consider two cells i and j connected by a flow path. The gravitational head, $g\rho_i(h_i - h_1)$, for the difference in elevation h between the center of cell i and the end (labeled 1) of the flow path attached to i is based on the gas and condensable density ρ_i in cell i. Similarly, the gravitational head, $g\rho_j(h_j - h_2)$, between the center of cell j and the end (labeled 2) of the flow path attached to j is based on the density ρ_j in cell j. The gravitational head developed within the flowpath, $g\rho_a(h_1 - h_2)$, is based on the average $\rho_a = (\rho_i + \rho_j)/2$ of the densities of the two cells.

The expression for the ΔP_{ij} in Equation (2-3), including the effects of the gravitational head within each cell and the acceleration due to gravity in the flow path, is

$$\Delta P_{ij} = P_i - P_j + g\,\rho_i\left(h_i - h_1\right) + g\,\rho_a\left(h_1 - h_2\right) - g\,\rho_j\left(h_j - h_2\right) \qquad (2\text{-}8)$$

Note that the use of the average, rather than donor, density precludes the modeling of certain effects such as siphoning. These effects, important for liquid flow, are believed to be minor effects for gas flow.

Caution: the ELEVFP, VELEVB, and VELEVF keywords give the user the flexibility to attach the end of a flow path to a cell at any elevation. This flexibility is often useful in modeling first-order gravitational effects on the pressure, as incorporated in Equation (2-8) above. However, second-order (and higher order) effects resulting from the variation in density within a cell due to gravity are, in general, not properly treated in Equation (2-8). The proper treatment of these second-order effects, in general, requires knowing the density variation that would be present in the cell if a finer nodalization of the cell were used. That information is clearly not readily available. First-order effects are sufficient to describe strong natural convection currents, such as those present in a containment with heat sources that represent a moderate fraction of the decay power present for the first few days after

shutdown. However, the improper treatment of second order effects will, in general, prevent the eventual equilibration of such convection currents. In some cases, it may also prevent the formation of a stable stratification. The difficulty is that the integral for the gravitational head around a closed loop formed by a set of flow paths will in general not be correct to second order and, in particular, may not vanish as it should at equilibrium.

An estimate of the importance of second-order effects can be made by assuming a uniform linear variation in density throughout the system. (Such a uniform linear variation does not address local effects such as those due to hot spots within one cell.) If the density ρ is assumed to vary as $\rho \approx \rho_0 (1 - ah)$, then it can be shown that the additional term

$$\Delta G_{ij} = -\frac{1}{2} a\rho_0 g \left[\left(h_i - h_1\right)\left(h_i - h_2\right) - \left(h_j - h_1\right)\left(h_j - h_2\right)\right]$$

should appear on the right of Equation (2-8), when effects through second order in h are correctly treated. Note that this term vanishes if the flow path ends are specified to be at the cell center elevations $\left(h_1 = h_i,\ h_2 = h_j\right)$, which is the default if ELEVFP, VELEVB, or VELEVF are not used. The use of these keywords to specify elevations different from those of the cell centers is not recommended unless either (1) the second-order correction terms ΔG_{ij} vanish from symmetry, (2) the configuration is such that the sum of ΔG_{ij} around all flow path closed loops important for natural convection vanishes, or (3) the sensitivity of the calculation to second-order effects is determined through separate hand calculations or refinements in the nodalization.

2.2.3.2.2 The Quasi-Steady Flow Model. The quasi-steady flow model is used with the quasi-steady flow option within the Runge-Kutta method and also for special models available with the implicit method, such as the suppression pool vent flow path model.

The flow resistance in the quasi-steady flow model is controlled by a linear flow coefficient (C_{LFC}) and a turbulent flow coefficient (C_{FC}),

which is discussed after Equation (2-4). The back pressure or flow resistance ΔP_{ij} for a given total flow rate W_{ij} is

$$\Delta P_{ij} = C_{LFC} W_{ij} + C_{FC} \left| W_{ij} \right| W_{ij} / \rho_{ij} A_{ij}^2 \qquad (2\text{-}9)$$

Note that this equation is obtained by setting the left side of Equation (2-3) equal to zero (i.e., neglecting acceleration) and adding the linear flow resistance term containing C_{LFC}. This term is modeled after laminar flow resistance, but its primary purpose is to remove a singularity at the point of flow reversal in quasi-steady flow. The linear flow resistance term is analogous to the artificial linear viscosity often used to stabilize fluid-in-cell hydrodynamic calculations.

The applications of Equation (2-9) with the implicit method are discussed elsewhere. The remainder of this section discusses quasi-steady flow in the context of the quasi-steady flow option available with the Runge-Kutta method. This option has a number of features besides the neglect of inertia to enable calculations to proceed quickly. It should be considered only if the user needs to assess integration errors. In general, the implicit method is the preferred method.

The modeling of the flows in the quasi-steady flow option distinguishes, for practical reasons, between two different flow regimes expected in containment analysis (see Figure 2-1). The transient regime is characterized by large pressure differences between cells. The flow is typically turbulent. The large pressure differences are generated by large sources within the cells. In general, the pressure differences change rapidly with time. Because of the magnitude of the sources, they cannot be sustained and are typically of short duration. The flow path resistance is modeled accurately in this regime.

The quiescent flow regime is characterized by pressure differences that are very small in comparison to the pressures in the cells. The cell pressures are expected to have nearly attained their steady state values. However, the pressures need not have fully equilibrated; the flow may

continue because of small sources and sinks within the cells. In this regime, the flow rate is expected to be controlled primarily by source rates within the cells rather than by the flow path resistance. Although the flow rates are low, the quiescent periods are relatively long. The cumulative effects of the flow in this regime may therefore be important. The flow may enter the transition or laminar flow regime.

The user may set the value of C_{LFC} through the "dpref" value, which is the pressure difference at which the flow resistance will cross over from turbulent to linear. By definition, when $|\Delta P_{ij}|$ is equal to "dpref", the two terms in Equation (2-9) are equal. It follows that

$$C_{LFC} = \left["dpref" C_{FC}/2\rho_{ij}A_{ij}^2\right]^{1/2} \qquad (2\text{-}10)$$

At much smaller pressure differences the linear term will dominate, while at much larger pressure differences the turbulent term will dominate. The default value for the cross-over point is "dpref" = 1000 Pa.

The artificial linear flow resistance term means that, in general, the flow resistance will not be modeled accurately for pressure differences less than "dpref". Two questions arise here: the magnitude of the flow into a given cell, and the distribution of the flow among parallel paths.

It is expected that the magnitudes of the steady-state flow rates into a cell under quiescent conditions will be determined by the sources in the problem and will not depend on the flow resistance. The inaccurate modeling of the flow resistance means, however, that the pressure differences between cells and therefore the pressures in the cells will be slightly in error. The inaccuracy in the cell pressures will be comparable to or less than "dpref". Therefore "dpref" should be set to a value that is negligible compared to the pressure within the cells.

The desired level of accuracy in the pressure calculation is problem-dependent, but consideration should be given to the sensitivity to pressure of pressure-dependent processes within the cell. In particular,

"dpref" should be chosen so that an inaccuracy in pressure on the order of "dpref" should have negligible effect on the source rate to the atmosphere.

The driving pressure that can be developed by certain sources could be much smaller than the default value of "dpref". These are typically heat sources with low potential for conversion of heat energy to work. Such sources lead to buoyancy effects such as natural convection, circulation, and stratification within an open volume. For reactor containments, buoyancy pressures on the order of 1 Pa are important. CONTAIN would run relatively inefficiently if "dpref" were reduced to the extent required to handle buoyancy pressures. For this reason, buoyancy effects are not modeled in the explicit option.

Another question that arises concerning the quiescent regime is the distribution of the flows among the possible parallel paths. (There is no such "flow-splitting" problem in the case of pure series networks.) The dependence of the flow path resistance on flow path dimensions is the same whether the flow resistance is dominated by the turbulent or the linear terms of Equation (2-9); the flow rate W_{ij} is proportional to the flow area in both cases. However, the dependence on the pressure difference is not the same. When the turbulent term dominates, W_{ij} is proportional to $(\Delta P_{ij})^{1/2}$. When the linear term dominates, W_{ij} is proportional to ΔP_{ij}.

This change in the flow law from square root to linear may affect the flow distribution among the possible parallel paths for the flow. This is clear from the example illustrated in Figure 2-3. Flow is occurring from cell 1 to cell 3 directly and also via cell 2. For simplicity, the gas densities, flow areas, and the turbulent flow coefficients are all set to unity. Mass sources at the indicated rates are provided to the cells based on a simple, steady-state solution of Equation (2-9). The ratio of the steady state flow distribution between paths (1,2) and (2,3) is 0.32:0.68 for a flow law that goes as the square root of the pressure difference and is 0.42:0.58 for a flow law which is linear in the pressure difference.

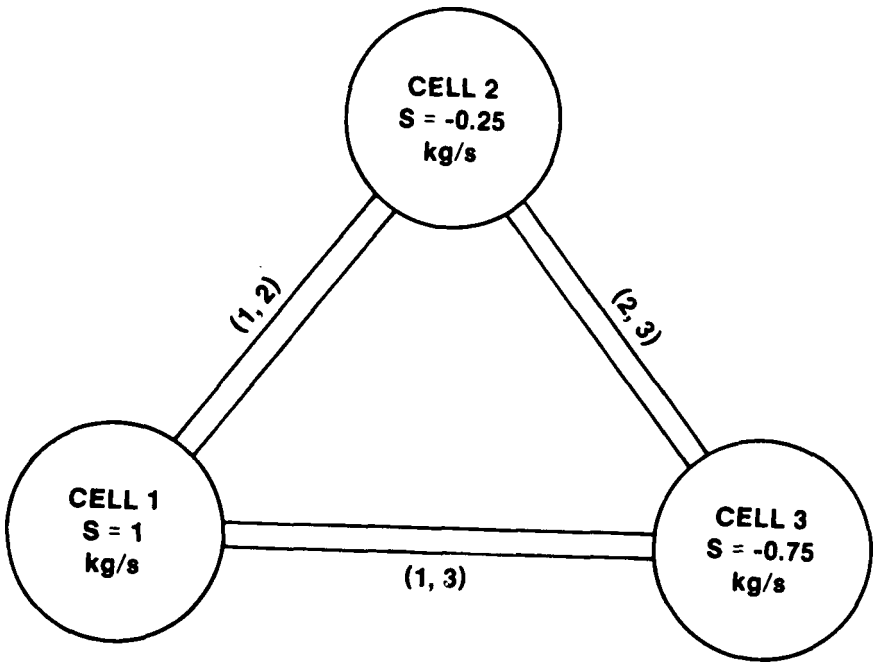

Figure 2-3. Flow in Parallel Paths Affected by Linear Viscosity

The user is encouraged to check the sensitivity of the calculation to the flow resistance modeling whenever the flow distribution is considered important. A reduction by a factor of four in "dpref" should be sufficient to check this sensitivity. In some cases, dominant paths exist that effectively make the configuration serially connected from the practical point of view. In these cases, the overall sensitivity to "dpref" should be slight.

2.2.3.2.3 User-Specified Flow Rates. The user may want to specify the flow rate as a function of time instead of the pressure difference between cells. With the regular flow paths, only constant mass or volumetric flow rates can be modeled. Although this flow can be turned on and off by opening and closing the flow path, the modeling is not very flexible. With the engineered vent, the flow rate versus time can be

specified with considerably more flexibility. The mass or volumetric flow rate can be directly specified as a function of time through tables.

Note that the flow rate for the regular flow paths with a user-specified flow rate may be completely different from that in versions prior to CONTAIN 1.1 if opening and closing options are used. In versions prior to 1.1, a constant flow rate (interpreted as leakage) would occur when the flow path was closed and pressure-driven flow would occur when the flow path opened. This logic is incompatible with newer features, such as aerosol settling through flow paths, which also use the area. The old logic has therefore been revised to permit flow (user-specified and pressure-driven) only when the flow path is open. If flow between two cells needs to be specified as a rate in one period and as a function of pressure difference in another, one can now simply use two parallel paths, which are allowed with the new engineered vent flow paths.

2.2.3.3 Flow Path Configurations and Control Options. The user may specify at most one regular flow path between a given pair of cells. However, any number of engineered vents may be specified in parallel. The suppression pool vent flow path may be placed in parallel with a regular flow path or any number of engineered vents. However, only one suppression pool vent flow path may be specified per problem. Note that the engineered vents and the suppression pool vent may be used only with the implicit solution method.

There is no additional restriction on the connectivity of the network of cells and flow paths. Futhermore, with the implicit method, the number of flow paths or vents has only a minimal impact on calculational efficiency. The reason is that the size of the solution matrix depends only on the number of cells and not on the number of flow paths.

A special option is available to increase the computational efficiency in problems with large cells, called environment cells, whose purpose is to provide a constant pressure boundary condition or to keep track of inventories released from other cells. If the environment cells are sufficiently large, they no longer need to be solved implicitly. In order to reduce the size of the solution matrix in problems with such

cells, the user should specify IMPLICIT = "nimpli", where "nimpli" is the number of interior (or nonenvironment) cells. In this case the implicit method will be used to solve for the first "nimpli" cells, and an explicit approach (not Runge-Kutta) will be used to solve for the rest. The interior cells should be numbered lower than the environment cells, and for the explicit approach to be stable, the environmental cells must be very large (on the order 10^{10} m^3).

Each flow path or vent may be opened at a specified time (using TOPEN or VTOPEN) or at a given pressure differential (using DP or VDP). Each can also be closed at a specified time (using TCLOSE or VTCLOS). Flow and aerosol settling will occur in a path or vent only if it is open.

The area of an open path or vent can be specified as a function of time or pressure difference through tables. For the regular flow paths, the table input is activated through the keyword VAR-AREA, and the independent variable in the table is either time or pressure difference across the flow path. The dependence on the pressure can either be reversible or irreversible, depending on the flag set by PDAFLAG. In the irreversible case, the area returned from the table for an open flow path can either stay the same or increase, but it cannot decrease. Note that upon closing of the flow path (through TCLOSE) the table values will be overridden, and the area will be set to zero.

Table input analogous to the above is also available for engineered vents. A new feature for the reversible area table is that the pressure used to determine the area from the table is the implicit, end-of-timestep pressure calculated in the flow solver. In contrast, in the analogous option for regular flow paths, the pressure used is the beginning-of-timestep pressure. The use of the end-of-timestep pressure eliminates chatter in the area chosen from the table when the change in area with respect to pressure in the table is rapid, as in the modeling of one-way doors in ice condenser plants. One disadvantage of this approach is that such rapid changes may cause convergence difficulties. In case of convergence difficulty in the flow solver, the change in area with respect to pressure in the table should be reduced.

2.2.3.4 BWR Suppression Vent Flow Path Model. The vent system of a BWR is a passive safety system designed to limit the pressure response of the drywell under accident conditions. Typically, drywell pressurization forces gas through the pressure suppression pool, which condenses steam and retains radionuclides. Although three different vent system designs are used in the U.S., the model in CONTAIN is of a generic nature; plant-specific modeling details are generated by specifying generic input parameters. Figure 2-4 shows the generic model parameters as defined for the nominally vertical vent configuration used in a General Electric Mark I or Mark II BWR; Figure 2-5 shows the generic model parameters as defined for a horizontal vent configuration used in a Mark III BWR. In these figures, "elevnt" is the elevation of the vent opening above pool bottom, "vntlen" is the length of the vent which can support water without overflow into the drywell, and "avnt" is the area of a single vent.

The vent model is activated at the global level by the keyword SPVENT and can be used only in conjunction with the implicit flow solver option. In the simplest configuration with a vent flow path, two cells are required, one for the wetwell and one for the drywell. A pool must be specified as part of the lower cell input of the wetwell cell, and this pool should include both the vent inventory and wetwell pool inventory. For a Mark III, it should also include the drywell annular pool inventory. The area of the pool specified in the lower cell input for the wetwell cell should include all of the free surface associated with these inventories. If present, the inventory of aerosols and fission products that have been scrubbed out of the gas passing through the pool is always associated with the wetwell lower cell inventory.

The SPVENT input block is used to specify the gas and liquid flow parameters in the vent and the suppression pool. It is also used to specify the aerosol and fission product scrubbing parameters in the pool. Other aspects of the suppression vent system can be modeled through other CONTAIN modules. For example, because the vent path can be specified independently of other types of flow paths, vacuum breaker operation between the wetwell and drywell can be treated by separately specifying a regular one-way flow path or an engineered vent from the wetwell to the

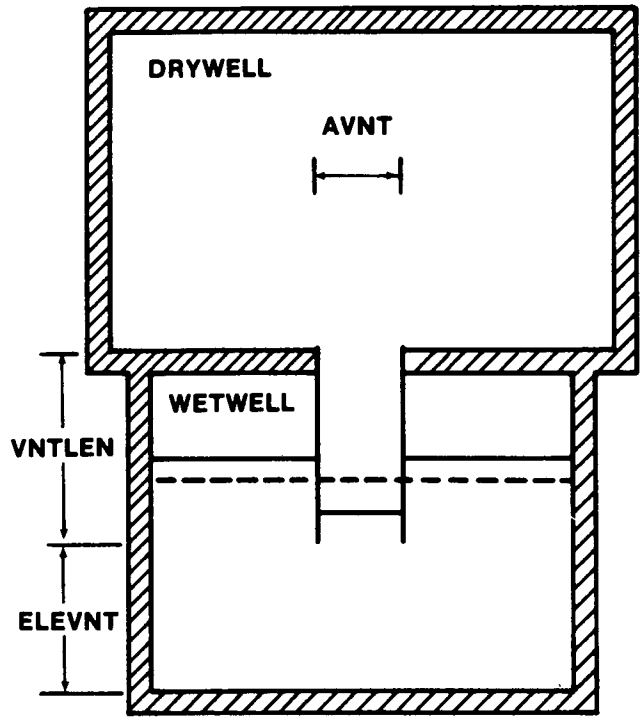

Figure 2-4. Vertical Vent System Schematic Used to Represent a Mark I or Mark II. The dashed line represents the normal water levels; the solid line, the displaced levels.

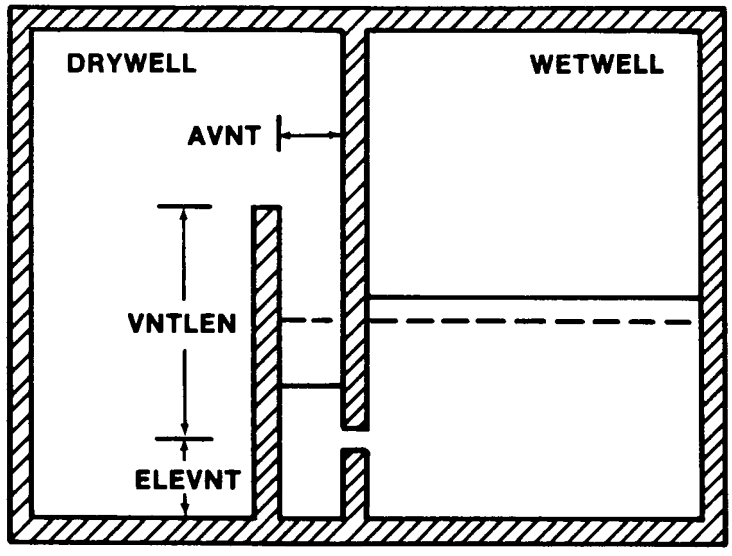

Figure 2-5. Horizontal Vent System Schematic Used to Represent a Mark III. The dashed line represents the normal water levels; the solid line, the displaced levels.

drywell. Other suppression pool features that can be modeled include recirculation cooling (simulated through the use of the Q-VOL lower cell volumetric heating model), discharge from the primary system safety relief valve lines (using the SRV discharge model), and return of pool overflow from the drywell back to the wetwell (using the engineered system overflow model).

2.2.3.4.1 Suppression Pool Vent Thermal Hydraulic Model. Liquid levels in the wetwell and vent (or wetwell and annulus of the Mark III design) are computed explicitly once per system timestep. The liquid levels are adjusted first according to any change in inventory and density of the pool over the timestep, and then according to a liquid velocity calculated from gas pressure differences and liquid heads. A quasi-steady liquid flow model is used to determine the liquid velocity. The equation for the liquid velocity is based on a Bernoulli mechanical energy balance equation [Bir60] for isothermal, incompressible fluid flow with an effective loss coefficient. For flow from the drywell to the wetwell, the balance equation is

$$\Delta P_{dw} + g\rho_{\ell}\Delta h_{dw} + (1/2)\rho_{\ell}\, v_{\ell}^2\, f_{dw} = 0 \qquad (2\text{-}11)$$

where $\Delta P_{dw} = P_{wet} - P_{dry}$, the difference in the drywell and wetwell gas pressures, $\Delta h_{dw} = h_{wet} - h_{dry}$, the difference in the liquid levels on the drywell and wetwell side of the pool, v_{ℓ} is the liquid velocity on the drywell side, ρ_{ℓ} is the liquid density, and $f_{dw} = \beta^2 - 1 + (1 - \beta)^2 +$ "fdw". The variable β is the ratio of the vent total area "nsvnts"*"avnt" to pool total area and "fdw" is the user-specified liquid loss coefficient for the drywell to wetwell direction. Here "nsvnts" is the user-specified number of vents of area "avnt". Note that the definition of f_{dw} explicitly includes, through the term $(1 - \beta)^2$, the loss coefficient for sudden expansion and that this should not be included in the user-defined "fdw". Turning and contraction losses, however, should be included. For flow from wetwell to drywell, there is an analogous equation to Equation (2-11) but with drywell and wetwell indices interchanged. In that equation, $f_{wd} = 1 - \beta^2 +$ "fwd". Note that in the gas

pressure difference in Equation (2-11) and in other equations used for the vent model no correction is made for the gas gravitational head between the cell centers, where P_{dry} and P_{wet} are defined, and the pool surface.

The vent, if covered, can have three possible states with respect to gas flow. It can be open in the normal forward direction, from drywell to wetwell; it can be open in the reverse direction, from wetwell to drywell; or it can be closed to gas flow. To avoid possible numerical difficulties in the gas flow calculation, the effective gas flow area A_{eff} is assumed to vary linearly from zero at the opening point to the value "avnt" over a pressure difference range specified by the user. This range is either "dpwet" or "dpdry" depending, respectively, on whether the flow is from the drywell to wetwell, or vice versa. The opening point is defined as the pressure difference required to support the liquid head present when the vents just begin to open. The flow rate of gas W_{sup} entering the pool is calculated as quasi-steady flow according to the formula

$$W_{sup} = \left[|P_{wet} - P_{dry}| \; \rho \; \text{"nsvnts"}^2 \; A_{eff}^2 \right]^{1/2} \qquad (2\text{-}12)$$

where ρ is the gas density of the upstream cell and P_{wet} and P_{dry} are the pressures of the wetwell and drywell, respectively. The actual effective gas flow area used is calculated self-consistently in the flow solver to eliminate numerical surging.

For vents in the bypass (uncovered) state, the flow equation used is Equation (2-3) with the i and j indices interpreted to refer to the vent flow. The turbulent flow coefficient used is $C_{FC} = 1$, the flow area used is A_{ij} = "nsvnts"*"avnts", and the gas inertial length used is L_{ij} = "ginlen", which is specified in the SPVENT input. The pressure difference ΔP_{ij} is taken to be ΔP_{dw}. Note that not all modeling features of a normal flow path are available for the vent in the bypass state. In particular, choked flow and gas gravitational head corrections are not modeled.

For a timestep during which the vent is calculated to open, the gas flow rate is scaled by the relative amount of time the vent is open. In the timesteps following the opening, the liquid head at the opening point (which coincides with the point at which the effective gas flow area goes to zero) is adjusted according to any change in pool conditions. If the gas pressure difference between the wetwell and drywell becomes inadequate to support the liquid head, the gas flow is set to zero. In the timesteps following the zero gas flow condition, the liquid velocity defined in Equation (2-11) is used to calculate the liquid levels dynamically. Note that once open in a given direction, the vent will remain open until the gas flow ceases. Because of this, it will take at least two timesteps for a vent to close in one direction and open in the reverse direction during a pressure reversal even though the liquid levels may adjust in a much shorter time.

Note that if more than one vent is specified ("nsvnts" > 1) , the vents are assumed to act in unison. There is at present no provision for the opening of vents at different elevations as present in a Mark III. To some extent one can accommodate vents at different elevations by defining the value of "dpdry" or "dpwet" to be the difference in pressure between that required to barely open the upper vents and that required to fully clear the lower vents, as opposed to that required to barely open and to fully clear a single vent.

The boiling of the suppression pool and the resaturation of bubbles of noncondensable gas passing through the pool due to vent flow is controlled by the lower cell BOIL keyword. If BOIL has been specified, the pool will flash as necessary to bring it down to saturation. Vent flow usually will cause additional vapor to evolve from the pool. If the vent is covered and noncondensable gas is present in the vent flow, this gas is assumed to come to temperature equilibrium with the wetwell pool and to saturate to 99 percent relative humidity, as determined from a self-consistently calculated bulk pool temperature and the wetwell cell pressure. The relative humidity limit removes the potential for evolution of a very large amount of vapor, compared to the noncondensable gas present in a bubble, for saturated pool conditions. The use of a 99 percent

humidity limit is probably more realistic than assuming complete equilibrium for a pool at saturation, due to the subcooling of the bubble wall when significant amounts of vapor are evolved. The use of a self-consistent bulk pool temperature, which takes into account the heat of vaporization of the vapor, also serves to limit the amount of vapor evolved and is important for shallow pools. If noncondensable gas is not present in the vent flow, vapor is condensed at the bottom of the pool and enough is flashed off at the top to leave the pool at saturation. The disposition of the vapor from the pool depends on the process generating it. Any vapor produced from the pool when it flashes down to saturation is directed to the wetwell cell atmosphere. The vapor evolved from the pool due to vent gas flow is conveyed to either the drywell or wetwell, whichever is the downstream cell. (The latter applies even when the vent flow is pure vapor.)

If the BOIL option has not been selected for the suppression pool, the vapor in the vent gas flow will condense in the wetwell pool. The noncondensable gas will come to temperature equilibrium with the pool, but there will be no resaturation of the noncondensable gas. (However, running the code without the BOIL option is not recommended.)

Suppression vents are designed to open from the drywell side; normally, they are prevented from opening from the wetwell side by vacuum breakers. Under some conditions, however, the pool may depress enough on the wetwell side to cause overflow of the suppression pool into the drywell. This overflow occurs in Figures 2-4 and 2-5 when the liquid level on the drywell side reaches "elevnt" + "vntlen". This liquid is transferred to the drywell pool, if specified; otherwise it is lost from the inventory. In modeling Mark I and II designs for situations where overflow may occur, it can be important to set up a second overflow system using an engineered system overflow model. (This requires specification of a lower cell pool in the drywell cell, which should not be confused with the suppression pool.) The reason is that the overflow should be allowed to drain back into the suppression pool when the wetwell pressure is relieved.

In the relatively unlikely case of reverse opening of the vents, one should note that there may be a problem with always using the wetwell pressure to calculate flashing and resaturation in the present single-pool representation of the suppression pool. In reverse opening, the relatively small amount of liquid in the vent for a vertical vent system or in the annulus for a horizontal vent system sees the drywell pressure rather than the wetwell pressure which is used to calculate the flashing and resaturation. This difference could be important in a transient situation. The problem with a more general two-pool description of the suppression pool is that the amount of liquid involved on the drywell side, neglecting amounts which have overflowed, is relatively small. The thermal mixing of this liquid with the bulk of the suppression pool, which provides the thermal reservoir for vaporization under transient conditions, would have to be modeled in order to calculate the vapor evolved at the drywell pressure. Use of the lower drywell pressure would increase the resaturation and flashing; limited thermal mixing would tend to decrease the resaturation and flashing. An appropriate thermal mixing model is presently not available.

For gas flow in the reverse opening case, the present use of the wetwell pressure and bulk pool temperature corresponds to the assumption that the sensible heat and vapor evolving from the pool on the drywell side are those for bubbles at equilibrium at the entry to the vent. If the thermal mixing is assumed weak and the water on the drywell side is assumed to have reached a quasi-steady-state temperature, the present model gives results close to the anticipated ones. The bubbles evolving into the drywell actually would be somewhat cooler, with somewhat more vapor in them, due to the exchange of sensible heat to vaporize more vapor into the bubbles, but this difference is not thought to be significant. With respect to flashing of the pool on the drywell side, one should note that in a transient in which most of the suppression pool water is available, reverse opening would result in a significant amount of liquid overflowing into the drywell. If a pool has been separately specified for the drywell, the flashing of the overflow will be calculated according to the proper pressure conditions. Thus the errors introduced by the use of the wetwell pressure in reverse opening for the drywell side of the suppression pool may not be significant.

As is generally the case for intercell flow in CONTAIN, nonaerosol suspended liquid and solid materials flow with the gas and are not trapped in the pool.

2.2.3.4.2 Suppression Pool Vent Aerosol Scrubbing Models. For thermal reactors, two models are available for scrubbing aerosol materials passing through vents; an adaptation of the SPARC code [Owc85b] and the model taken from the VANESA code [Pow86], which is referred to in CONTAIN as SCRUB. For fast reactors only SCRUB is available. These models are also used for the safety relief valve (SRV) discharge model described in Section 2.3.4. The SCRUB model is also used in conjunction with CORCON/VANESA. These models calculate the decontamination factors that arise from the scrubbing which takes place in the gas bubbles rising in the pool. The particle-size-dependent decontamination factors returned from these models are taken to lie in the range between 1 and 10^5. The upper limit is an attempt to account for effects not modeled, such as resuspension due to bubble breaking at the pool surface. Both of the models have been modified slightly for integration into CONTAIN. Note that these models make their own assumptions about the vapor evolution into rising bubbles; the discussion in the section above on vapor evolution in the thermal hydraulic calculation does not apply.

The original SCRUB model from VANESA, which assumes initially saturated bubbles, has been modified for CONTAIN through the addition of a decontamination factor which takes into account steam condensation in bubbles at the inlet. This calculation is identical to that used in the SPARC code. The SCRUB model is a direct application of Fuchs [Fuc64] treatment of the processes of sedimentation, impaction, and diffusion in spherical bubbles. In this model, the scrubbing efficiency is sensitive to the ratio of the gas circulation velocity to bubble rise velocity. The default ratio of 1.0 corresponds to the value used in the standard version of VANESA. If desired, the user may specify a larger value (e.g., to simulate elliptical bubbles with enhanced scrubbing) or a smaller value (e.g., to simulate the effect of surface impurities which inhibit circulation). The effects of bubble expansion during its rise through the pool are calculated assuming a constant number of moles of

gas in the bubble; a possibly significant approximation is the neglect of vapor evolution effects in rising bubbles.

The SPARC code [Owc85b], developed at Pacific Northwest Laboratories, is a much more detailed model that attempts to mechanistically treat a number of processes. As implemented, that code extends Fuchs' model explicitly to elliptic bubbles, treats deposition due to initial steam condensation, and includes sedimentation, diffusion, and inertial deposition in rising bubbles. It mechanistically accounts for bubble growth and the deposition limiting effects of vapor evolution during bubble rise. Details of the model can be found in Reference Owc85b. Several options in the original code are not implemented as they are either not recommended by the developers or not compatible with CONTAIN models. Particle growth due to condensation, bubble interior heat transfer, and particle solubility effects are examples of models which are either incompatible or not recommended. The pool equilibrium temperature calculation is also not implemented as it conflicts with the CONTAIN pool calculation.

The scrubbing depth for flow through the vents is the continually updated height of liquid covering the vent on the downstream side. If the vents bypass the pool, no scrubbing occurs. Any aerosols removed from the gas passing through the pool are considered deposited in the wetwell pool, along with any fission products hosted by these aerosols. Note that the scrubbing of fission products not hosted by aerosols, such as vapor phase iodine, is not modeled. These fission products pass through the pool without being affected. The targeted release and acceptance formalism may be useful in simulating iodine scrubbing; see Section 5.2.6.

2.2.4 Aerosol Behavior

Overview

Subjects discussed include general features of the aerosol modeling, initial aerosol and aerosol source size distributions, numerical considerations in the description of aerosol processes, modeling of agglomeration and deposition processes, condensation on and evaporation from aerosols, and transport of aerosols

by intercell flow. Aerosol processes are required for the mechanistic treatment of liquid water in the atmosphere and of removal of fission products in aerosol form from the atmosphere. Water aerosol removed from the atmosphere is transferred to the structure film or the lower cell pool. Once removed from the atmosphere, additional transport of solid aerosols is not modeled; however, the transport of fission products in liquid pathways may be modeled, including fission products that were previously carried by airborne aerosols.

One of the purposes of CONTAIN is to characterize the radiological source term to the environment in the event of containment failure. Released fission products are most effectively transported within containment and into the environment as gases and aerosols. The MAEROS aerosol model, a state-of-the-art code for modeling aerosol behavior in either wet or dry environments, forms the basis for the aerosol behavior model in CONTAIN.[Gel82] MAEROS uses a number "nsectn" of size classes, or sections, to represent the particle size distribution for the suspended aerosols. In addition, the code is designed to cope with the fact that certain aerosols, particularly the radiologically significant ones, may behave quite differently from other aerosols. Therefore, one may specify a number "nac" of aerosol species, or components, which are tracked individually and which can have independent source size distributions and source rates. Up to eight aerosol components can be specified. Thus MAEROS is said to be a multisectional, multicomponent aerosol model. Because particle size is an important characteristic governing the respirability of an aerosol, and because composition is important in determining consequences, MAEROS is particularly suited to applications where health effects are important.

The degree of cooperative behavior among the aerosol components is determined by the extent of agglomeration among different particles and condensation on the particles. MAEROS tracks the composition of a particle as a function of particle size according to the agglomeration and condensation history of the particle. For an LWR, condensed water can be one of the aerosol components; the condensation and evaporation of water vapor, as they affect the aerosol composition and size, are

modeled. There are, however, no corresponding models for the case of an LMR with sodium coolant.

The aerosol processes considered in CONTAIN are discussed in Sections 2.2.4.3 through 2.2.4.6. A more complete discussion is given in Reference Gel82. Aerosol processes are modeled for each of the upper cell atmospheres. The atmospheres are taken to be well mixed and stagnant in the sense that the average velocity of the cell atmosphere is assumed to be zero. Some degree of convection or turbulence is required to keep the atmosphere well mixed in the presence of stratification effects caused, for example, by settling. However, the degree of turbulence is assumed to be small. Turbulent agglomeration is modeled but has a small effect when the aerosol physics parameters are set to their default values. Turbulent deposition is not modeled (except in conjunction with certain ESFs, as described in Section 2.3.3.4). The flow of aerosols between cells via the intercell gas flow paths is modeled. The aerosol flow velocity is taken to be the gas convective velocity when an explicit flow option is used, and the sum of the gas convective velocity and the component of the aerosol settling velocity parallel to the flow path axis when the implicit flow option is used.

To run an aerosol calculation with nominal aerosol parameters, the user should specify the aerosol names and size distribution parameters ("amean" and "avar") for each aerosol component in the global AEROSOL block. The aerosol component names may be selected from either the AERNAMES or the COMPOUND material list (see Section 3.2.1). The size distribution parameters govern the initial distribution and the distribution of sizes in a source of new particles. For an LWR, H2OL should be specified as the last aerosol component if modeling of condensation on or evaporation from aerosols is desired. If H2OL is specified as the last aerosol component, the amounts of any water vapor condensed on aerosols will be added to the mass of that aerosol component. One may also specify an aerosol source table for H2OL to introduce water droplets directly into the problem, with a size distribution given by the "amean" and "avar" parameters. Initial aerosol masses and aerosol sources are specified in the cell AEROSOL block (see Section 3.3.1.8).

2.2.4.1 Initial and Source Size Distributions. Although the distribution of airborne particles among the "nsectn" size classes is generally unrestricted, the initial airborne size distribution and the distribution of sizes in a source of new particles are taken to be lognormal. The lognormal size distribution parameters governing the latter types of distributions are "amean" and "avar". Normally, these parameters are constants independent of time. However, the AERTIM option may be used to specify these parameters for aerosol sources as a function of time. A different size distribution may be specified for each aerosol component or species.

The lognormal distribution of mass m(D) in particles with a spherical equivalent diameter between D and D + dD is given by the standard expression

$$m(D)dD \propto \exp\left\{ -\frac{1}{2}\left[\frac{\ln^2(D/\text{"amean"})}{\text{"avar"}^2}\right]\right\}\frac{dD}{D} \qquad (2\text{-}13)$$

In aerosol terminology, "amean" is the volume-equivalent mass median diameter (i.e., the diameter of a fully dense spherical particle with the same mass as the mass median particle), and "avar" is the natural logarithm of the geometric standard deviation with respect to diameter.[Yos79] In CONTAIN, the above distribution function is integrated over each size class to determine the amount of aerosols within each size class. The parts of the distribution function lying outside the range of particle sizes considered by CONTAIN are truncated, and the distribution function within the range is renormalized.

2.2.4.2 Numerical Considerations. The CONTAIN aerosol module, as with MAEROS, is designed to use a small number of size classes, or sections, for computational efficiency. A sensitivity study has shown that a particle diameter range between 10^{-7} and 10^{-4} m can be handled adequately by ten sections in a typical case.[Lei84] However, because the aerosol calculation in CONTAIN is typically not a time-limiting factor in a general containment calculation, it is recommended that no fewer than 20 size classes (the default number) be used without testing. The upper

limit on the number of size classes that can be used is dictated by the constraint given in Equation (2-15) below.

The lower and upper diameters for the particle sizes considered in the calculation are given by "diam1" and "diam2", respectively. These are defined as the diameters of fully dense, spherical particles having the same masses as the irregularly shaped aerosol particles. The "nsectn" + 1 size class boundaries are determined by partitioning the interval ["diam1","diam2"] geometrically; that is, the interval [ln("diam1"), ln("diam2")] is divided evenly. The default values of "diam1" = 10^{-7} m and "diam2" = 10^{-4} m give satisfactory results in a number of containment situations. The user is cautioned that a value smaller than 10^{-7} m for "diam1" may introduce stiffness into the calculation and increase the execution time considerably.

A lower bin and an upper bin have been added to keep track of the mass of particles that become undersized or oversized, respectively. (Such masses are referred to as "mesh" losses in the following discussion.) A particle can become undersized through evaporation of water. It can become oversized through condensation of water vapor or agglomeration. The disposition of the mass that leaves the mesh is controlled by the cell OVERFLOW option discussed in Section 3.3.1.11. (This OVERFLOW option should not be confused with the engineered systems OVERFLOW component.) By default, the mass in the lower bin is assumed to be deposited onto the floor structures, if present, in the cell in which the mesh losses occur. Likewise, the mass in the upper bin is assumed to be deposited instantly onto the floor structures. If more than one floor structure is in the cell, the mass is divided among the structures according to surface area. If no floor structures are available in the cell then the mass leaving the mesh will be diverted to the pool if one is available. Finally, if a pool has not been defined, the mass will be lost from the problem and placed into a waste holding location. The cell to which the mesh losses are directed may be specified through the cell OVERFLOW option. (This is the same option that determines the destination of the condensate runoff from structures.) If the specified overflow cell number is positive, the mesh losses will be diverted to the specified cell. The rules concerning the repositories in which the mesh

losses are placed in the specified cell are the same as those for the default cell. If the specified cell number is negative, all undersized aerosols are returned to the smallest size class. Oversized aerosols are considered to be lost from the mesh as usual and are directed to the cell given by the absolute value of the specified cell number. If the overflow cell is specified by the user to be zero, all aerosol mesh losses, including water, are removed from the problem and placed in the waste holding array.

Note that a default settling surface is not automatically defined, as in versions prior to CONTAIN 1.1, for cells without structures. Also mesh losses are no longer placed in the floor deposition location if floors are not present. For cells without floors, aerosol settling through flow paths should be activated (e.g., by giving the FPCOSN keyword in the FLOWS input block) and natural circulation should be modeled. Otherwise, substantial mesh losses will most likely occur (especially under condensing conditions) and will then be placed into the pool or waste holding location.

The large range of diameters that must be represented by a small number of size classes implies that standard finite difference methods, which attempt to represent a continuous function by its value at closely spaced mesh points, have little utility. The aerosol module, as with MAEROS, for the most part makes no attempt to model the overall particle size distribution as continuous. Instead, it models the aerosol behavior of bins of particles, each bin representing particles within a size class. The distribution of particles within a size class is not interpolated from adjacent size classes; rather, it is assumed to be fixed and logarithmically distributed. The amount q(D)dD of mass per cubic meter present as particles with diameters between D and D + dD is assumed to vary as

$$q(D)dD \propto d(\ln D) = dD/D \qquad (2\text{-}14)$$

Equation (2-14) is used to convert the integro-differential aerosol behavior equations to ordinary differential equations in time.

To integrate the ordinary differential equations forward in time, the kernel for agglomeration and the rate constants for aerosol deposition and condensation on aerosols need to be known on the basis of the size classes used. For example, the kernel β_{ijk} might be the kernel for agglomeration of all particles in size class i with those in size class j, which results in a particle in size class k. When defined on the basis of size classes, the agglomeration kernel and the rate constants are referred to collectively as coefficients. Most of the coefficients involve the kernel and require a two-dimensional integration over particle sizes, using Equation (2-14) for the functional dependence within a size class.

A simplification in the coefficients occurs if the geometric constraint

$$m_{i+1}/m_i > 2 \qquad (2\text{-}15)$$

is satisfied, where m_i is the particle mass at the i-th size class boundary. The geometric constraint ensures that the agglomeration of two particles results in a new particle which will fit into either the size class which contains the larger of the two original particles or the size class above it. This constraint thus reduces the number of agglomeration coefficients; it is assumed to hold in CONTAIN and in MAEROS. The input mesh values should be checked to ensure that it is satisfied, since CONTAIN does not check.

The calculation of the coefficients is somewhat costly; a full calculation for 20 size classes requires about 10 CPU seconds on a CRAY 1S computer. Therefore, the coefficients are either read in from a tape or calculated on the first call to the aerosol model for use throughout the entire problem. Using a constant set of coefficients imposes some modeling constraints, however. This is because parameters embedded in the coefficients are also effectively held fixed, despite the fact that

they should vary with changing conditions during the problem. A simple multiplier in a coefficient should not be considered embedded because the coefficient can be calculated for a unit multiplier and rescaled when used. In fact, the deposition coefficients, except for settling, are calculated for a unit forcing factor. The coefficient set employed in CONTAIN 1.1, uses $8(\text{"nsectn"})^2 + 28\text{"nsectn"} - 8$ storage locations.

The following constraints pertain to the current coefficient set:

- The aerosol material density is assumed to be the same for all components.
- The particle shape, as modeled by the dynamic and agglomeration shape factors, is independent of the particle composition.
- The medium in which the aerosol processes are assumed to occur has fixed composition and is taken to be air.
- The degree of turbulent agglomeration, is fixed throughout the problem. This is controlled by the turbulent dissipation coefficient, "turbds".
- Other parameters that control deposition rates do not depend on particle composition. For example, the ratio of the thermal conductivity of air to that of the aerosol material, "tkgop", is fixed.

The pressure and temperature of the atmosphere are embedded in these coefficients and are fixed for a single set of coefficients. However, the aerosol module actually calculates four sets of coefficients at points given by combinations of two temperatures ("tgas1", "tgas2") and two pressures ("pgas1", "pgas2"). Changing thermal-hydraulic conditions during the problem are accommodated by interpolating between these sets of coefficients. The "tgas1", "tgas2", "pgas1", and "pgas2" parameters should be chosen to bound the temperatures and pressures expected.

At the expense of larger sets of coefficients, some of the constraints above can be removed by interpolating to accommodate other changing parameters or by separating the coefficients so that a relevant parameter is not imbedded. For example, by neglecting turbulent agglomeration and approximately doubling the number of coefficients, the constraint that the material density be the same for all components can be removed.

However, for most aerosol problems, and in particular for LWR containment applications problems that do not model the reactor coolant system, the present choice for the coefficient set appears adequate.

The ordinary differential equations governing agglomeration, deposition, and condensation on aerosols are integrated forward in time using a Runge-Kutta method with its own timestep control. The parameters "reltol" and "abstol" control the error tolerance during this integration. Agglomeration, deposition, and condensation are assumed to occur in a closed cell during the Runge-Kutta integration, and changes in the aerosol population due to intercell flow are incorporated separately at every system timestep.

2.2.4.3 Agglomeration. The CONTAIN aerosol module treats the same three agglomeration processes included in the MAEROS code: Brownian, gravitational, and turbulent agglomeration. The aerosol input parameters controlling these processes are the material density "densty", the dynamic shape factor "chi", and the agglomeration shape factor "gamma". In addition, the degree of turbulence and the amount of turbulent agglomeration are controlled by the turbulent dissipation coefficient "turbds". The user also has control over the collision efficiency during gravitational agglomeration. The collision efficiency can be either set to a nonzero user-specified constant value "coleff" or otherwise defined in terms of an internal analytic expression.[Gel82] Use of the default value for all parameters should give reasonable results for LWR containment conditions in the absence of a large degree of turbulence. As noted in Section 2.2, CONTAIN is not designed to model aerosol processes in conjunction with highly turbulent jets or pipe flow.

2.2.4.4 Deposition. The CONTAIN aerosol model treats four mechanisms for deposition onto surfaces of heat transfer structures: gravitational settling, diffusiophoresis, thermophoresis, and particle diffusion. Diffusiophoresis as defined here is the migration of aerosol particles to surfaces in the flux of coolant vapor condensing on the surfaces. Note that these and other deposition mechanisms are also modeled in conjunction with the operation of engineered safety features and with scrubbing in the suppression pool of a BWR.

The driving forces for all deposition mechanisms except particle diffusion are calculated mechanistically. The diffusiophoretic velocity, which is related to the drift velocity of the coolant vapor condensing onto structure surfaces, is calculated if the CONDENSE option is specified. The diffusiophoretic velocities are calculated for each structure surface lying in the cell in which the structure is defined. The temperature gradient in the gas boundary layer at a structure surface is the driving force for thermophoresis. It is also determined for each surface and is calculated on the basis of the sensible heat flux to the surfaces and the gas conductivity in the boundary layer. The parameter "tkgop", the ratio of the gas thermal conductivity to that of the particle, enters the expression for thermophoresis. It is used in the same way in CONTAIN as it is in MAEROS.[Gel82]

The driving force for particle diffusion is represented by the inverse of the particle diffusion boundary layer thickness "deldif", which has a default value of 10^{-5} m. In general, particle diffusion is considered to be a relatively unimportant deposition process. Decreasing "deldif" increases diffusion, and the user can employ this sensitivity to determine whether his problem could be affected by diffusion modeling.

The user should note that if the outer face of a structure is specified to be adiabatic or outside of the cell in which the structure is defined, then aerosols will not deposit onto this surface, even if aerosols are present in the cell where the outer face resides. The user should also note that the outer surface of a ceiling structure is considered a floor deposition area and that the outer surface of a floor structure is considered a ceiling deposition area. Also, for a half-cylindrical or hemispherical structure, the actual surface area and not the area projected on a horizontal plane is used for the settling area.

Beginning with CONTAIN 1.1, a floor is no longer created by default when structures are not explicitly defined by the user. One reason for this change is that not all cells should have a settling surface. A cell could have an open bottom connected to a cell below, and settling may occur through the opening to that cell and not to a surface in the cell above. The opening should be modeled as a flow path. Aerosols are

transported through flow paths by settling if the new FPCOSN option or VCOSN option is selected in the FLOWS or ENGVENT input blocks, respectively.

Direct natural deposition (e.g., settling) into the lower cell is not modeled; however, aerosol mesh losses may accumulate in a lower cell pool, as discussed above in Section 2.2.4.2. When this happens the coolant component is added to the mass of water in the pool. Also, aerosols may accumulate in the pool through the action of containment sprays, ice condensers, or fan coolers.

Not all phases of aerosol transport are modeled. The processes that first remove aerosols from the atmosphere are, in general, modeled. An example of such a process is one such as deposition on surfaces. The aerosols may not adhere to the surfaces but might be washed into a pool by the condensate draining from the surface. This is considered a secondary process because aerosols must first deposit out in order for it to occur. An example of a tertiary process is resuspension, during pool flashing, of the aerosols washed into a pool.

One secondary process, the draining of the coolant component of aerosols deposited on heat transfer structures, is modeled. If the CONDENSE option has been specified, the coolant component is added to the condensate film on the deposition surface (see Section 2.3.1.4). This film may become too thick, in which case the excess coolant will run off to the pool of the overflow cell. By default, that cell is the cell in which the structure is defined. The OVERFLOW option discussed in Section 3.3.1.11 can be used to divert this runoff to another cell. (This is the same option used to divert aerosol mesh losses to a nondefault cell.) If a pool is not present in the overflow cell, or if the overflow cell is set to zero, then the runoff will be lost from the problem. Since the noncoolant components of deposited aerosols do not have further physical effects that are presently modeled, they are held on the surface. (However, the washdown of the associated fission products may be simulated with the FPLIQUID or targeted release model--see the next paragraph.)

The fission products carried by aerosols that deposit onto a surface normally remain on that surface. This can be changed in two ways. First, if the transport efficiency factor for a fission product is set to a nonzero value in the FPLIQUID input discussed in Section 2.2.5.5, then that fission product will be carried with the condensate film runoff to a pool. Second, the user may specify a fission product transfer rate from the structure surface to a pool or any other host in the same cell through the targeted release formalism discussed in Section 2.2.5.3.3.

2.2.4.5 Condensation and Evaporation of Water on Aerosols. The CONTAIN aerosol model for an LWR models the condensation of water vapor onto aerosols and the evaporation of water from them. The user may employ the keywords NOCOND to suppress condensation and NOEVAP to suppress evaporation. Considerable development work has gone into assuring that CONTAIN runs efficiently for the maximum aerosol loadings that can result from condensation.

The rate equation for diffusion of water vapor to and from the particle is not that used in the MAEROS stand-alone code but is one taken from Reference Bye65. It accounts both for the diffusivity of water vapor in air and for the conduction of the heat of condensation away from the particle. The rate of condensation on a particle is assumed to correspond to the rate for a fully dense spherical particle. Condensation is assumed to begin on existing particles, which are assumed to have a spherical core composed of the solid materials, as shown in Figure 2-6. The Runge-Kutta integration method is used for condensation.

For evaporation, two methods are used. For high superheat, when the evaporation of the aerosol water is insufficient to keep the atmosphere saturated, a method of characteristics is employed. For evaporation under saturated conditions, the Runge-Kutta method is used. However, use of the spherical particle rate poses problems because the discontinuous change in rate at dryout causes the Runge-Kutta integrator to become very inefficient. Therefore, when the Runge-Kutta method is used during evaporation, the solid materials are assumed to inhibit evaporation when the mass of water and the mass of solid are comparable. The rate during evaporation is assumed to be

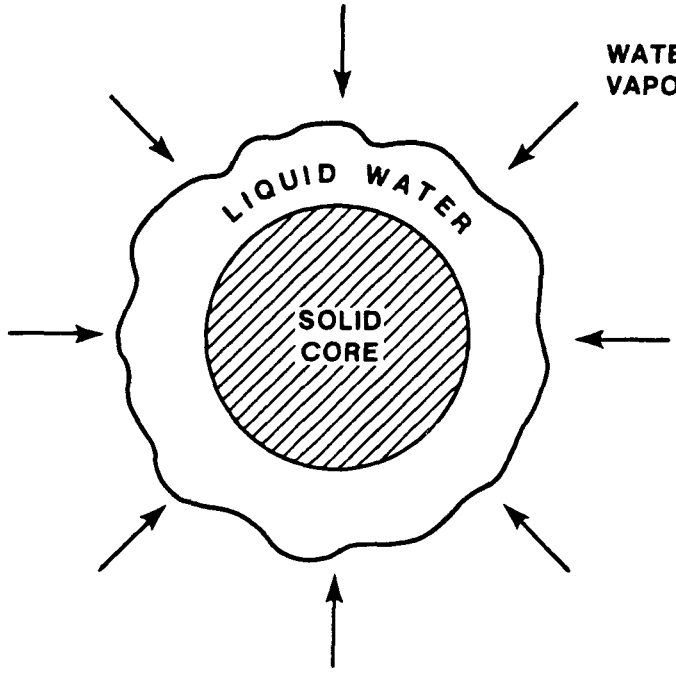

Figure 2-6. Model for Condensation of Water on Aerosols

$$W_{d,evap} = 1.037 W_d \tanh(2m_{H2OL}/m_{TOT}) \qquad (2\text{-}16)$$

where W_d is the uninhibited rate of evaporation from a spherical particle, and m_{H2OL} and m_{TOT} are the mass of water and total mass, respectively, of the particle. The amount of water present on aerosols when the rate is strongly inhibited is typically not significant.

Seed nuclei for condensation can alter the condensation rate on aerosols considerably. Even if a large number of aerosol particles are available as nucleation sites, the condensation rate can slow down if these have grown in size. In CONTAIN, seed nuclei are automatically generated as needed. They are provided to promote condensation if it would not otherwise occur or if it would occur but at a significantly impeded rate. The seed aerosol is placed in the smallest size class. The mass added is

proportional to the absolute error tolerance ("abstol") and is typically much less than the error tolerance used in integrating the masses in each size class.

To implement condensation or evaporation, the user should specify H2OL as the last aerosol component in the "mapaer" input under the global AEROSOL keyword. This is discussed in Section 3.2.4. The condensation/evaporation modeling for aerosols is available only for an LWR.

2.2.4.6 Intercell Flow of Aerosols. Aerosols are allowed to flow between cells through regular flow paths and engineered vents. They are considered to flow at the sum of the gas convective velocity and the component of the aerosol settling velocity along the flow path axis. The angle of inclination of regular flow paths and engineered vents, for the purpose of calculating the settling velocity, is specified through the FPCOSN and VCOSN keywords in the FLOWS and ENGVENT input blocks, respectively. Deposition within such flowpaths is not modeled. However, the scrubbing of aerosols passing through the suppression vent system of a BWR is modeled (see Section 2.2.3.4.2).

To account for the effects of flow, the aerosols are redistributed once per system timestep. The user is warned that no check is made on the adequacy of the system timestep for aerosol behavior if intercell flow occurs. The effects of aerosol agglomeration, deposition, and condensation within a cell are calculated with automatic timestep control through a Runge-Kutta method in a calculation that disregards flow. The flow of atmosphere gases is also calculated with automatic timestep control. However, the timestep controls for each process individually may not ensure that the coupled problem is described adequately. In general, the user should check the sensitivity of the calculation with respect to the system timestep whenever both aerosol processes within a cell and intercell flow result in large effects on the aerosols within a cell during a timestep.

As an example of difficulties that may be encountered in a calculation with too large a system timestep, the code may predict that the aerosols agglomerate and settle rapidly in a cell with a large source of aerosols

before they have a chance to flow out of the cell. A more accurate calculation may predict that the aerosols may flow out of that cell before significant agglomeration occurs. Because of dilution effects in the other cells, agglomeration and settling may not be as rapid in those cells, and the total aerosol deposition may be significantly less.

2.2.5 Fission Product Decay, Heating, and Transport

Overview

Detailed modeling of fission product behavior is described. Fission products can be tracked as individual nuclides and/or as user-defined fission product groups. An unlimited number of radioactive decay chains can be specified with any number of elements in any one chain. Decay heating can be included both for individual species and for the user-defined groups. Fission products are associated with various "hosts", or repositories. Transport of fission products associated with atmospheric hosts (i.e., gases and aerosols) is modeled mechanistically, as is the removal from the atmosphere of fission products on aerosol hosts. Except for removal of gaseous iodine species by certain engineered systems (see Section 2.3.3), the removal of gaseous fission products from the atmosphere is not modeled mechanistically. Further transport of fission products, once removed from the atmosphere, is generally not modeled, with the exception of that resulting from condensate films draining from heat transfer structures and from pool-to-pool liquid transport. Simple, yet partially mechanistic, models are available for the latter processes. Fission product transfers among the hosts can also occur in accordance with user-specified transfer rates. Such rates can depend on the host temperatures; however, no mechanistic models are provided for the determination of these transfer rates.

Modeling of decay heating from explicitly specified fission products requires specification of nonzero power coefficients in the FISSION input. (A heating rate based upon the ANSI standard for decay heating can also be used in the lower cell as discussed in Section 2.3.2.2.) Except for effects related to decay heating, other CONTAIN models should be unaffected by the presence or absence of fission product modeling.

2.2.5.1 Introduction. In any reactor accident, the major concern is the possible escape of radionuclides from the containment system to the outside environment. The term "fission product" is used throughout this manual to represent all radionuclides, including actinides and other neutron activation products. With CONTAIN, the user can track as many fission products as desired. The fission products can be specified as nuclides, elements, compounds, and release groups. Decay of one species into another is allowed if such decay can be modeled as an exponential process. The code follows the birth and decay of each fission product specified, and also accounts for the associated decay heating. It tracks the movement of fission products throughout the containment system, and, if a breach of containment occurs to a cell that represents the outside environment, the code will predict the extent of fission product releases.

For a typical reactor accident analysis, identifying and tracking the large number of radionuclides present as individual species would be tedious. Therefore, three levels of resolution of these species are available to the user:

- Individual radionuclides, which are explicitly represented in the decay chains and which have constant half-lives and constant specific decay powers. These species are associated with various hosts within a cell, can move with hosts from cell to cell, and can change hosts.

- Fission product groups, which differ from individual radionuclides in that the decay of groups generally is not explicitly modeled, except through a decay power that changes with time.

- A lumped stationary radioactive inventory, which is modeled in terms of its heating of various layers in the lower cell model.

The user must decide which parts of the radioactive inventory should be handled at the first or second levels. The species modeled at these levels are typically important with respect to biological consequences upon release or with respect to the transport of their decay heat within

containment. In the following discussions, the term "fission product" is used only to describe radionuclides modeled at the first or second level.

The decay heating model implemented at the third level is discussed in Section 2.3.2.2. The model ensures that the sum of the decay power from the inventories at all three levels equals the ANSI-standard decay power appropriate to the reactor operating power and fuel burnup.[Ame79] Since only the decay power at the third level is adjusted to bring the total power into agreement with the ANSI standard, it is referred to as "makeup decay power."

Fission products in CONTAIN are associated with various "hosts," or repositories. Some hosts, such as the upper cell atmosphere gas or aerosols, are mobile, while others, such as the wall surfaces, are fixed. In general, the initial introduction of fission products onto various hosts is specified by the user. CONTAIN then tracks the transport of the fission products according to a variety of mechanistic and nonmechanistic models enumerated in Section 2.2.5.3. One way in which fission products are transported is through the movement of the mobile hosts, such as that resulting from the flow of the atmosphere gas and the deposition of aerosols on surfaces. Other processes may cause fission products to change hosts. The depletion of fission products from the atmosphere due to the action of various ESFs typically results in the transfer of these fission products to pools.

Fission products also tend to move from one host to another on the basis of physical or chemical compatibility. For example, when a fission product decays, the daughter may have different chemical and physical characteristics, and therefore the subsequent transport may be different from that of the parent. As an example, a solid fission product trapped in fuel material may decay to a noble gas, which then escapes. User-specified release rates within the targeted release and acceptance formalism discussed in Section 2.2.5.3.3 provide a flexible, although nonmechanistic way to simulate the change in the affinity of a fission product for its host when it decays. User-specified release rates may also be useful in modeling other processes, such as resuspension.

2.2.5.2 Fission Product Decay. The decay of fission products and the accumulation of daughters are modeled by using the technique of linear chain resolution.[Eng68] The differential equations for decay are decoupled by breaking the branched decay chains into a system of linear chains. These chains are independent in the sense that only the masses in one chain are needed to solve for the effects of decay at any time. This is illustrated by the example below.

The system shown in Figure 2-7 can be formulated in terms of the three linear chains shown in Equation (2-17).

$$\begin{array}{l} B \rightarrow C^{*} \rightarrow D \rightarrow \\ B \rightarrow C \rightarrow D \rightarrow \\ X \rightarrow Y \rightarrow C \rightarrow D \rightarrow \end{array} \qquad (2\text{-}17)$$

Because the same fission product can appear in more than one linear chain, the rules for determining initial masses and half-lives to be used in the linear chains are not obvious. It can be shown, however, that the half-life to be used for a given fission product in any linear chain should be the net half-life from all decay branches, even though only one branch is taken in any linear chain.[Eng68] The initial mass of the fission products in a linear chain upstream of a branch should be distributed according to the branching ratio for that chain. In the example below, the initial mass of B (if any) should be distributed so that the first chain has a mass

$$m_{B,1} = m_B \frac{\lambda_{B\rightarrow C^{*}}}{\lambda_{B\rightarrow C^{*}} + \lambda_{B\rightarrow C}} \qquad (2\text{-}18)$$

and the second chain has mass

$$m_{B,2} = m_B \frac{\lambda_{B\rightarrow C}}{\lambda_{B\rightarrow C^{*}} + \lambda_{B\rightarrow C}} \qquad (2\text{-}19)$$

where the λ's are the decay constants. The same fission product can also occur in more than one linear chain if the same daughter can be formed in more than one decay path, such as fission product C in Equation (2-19). A merging of decay paths occurs in this case instead of a branching. The distribution of the initial mass of a fission product that occurs in more than one linear chain as a result of merging is arbitrary, as long as the individual masses give the correct total mass. For complicated decays, the user may find it helpful to break up the decay sequence into linear chains one step at a time. Each step corresponds to removing one branching or merging chain. It may be easier to distribute the mass of a fission product over all chains if this is done.

Because a fission product or radionuclide can appear in more than one decay chain, its inventory may be divided among several locations in the linear chain structure. The code makes a distinction between the number of radionuclides and the number of positions in the linear chain structure. The number of radionuclides corresponds to the number of unique fission product names used in the linear chain structure. The term "fission chain element" has been adopted to designate a particular position in the linear chain structure. Because a radionuclide may appear more than once in the structure, the number of fission chain

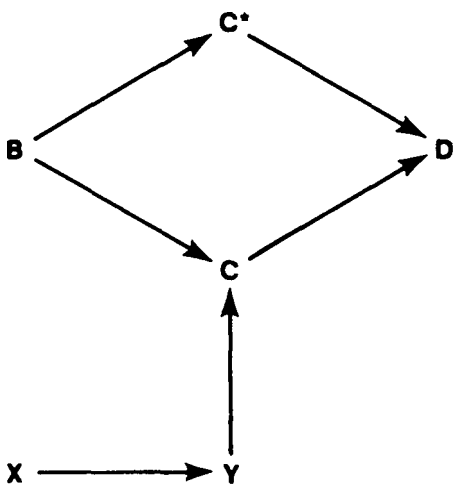

Figure 2-7. Example of Fission Product Decay Chains. This configuration can be broken down into three equivalent chains.

elements, "nfce", is therefore greater than or equal to the number of radionuclides, "nnuc". For example, "nnuc"=6 and "nfce"=10 in the above three chain example (see Figure 2-7 and Equation (2-17)). A fission chain element may also represent a fission product group, in which case it will normally be the only element in its decay chain.

At any time, the inventory of a radionuclide for a given host is given by the sum of the masses of the linear chain elements that have that radionuclide name. CONTAIN does not sum over chains. Instead, the mass for each linear chain element is tracked and displayed separately.

Because the differential equations for decay are linear, a source of fission products that occurs after the start of the problem can be taken into account by adding the source masses to existing masses. If fission product masses are specified through source tables, it is the user's responsibility to specify amounts for each fission chain element associated with the radionuclide. Only the species specified in the tables will be introduced at each timestep; decay to daughter species begins only after the material enters the active inventory in the problem. (See Section 3.3.1.9 for a detailed discussion of fission product source table input.)

Fission product masses, as treated by the code, do not influence the dynamics of their hosts, except through possible heating effects. For example, fission products associated with aerosol hosts will not influence the dynamics of the aerosols. In effect, the fission products are treated as being massless. Similarly, the mass of airborne fission products does not influence intercell flow (other than by possible heating effects), nor does the mass of fission products in the lower cell add to the mass of materials in the lower cell. In some cases, the neglect of the fission product masses can be rectified by augmenting the masses of the hosts; see the discussion in Section 5.3 concerning the augmentation of aerosol masses.

2.2.5.3 Fission Product Inventory and Transport. The transport of fission products in CONTAIN can occur in the following ways:

- Airborne fission products flow with the atmosphere gas as it passes from one cell to another. Fission products hosted to aerosols flow with the sum of the gas convective velocity and the component of the aerosol settling velocity parallel to the flow path axis.

- Liquid transfers between pools may result in the transport of fission products from the donor pool to the recipient pool. Fission products may also be carried from cell walls to a lower cell pool by condensate film runoff. The amounts of fission products transferred between pools and carried by the runoff are controlled by the transport efficiency factors specified in the FPLIQUID input block discussed in Section 2.2.5.5.

- The deposition of aerosols bearing fission products occurs on surfaces of heat transfer structures. The deposition is calculated mechanistically for the dominant processes as discussed Section 2.2.4.4.

- The operation of engineered safety systems removes gaseous iodine fission products and fission products hosted to aerosols from upper cell atmospheres according to mechanistic decontamination models, as discussed in Section 2.3.3.

- Fission products residing on aerosols vented into pools are scrubbed according to mechanistic models and deposited in the pool. The scrubbing resulting from flow through suppression pool vents and discharge through safety relief valves is discussed in Sections 2.2.3.4.2 and 2.3.4, respectively.

- Fission products may transfer from one host to another. For instance, a solid fission product could decay to a noble gas, which would then tend to escape to the atmosphere. In the targeted release model discussed in Section 2.2.5.3.3, this movement may be simulated nonmechanistically by user-specified release rates specific to each combination of fission product and host.

- Mechanistic models for resuspension or release of fission products from the lower cell to the upper cell atmosphere are not provided at present. The user may, however, simulate resuspension or release to the upper cell through the targeted release model.

2.2.5.3.1 Fission Product Hosts. Modeling of the above phenomena is made possible through an inventory scheme in which fission products are assigned to various hosts. The user should assign fission products to a host based primarily on the chemical affinity and physical characteristics of the fission product. These assignments may be made for the initial fission product inventory and for time-dependent sources of fission products. For tracking purposes, VANESA[Sci84] constituents may also be

assigned as CONTAIN fission products to CONTAIN aerosol hosts through the FPTRACK option as described in Section 3.3.2.3.

The upper cell atmosphere gas and each component of the suspended aerosols are always hosts in every cell. The code automatically defines surfaces of heat transfer structures and lower cell layers as hosts. Both surfaces of each structure and each lower cell layer (including the lower cell atmosphere layer if a lower cell model has been defined) are all taken to be individual fission product hosts. Therefore, each cell will generally have a different number of fission product hosts. In contrast to prior versions, in CONTAIN 1.1, individual lower cell layers rather than lower cell materials are taken to be hosts. (Note: this is a non-upward-compatible change from versions prior to revision 1.1; see Appendix D for details on how the obsolete material hosts are handled.) The capability to specify a host not associated with any other entities in a cell has been maintained by introducing a DUMMY host in each cell.

The transport of CONTAIN host materials within the cell may cause the fission product to change hosts; for example, aerosol deposition causes a fission product attached to the aerosols to become attached to the deposition surface. Mechanistic models for changes in host assignments are discussed in the descriptions of heat transfer to structures (Section 2.3.1.4) and the ESF models (Section 2.3.3.2 and 2.3.3.11). A semi-mechanistic model for the washdown of fission products from structure surfaces to a pool is discussed in Section 2.2.5.5. In general, however, host changes need to be specified by the user through the targeted release and acceptance formalism described below.

2.2.5.3.2 Host Temperatures. A temperature is associated with each fission product host. This temperature is used in the targeted release and acceptance formalism to model transfer rates, as described in the next section. The gas and aerosol host temperatures are assumed to be the cell gas temperature. The temperature of the first and last nodes of a structure are used for the host temperatures of the inner and outer surface, respectively, of structures. In the lower cell, the layer average temperature is used as the host temperature for all layers except the concrete layer. The temperature of the uppermost concrete node is used

as the host temperature in concrete layers since fission products are not expected to penetrate below that node.

2.2.5.3.3 Targeted Release and Acceptance. A nonmechanistic fission product transfer model is included in CONTAIN. It uses a flexible targeted release and acceptance formalism. In this formalism, the user may specify transfer rates for individual fission products between any number of pairs of hosts. For a given pair of hosts (i,j), the fractional transfer rates per second, $r_{i\to j}$, for a particular fission product may depend on the host temperatures, T_i or T_j, according to the following expressions:

$$r_{i\to j} = \left\{ \begin{array}{ll} a\, e^{-b/T_i} & T_i \geq T_{threshold} \\ 0 & T_i < T_{threshold} \end{array} \right\} \text{ if } a > 0;$$

(2-20)

$$r_{j\to i} = \left\{ \begin{array}{ll} -a\, e^{-b/T_j} & T_j > T_{threshold} \\ 0 & T_j < T_{threshold} \end{array} \right\} \text{ if } a < 0$$

where a, b, and $T_{threshold}$ are user-specified parameters and where i is the host specified after the FROM keyword in the TARGET input block and j is the host specified after the TO keyword (see Section 3.3.1.10). Fission products are assumed to transfer at mass rates proportional to the amount of fission product mass present. For example, the simple case of the transfer between one pair of hosts at the fractional rate $r_{i\to j}$ per second is represented by the coupled equations:

$$\dot{m}_i = -\, r_{i\to j}\, m_i \quad , \quad \dot{m}_j = r_{i\to j}\, m_i \quad \text{if } a > 0;$$

(2-21)

$$\dot{m}_j = -\, r_{j\to i}\, m_j \quad , \quad \dot{m}_i = r_{j\to i}\, m_j \quad \text{if } a < 0,$$

where m represents the fission product mass.

For simple coupled equations like those given in Equation (2-21), fission product mass redistributions are calculated using the analytic solution. More complex coupled equations are solved by a highly accurate exponential operator method.[Lee80] Note that array space for the targeted release model must be provided through the "ntgt" parameter in the global CONTROL block.

Targeted release rates, if used, are associated with fission product names and are applied to all fission chain elements having the specified name. Therefore, all chain elements having the same fission product name will transfer at the same rate. For example, suppose a release rate is defined for nuclide B in Figure 2-7; the masses of the first elements in chain 1 and chain 2 in Equation (2-17) would then be transferred at the specified rate.

To illustrate the flexibility of the targeted release formalism when coupled with fission product decay, consider how iodine and iodine decay products are affected by the release rates of Figure 2-8. The decay chain is as follows:

$$^{137}\mathrm{I} \xrightarrow{\beta^-} {}^{137}\mathrm{Xe} \xrightarrow{\beta^-} {}^{137}\mathrm{Cs} \qquad (2\text{-}22)$$

The hosts involved in this illustrative problem are called GAS (for the upper cell atmosphere), AEROSOL 1 (for aerosol component 1), INNER STRUC (for the inner surface of a structure), and LAYER 1 (for a lower cell layer representing fuel).

The release rates in Figure 2-8 simulate a variety of processes that may occur within a cell. It is assumed that melted fuel is represented by a lower cell layer. The gaseous iodine and xenon are assumed to transfer from the fuel to the atmosphere at the rate of 0.1% per second. The transfer rate of cesium vapor is assumed to be two orders of magnitude lower. The rapid release of iodine and cesium from molten fuel in the

Nuclide	From	To	Rate (s^{-1})	Process Represented
^{137}I	LAYER 1	GAS	10^{-3}	Vaporization
^{137}I	LAYER 1	AEROSOL 1	0.1	Aerosolization
^{137}Xe	LAYER 1	GAS	10^{-3}	Outgassing
^{137}Xe	AEROSOL 1	GAS	5.0	Rapid gas escape
^{137}Xe	INNER STRUC	GAS	5.0	Rapid gas escape
^{137}Cs	LAYER 1	GAS	10^{-5}	Vaporization
^{137}Cs	LAYER 1	AEROSOL 1	0.1	Aerosolization
^{137}Cs	GAS	AEROSOL 1	0.1	Aerosol adsorption

Figure 2-8. Illustrative Fission Product Targeted Release Rates

form of aerosols is assumed to occur at the rate of 10% per second. Any xenon hosted to the aerosols or to the inner surface of the structure (as a result of iodine decay) is assumed to be transferred to the atmosphere at an essentially instantaneous rate. Finally, cesium hosted to the atmosphere (as a result of xenon decay) is assumed to adsorb on the aerosols at the rate of 10% per second.

Figure 2-9 illustrates how the above targeted release processes fit into the overall fission product transport picture. In Figure 2-9, all of the initial mass is assumed to be iodine and hosted to the first lower cell layer (in this case an intermediate layer). Decay processes govern the formation of xenon and eventually cesium. Targeted release processes affect the mass distribution among host materials. Intercell flow transports fission products hosted to the gas and aerosols to and from other cells in multicell problems. Finally, fission products in aerosol form deposit on the structure surfaces in the cell.

2.2.5.4 Fission Product Decay Heating and Groups. Fission product modeling is coupled to the thermal-hydraulics models in CONTAIN through the effects of fission product decay heating. The decay heat of fission products hosted to the gas and to aerosols is assumed to be deposited in the atmosphere. The decay heat of fission products on structure surfaces is assumed to heat the structure node immediately below the surface. The

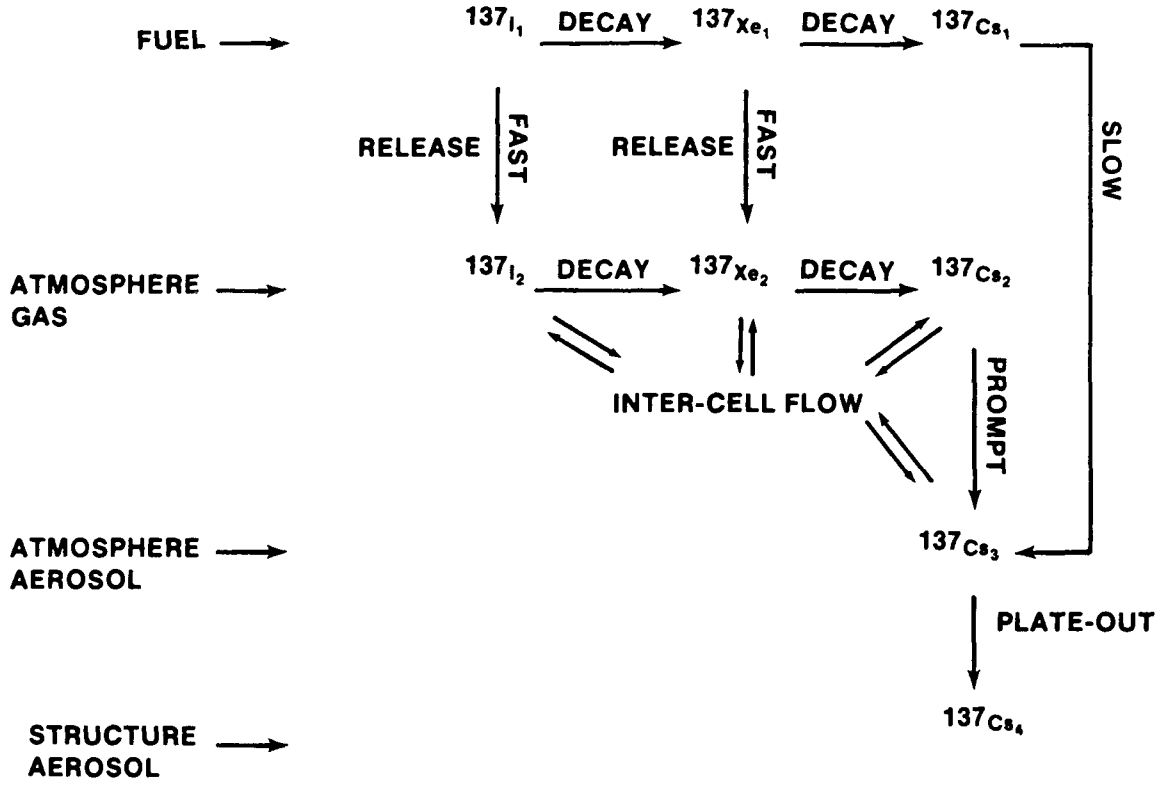

Figure 2-9. Example of Decay and Redistribution Transport Paths for Fission Products Initially Located in the Lower Cell Fuel Layer

decay heat of fission products in the lower cell layers is assumed to be distributed uniformly in the layer, with the exception of the concrete layer where it is always deposited into the uppermost node.

For fission chain elements representing individual radionuclides, a constant decay power in watts per kilogram may be specified by the user. To accommodate the representation of fission product groups, a time-dependent decay power option is available through the FGPPWR keyword (see

Section 3.2.5). Up to four coefficients (a_1 through a_4) may be specified for each fission chain element, where the specific power p for that element is taken to be

$$p = a_1 \exp(-a_2 t) + a_3 \exp(-a_4 t) \quad (W/kg) \tag{2-23}$$

A coefficient not specified is taken to be zero; for example, if three coefficients are given, a_4 will be zero. Note that the time t in seconds is the somewhat arbitrary problem time and not necessarily the time from shutdown or the start of the problem.

2.2.5.5 Fission Product Transport in Liquid Pathways. The materials transported in liquid pathways between repositories of coolant liquid are presently restricted to the coolant and to fission products carried by the coolant. Although materials such as deposited noncoolant aerosols are not transported, the transport of fission products along with the coolant allows the user to assess the radiological inventories and the decay heating resulting from such transport.

The transport of fission products in liquid pathways occurs in two instances. Fission products present on structure surfaces as the result of aerosol deposition and other mechanisms may be transported with the condensate film draining from the surfaces. Note that the formation of such a film from vapor condensation and its drainage is controlled by the CONDENSE cell level input in each cell, as discussed in Section 2.3.1.4. In addition to vapor condensation, coolant aerosol deposition may also contribute to the film, as discussed in Section 2.2.4.4. Fission products deposited in coolant pools may also be transported along with the coolant in the flow between two pools, provided the flow is modeled through an engineered system component such as a PIPE. The components which may connect two pools are discussed in Sections 2.3.3.5 through 2.3.3.9 and in Section 2.3.3.11. Note that fission products already in pools are presently not transferred as a result of the operation of engineered safety features constructed of several components, such as the SPRAY engineered system discussed in Section 2.3.3.2, even though they

may have the effect of transferring coolant between pools, as when the spray is run in the recirculation mode.

The optional FPLIQUID input block is used (see Section 3.2.5.1) to specify transport efficiency factors which determine the rate of transfer of fission products relative to the rate of transfer of coolant. Only those fission products assigned a finite value of "fpliq" in the FPLIQUID input will be transferred with the condensate runoff and the flow of coolant between pools. The value of "fpliq" is defined to be the ratio of the fraction of the fission product transferred from a repository per timestep to the fraction of liquid transferred from that repository.

The value of "fpliq" is assigned by fission product name and applies globally to liquid pathway transfers of that fission product. Fission chain elements that have the same fission product name are automatically assigned the same liquid pathway transport efficiency factor.

2.2.6 Calculational Timestep Control

This section discusses the calculational timestep hierarchy under which the physical models are integrated forward in time. There is a separate hierarchy that controls the various output frequencies (long edit, plot, and restart); this is discussed in Section 3.2.6.

The modular nature of the code requires that processing of different models be performed in some sort of sequenced loop. Figure 1-3 shows the bi-level sequence of calculations, i.e., the global versus cell level processing. However, it does not show the sequence of physics model calculations at each of these levels. Section 2.2.6.1 provides additional information concerning the timesteps used for different models and the manner in which the models are coupled.

Section 2.2.6.2 provides some guidance to the user in selecting reasonable maximum system and cell timesteps. These suggestions consider only some of the interactions among the explicitly coupled models. The user should be aware that other inaccuracies (not necessarily instabilities)

may result from insufficiently frequent updating of information between explicitly coupled models. Depending on the level of the model, the updating frequency is controlled by either the cell or system timestep. The testing of calculated results for sensitivity to user-specified timesteps is always encouraged.

2.2.6.1 Timestep Hierarchy. Four different types of calculational timesteps are used. Two of these, the system timestep and the cell timestep (DT4 and DT5 in Figure 1-3), are primarily under user control. The third type, the Runge-Kutta timestep, is selected automatically and used within certain models. The fourth timestep is that used by the CORCON model. The maximum and minimum allowed values of this timestep are user-controlled. The VANESA timestep is a user-controlled fraction of the CORCON timestep.

The models in CONTAIN are processed in parallel. This type of processing is somewhat different from the sequential processing normally found in single purpose codes. In parallel processing, each model, or in some cases each group of models, is integrated forward in time over the current system timestep. State variables that are external to the model or model group being processed at any given time are held fixed, for example, at the values existing at the beginning of the system timestep. State variables that belong to the model or model group being processed may be updated at many subintervals within the system timestep. These subintervals are determined by the model internal timestep. (In some cases, this is just the cell timestep.) After a model is integrated forward in time to the end of the system timestep, the state variables are updated to the end of timestep values for use in the next system timestep.

The CORCON model uses its own user-specified timestep, which is chosen independently of CONTAIN timesteps. Thus, CORCON can advance beyond the end of a system timestep and generate source rates which CONTAIN will use until the CONTAIN time advances to the CORCON value. Alternately, CORCON can be run with a step smaller than the CONTAIN cell timestep. In this case, the fluxes computed by CORCON are integrated over the CONTAIN cell timestep.

In general, the values of the state variables at the subinterval points are not available outside the model or model group. For example, the suspended aerosol concentrations are calculated every Runge-Kutta time-step. However, the values are not available outside the aerosol model except at the end of the system timestep. The exceptions occur in the models that update their state variables every cell timestep.

The maximum system and cell timesteps are specified through input. These control the frequency with which the control loops in Figure 1-3 are traversed. There is little in the way of automatic control of these timesteps; the maximum timesteps are normally the timesteps that are actually used. The exceptions are as follows: (1) Because a hydrogen burn is a common event whose timing cannot be predicted, the system timestep is adjusted automatically during hydrogen burns. (2) Because the cell timestep cannot exceed the system timestep, the cell timestep is also adjusted during hydrogen burns. (3) The cell timestep is reduced if necessary so that it does not straddle a time point in a source table; that is, the end of the timestep is chosen to correspond to any intervening time point. This adjustment eliminates interpolation errors in the integration of source table rates. (4) With CORCON active, the cell timestep is adjusted so that it does not advance beyond the time to which CORCON has advanced.

Table 2-2 lists the internal timesteps used for various models. The internal timestep determines the frequency with which the state variables belonging to the model are updated for internal use. With respect to the integration methods listed, the word "integral" implies that a closed-form solution is used. The words "explicit" and "implicit" refer to the discrete integration method used internally, as defined in numerical analysis. (The integration method with respect to the variables at the model interface is always explicit.) The interface timestep determines the frequency with which the internal variables are updated for use outside the model in question.

For example, according to Table 2-2, the temperature profile in heat transfer structures is computed every cell timestep. The method used is

Table 2-2

Internal Timesteps Used Within Various CONTAIN Models

Model	Internal Timestep	Integration Method	Interface Timestep
Fission Product	System	Integral/ Matrix	System
Flow/Thermodynamics	Runge-Kutta or Convection	Explicit or Implicit	System
Aerosol Processes	Runge-Kutta	Explicit/ Integral	System
Heat Transfer Structures	Cell	Implicit	Cell
Engineered Systems	Cell	Explicit	Cell
Lower Cell Model	Cell	Implicit	Cell

fully implicit with respect to the internal variables (the node temperatures). However, as a result of the explicit coupling at the interface (such as that with the atmosphere), an instability in the profile may result from too large a cell timestep. The next section will discuss the maximum stable timestep due to this coupling.

2.2.6.2 Suggested Criteria for User-Specified Timesteps. This section will discuss two criteria for selecting user-specified timesteps. The first criterion specifies the system timestep required to incorporate properly the effects of flow on aerosols and fission products. The second criterion specifies the cell timestep required for stability in the presence of the explicit coupling between atmosphere thermodynamics and heat conduction in the structures.

2.2.6.2.1 Aerosol and Fission Product Flow Timestep. To reduce the length of the solution vector to be considered at any one time, the aerosol and fission product behavior within a cell are calculated separately from the effects of intercell flow. The effects of intercell flow are incorporated at the end of every system timestep by redistributing the suspended aerosols and fission products according to the gas convection and aerosol settling rates occurring during the timestep. Although the timestep used to calculate the flow of atmosphere gases is chosen internally, the timestep used for the redistribution of aerosols and fission products due to intercell flow is the system timestep. Under some conditions, a system timestep that is too long may result in inaccuracies in the overall aerosol and fission product behavior.

One time constant of interest with regard to accuracy in the calculated aerosol and fission product behavior is the convection time t_c for a cell. The convection time defines the rate at which the composition of the atmosphere can change. It controls the changes in the aerosol population, the fission product inventory, and the composition of the atmosphere gases.

A general discussion of timestep selection is beyond the scope of the present manual. Nonetheless, a conservative selection criterion can be given. A conservative choice of the system timestep requires that the system timestep be smaller than the time constants for aerosol and fission product dynamics within a given cell. A 20% change in aerosol quantities per system timestep is probably acceptable. For example, deposition of 20% of the suspended mass per timestep is usually acceptable, as is a source which injects mass at a rate of 20% of the suspended mass per timestep.

In the event that the conservative system timestep is too restrictive, one should try a system timestep on the order of 20% of the cell convection time. The effects of engineered systems operation on aerosols, in particular, may be quite large, and it may not be feasible to choose a system timestep conservatively as described above. For nonconservative timesteps, one should check on the sensitivity to the system timestep by reducing it by a factor of two or more in the time domain of interest.

The convection time will depend on the relative pressure differences between cells. The contents of a cell held at much higher pressure than its neighboring cells and then allowed to blow down will convect out with a time constant equal to the pressure relaxation time. A simple rule of thumb for such transient conditions is that if the system timestep is short enough to resolve a 20% change in the pressures, it should be adequate with respect to the cell convection time of the blowdown cell.

If the initial pressure difference is not large, the cell contents will not convect out significantly during the pressure relaxation to the steady state. In this case, most of the convection, if any, will occur under low, steady-state pressure differences. The timestep to use in this case is less obvious than the one to use for transients. The steady-state convection time, t_c, for cell i should be obtained from

$$t_c = \frac{m_i}{\sum_j W_{ij}} \qquad (2\text{-}24)$$

where the j sum is carried out for all flows out of cell i. (See Section 2.2.3.2 for definition of variables.) The sum over j is most easily evaluated from the code output for the flow rates. The steady-state convection time is typically much longer than the pressure relaxation time.

2.2.6.2.2 Atmosphere-Structure Time Constant. Another important potential source of inaccuracy or instability due to explicit coupling occurs at the cell level, where the atmosphere may transfer an excessive amount of heat into the first node of a heat transfer structure, because the effect on the surface temperature is not properly taken into account. A criterion for the maximum cell timestep can be obtained if the atmosphere-structure heat transfer coefficient h is known. By requiring the temperature rise in the first node during a single timestep Δt to be less than the atmosphere-structure temperature difference, one obtains for an insulated first node,

$$\Delta t < \rho C_p L/h \tag{2-25}$$

and for a node backed by similar material,

$$\Delta t < \rho C_p k/h^2 \tag{2-26}$$

where L is the first node thickness. These expressions should be used as first estimates for setting cell timesteps. Stable behavior may occur even if cell timesteps are two or three times these values, but exceeding these criteria by large factors will generally result in surface temperature oscillations. Sensitivity to the cell timestep should always be checked by varying the timestep. A typical heat transfer coefficient for condensing conditions would be h = 300 W/m^2-K.

2.3 Cell Models

The cell is the basic calculational unit used in the code. A CONTAIN cell is intended to model an entire room, vault, compartment, etc. Difficulties may arise if the user tries to represent such a volume by more than one cell. In particular, the flow equations are not intended to model a continuum, and thus unrealistic flow patterns may occur within the volume.

Each cell can consist of two parts: an upper cell portion containing the cell atmosphere and a number of heat transfer structures, and a lower cell portion that may include a pool, fuel debris, concrete, and various other layers. Various physical and chemical processes can occur in both the upper and lower portions of a cell. The upper cell processes are discussed in Section 2.3.1, and the lower cell processes are presented in Section 2.3.2.

2.3.1 Upper Cell Models

The upper cell is the collection of models that determine the rate of chemical reactions (burns) in the atmosphere and that control transfers of energy and mass between the cell atmosphere and the structures in contact with it. Every cell must have an upper cell, though there may be many situations in which a lower cell need not be specified. Heat transfer structures are optional in the upper cell, but the atmosphere is not. There are two ways to specify a floor in a cell: if the floor is in contact only with the atmosphere, it can be treated as an upper cell heat transfer structure. Otherwise, it can be treated as a layer in the lower cell structure, where it can be in contact with the atmosphere, a coolant pool, or other layers.

In this section, the basic features of the upper cell models and their interactions with other models in the CONTAIN system will be described. Atmosphere source tables provide a way for the user to introduce conserved quantities into the cell atmosphere. These source tables typically represent phenomena not modeled by CONTAIN, e.g., releases from the primary system, or from core-concrete interactions if the user prefers not to use the internal CORCON/VANESA module. The quantities which can be introduced through tables include mass, heat, aerosols, and fission products. Also discussed in this section are the models for heat transfer to structures. Condensation of coolant vapor onto structures may be modeled, along with normal dry convective heat transfer. Two levels of modeling are available regarding radiative heat transfer among the structures and the atmosphere. In conjunction with the radiation models, there are also two options available for modeling the emissivity of gas mixtures in the atmosphere. Finally, the hydrogen and carbon monoxide combustion models are discussed.

2.3.1.1 Cell Geometry. The upper cell representation in CONTAIN includes only two geometrical characteristics, a cell volume and a height. The cell volume is the free volume of the gases present. The height is used as a default to compute containment spray droplet fall times.

The cell volume remains constant throughout a CONTAIN calculation, even though coolant or other nongaseous material is added to the cell. A reduction of the cell volume, for example, by flooding with coolant is not modeled by the code.

Various heat transfer structures can be included in the upper cell to simulate roofs, walls, floors, and internal structures and equipment. The basic cell does not include any such structures automatically. They must be separately specified for each cell (see Section 2.3.1.3).

2.3.1.2 Cell Atmosphere Initial Conditions and Sources. The user must specify the initial conditions for the atmosphere in each cell. These initial conditions can be different from one cell to the next. Given the cell atmosphere mole fractions, pressure, temperature, and volume, the code calculates the mass of each gas present. Alternatively, the user may specify the constituent masses and temperature. Gases and superheated coolant vapors are treated as ideal gases. Saturated coolant vapors are treated according to a two-phase equation of state.

External sources of mass and energy can be provided to a cell atmosphere. Such sources can be useful for representing phenomena such as the blowdown of coolant from the reactor coolant system into the containment. External mass and energy source rates are specified as a function of time through tables.

Atmosphere sources may consist of three types of materials: gases, coolant, and other dispersed solids or liquids. Materials of all three types contribute enthalpy to the atmosphere, but the ways in which their masses affect atmosphere physics are different. Gases and coolant are considered in both the intercell flow calculation and the atmosphere thermodynamics. As described in Section 2.2.3.1, the coolant is treated properly as a two-phase material. The specific heat of dispersed noncoolant liquids and solids is not taken into account in the thermodynamics; however, if introduced through source tables, such materials give up their enthalpy to the gases present. Therefore, the use of dispersed solid or liquid materials is somewhat limited, except as a way to inject energy into the atmosphere.

There are four material names associated with the coolant. For water, the names are H2OV and H2OL, and for sodium they are NAV and NAL. There is an important difference between the way vapors are treated as atmosphere sources and the way the liquids are treated. H2OV and NAV sources couple to the two-phase atmosphere thermodynamics, and the mass injected can end up as a two-phase mixture (a liquid-gas suspension), as superheated vapor, or (in the case of water) condensed onto aerosols. H2OL and NAL atmosphere sources are treated in a manner similar to that for sources of noncoolant dispersed solids and liquids. In particular, these are sources are not allowed to change phase in the atmosphere. In the discussion in the previous paragraph, therefore, the word "coolant" refers only to H2OV or NAV. (However, it would be a mistake to think of these materials as vapor, because they are truly two-phase materials.)

The user is cautioned not to use atmosphere source tables for materials that are aerosol materials, except for H2OV and NAV. There should be no materials that are named both as aerosol materials (in the global AEROSOL block) and as atmosphere materials (in the cell ATMOS block), with these same two exceptions.

2.3.1.3 Structures and Heat Conduction. This section includes guidance on how to nodalize heat transfer structures. Rules for defining structures, the internal heat transfer algorithm, and structure boundary conditions are discussed. Fission product heating of structures is also discussed.

2.3.1.3.1 Structures, Heat Conduction, and Boundary Conditions. Heat transfer structures in the containment building (including walls, roof, floors, and internal structures) are repositories of the heat released by the reactor fuel, by fission products, and by chemical reactions. The pressure and temperature of the atmosphere are determined largely by the competition between numerous sources of heat on the one hand and the removal of heat by transfer to the structures on the other hand. Heat transfer between the structures and the atmosphere takes radiation, convection, condensation, and evaporation into account (see Sections 2.3.1.4 and 2.3.1.5). Heat transfer within each structure is handled by

solving a one-dimensional heat conduction equation for the materials specified for the structure.

Three choices for the one-dimensional structure geometry are available: planar, cylindrical, or spherical. Structures that are labeled spherical or cylindrical are actually hemispheres or half-cylinders. Each structure can consist of arbitrary combinations of layers of different materials. The thermal properties used in the conduction equation are obtained from the property library or from property tables for user-defined materials. Material names for structure layers must be taken from Table 2-1 or be included in the list of user-defined materials following the USERDEF keyword in the global MATERIAL block. Note that through the user-defined material input it is possible to redefine the properties associated with the materials in Table 2-1.

The number of heat transfer structures in each cell and their shapes, thicknesses, areas, material compositions, and boundary conditions are specified through input. Figure 2-10 shows an example of a heat transfer structure. This is a cylindrical structure consisting of a steel liner, an air gap (modeled as nitrogen), and a thick concrete wall. The type or orientation of the structure may be either a ROOF, WALL, or FLOOR. Different structure types use different heat transfer correlations and are treated differently with respect to aerosol deposition. The user must specify the nodalization of each layer and should take care not to change the node thicknesses too abruptly from one node to the next. (Generally, any change in thickness by a factor of two or less should be acceptable.) To determine how finely the structure should be nodalized, it may be useful to consider the thermal diffusion length,

$$\delta = (4kt/\rho C_p)^{1/2} \qquad (2\text{-}27)$$

where t is the shortest time scale of interest. The nodes that are in contact with the atmosphere should be a small fraction of this length, if accuracy in the heat transfer to and from the atmosphere is desired. The user should also consider the stability criteria in Equations (2-25) and (2-26) in nodalizing structures. For low conductivity materials or very

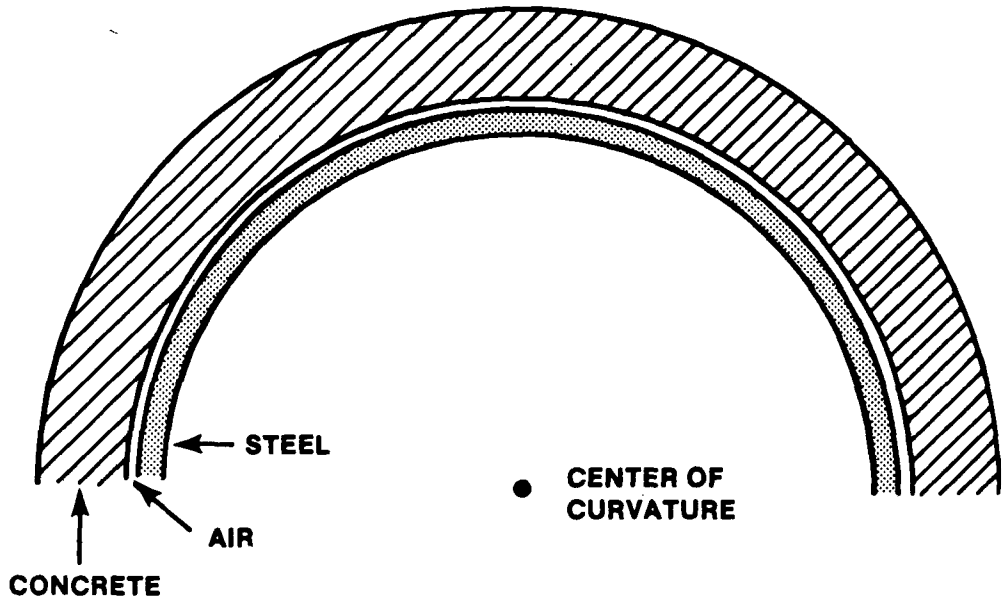

Figure 2-10. Cylindrical Structure Consisting of a Steel Liner, Air Gap, and Thick Concrete Wall

high atmosphere-structure heat transfer coefficients, a surface node thin enough to resolve the thermal diffusion length may lead to unstable structure temperatures. The stability criteria are equivalent to requiring that the cell timestep not be so long that proper account is not taken of the feedback between the first node temperature and the atmosphere-structure heat transfer process. An unstable condition is most easily remedied by reducing the ratio of cell timestep to system timestep, "ctmfr".

Each structure has two surfaces designated as the "inner" and "outer" surfaces. The precise meaning of the "inner" surface is that its location is given by the first number in the list of node positions in the input for the structure (see Section 3.3.1.3). For spherical or cylindrical structures, the coordinate given in the list is the radius. The center of curvature of spherical or cylindrical structures is determined by whether the radius is increasing or decreasing in the list. If it is increasing, the inner surface is concave; otherwise, it is

convex. The inner boundary is always inside the cell in which the structure is defined and exchanges heat with the atmosphere through convective heat transfer and through condensation or evaporation of coolant if the CONDENSE option has been specified (see Section 2.3.1.4), and through radiation if a radiation model is used.

Several options are available for the outer boundary condition: The outer boundary can be declared either (1) adiabatic or (2) "isothermal." (Isothermal boundaries are treated as if exposed to a gas held at a fixed, user-specified temperature and coupled through a fixed surface heat transfer coefficient of 6.08 W/m^2-K, a value typical of turbulent convective heat transfer to walls.) The outer boundary can also be (3) declared to be within the same cell as the structure or (4) in another cell. Special rules apply in the latter two cases.

If the outer boundary is within the same cell, then condensation and convective heat transfer can take place on the outer surface just as they do on the inner surface. However, radiative heat transfer between the atmosphere and the structure may occur only with respect to the inner surface or with respect to both the inner and outer surface, depending on the radiation model chosen. Radiative heat transfer to a heat transfer structure from the lower cell may occur only with respect to the inner surface.

If the outer boundary is in another cell, it exchanges heat with that cell's atmosphere at a rate determined by a surface heat transfer coefficient of 6.08 W/m^2-K. Also, radiative heat transfer and condensation heat transfer do not take place at the outer boundary. If radiative heat transfer or condensation heat transfer are important on both sides of a wall which joins two cells, then it may be better to divide the wall down the middle, put one half in each cell, and use an adiabatic boundary condition at each of the adjoining surfaces. Note, however, that there will be no transport of heat from one half of the wall to the other half when this is done.

2.3.1.3.2 Fission Product Heating of Structures. Fission products may become attached to structure surfaces as a result of aerosol deposition,

user-defined targeted release rates, initial conditions, or fission product source tables. The inner and outer surfaces of structures may be heated by decay heat from these fission products. The decay heat of fission products residing on a structure surface is deposited into the node immediately below that surface. Long range heating effects due to the gamma and beta rays, which would result in some of the decay heat being deposited in the atmosphere, interior nodes, or other structures, are not modeled.

It should be pointed out that, unlike earlier versions of the code, CONTAIN 1.1 no longer groups structure surfaces into generic ROOF, WALL, or FLOOR repositories. Each surface is now a separate repository and is heated specifically by fission products in that repository. (The ROOF, WALL, or FLOOR surface orientation is used primarily to determine the appropriate heat transfer coefficient and aerosol deposition rate. It is also used to report aerosol and fission product inventories on that type of surface when a summary is requested.)

2.3.1.4 Convection and Condensation. In this section, the model for atmosphere-structure heat transfer by convection and condensation is described, including the CONTAIN forced convection option. The role played by the condensate film thickness is discussed. The user should note that the modeling described in this section is available only if the CONDENSE option has been specified. If CONDENSE has not been specified, a nominal dry heat transfer coefficient of 6.08 W/m^2-K is assumed for all nonadiabatic surfaces, and condensation on structures and the formation of the condensate film are ignored. The user should also note that condensate draining from structures will be lost from the problem unless a lower cell with a pool is specified (see Sections 2.3.2 and 2.3.2.5).

The heat transfer between the atmosphere and structures described in this section occurs by two processes, convection (which can also be considered conduction through a turbulent gas boundary layer) and condensation (which for the purposes of this discussion includes evaporation). The next section describes a third process, radiation. Figure 2-11 shows the heat transfer configuration assumed for the calculation. A gas boundary layer in the atmosphere contributes the principal thermal resistance

under condensing conditions. This is because the coolant vapor must diffuse through a region of enhanced noncondensable concentration and depleted condensable vapor concentration. The modeling for this process is based largely on Chapter 10 of Reference Col81. For most calculations, it would be sufficient to calculate only this boundary layer resistance. However, this resistance can occasionally become quite small, and it is therefore desirable to include the other resistances that are in series with it. These include the condensate film and a layer of oxide or paint at the structure surface. Figure 2-12 illustrates schematically the various resistances affecting heat and mass transfer to structures (although the figure should not be taken literally as an equivalent thermal circuit, since convection is driven by a temperature difference, while condensation is driven by a partial pressure difference).

After deriving expressions for the mass and heat fluxes across a boundary layer using an analogy between heat and mass transfer, Reference Col81 describes an iterative process for correcting the fluxes to account for the presence of an interfacial liquid film. However, for containment applications, the film resistance is expected to be quite small compared with other resistances in series with it, so the computationally expensive iterations can be bypassed by making use of a first-order Taylor series expansion in $(T_i - T_{wall})$ where T_i is the temperature of the film surface and T_{wall} is the wall temperature. (Note: for convenience, the term "wall" as used throughout this section refers to any type of heat transfer structure - ROOF, WALL, or FLOOR.) In the following, we use a superscript zero in parentheses to refer to the lowest order term in the Taylor expansion, which is obtained by setting $T_i = T_{wall}$.

The mass flux J (units of kg/m^2-s) is approximated by

$$J^{(0)} = K_g M(P_{vb} - P_{vw}) \qquad (2\text{-}28)$$

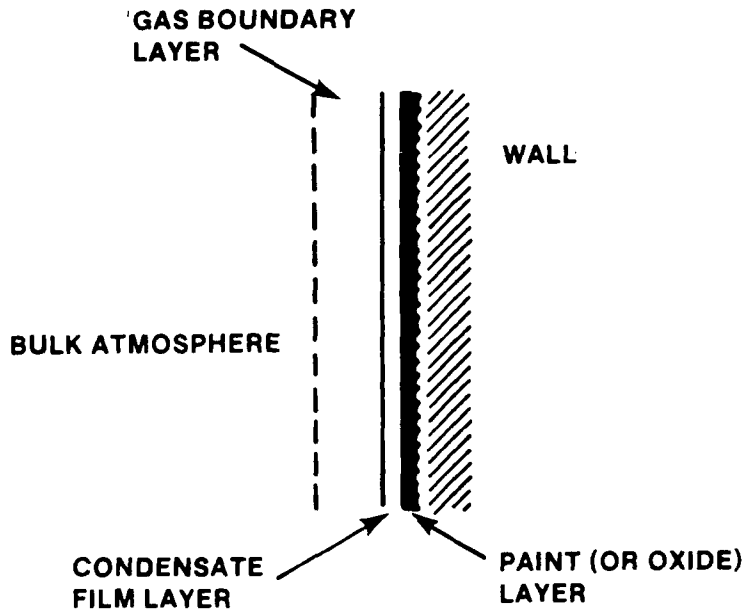

Figure 2-11. Heat Transfer Configuration

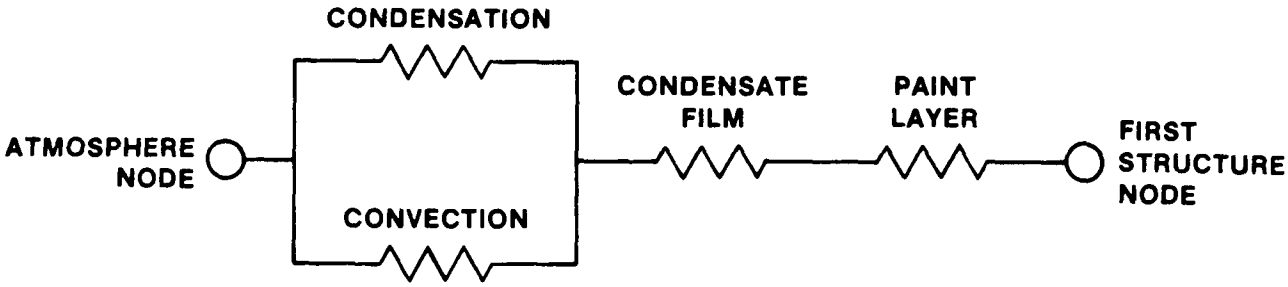

Figure 2-12. Lumped Parameter Equivalent Circuit for the Heat Transfer Configuration of Figure 2-11

where

M = vapor molecular weight,
P_{vb} = partial pressure of vapor in bulk atmosphere (at the bulk temperature T_{bulk}),
P_{vw} = saturation pressure at the temperature T_{wall},

and

$$K_g = \frac{Sh\ P\ D_v}{R\ T\ P_{nm}\ L} \tag{2-29}$$

where

P = cell pressure,
D_v = mass diffusivity of vapor in the noncondensable gas [Bir60],
R = gas constant,
T = the average of T_{bulk} and T_{wall},
L = characteristic length,

and

$$P_{nm} = (P_{vb} - P_{vw})/\ell n\left[(P - P_{vb})/(P - P_{vw})\right] . \tag{2-30}$$

The Sherwood number Sh itself is determined by using an analogy between heat transfer and mass transfer:[Kre58]

$$Sh = Nu(Sc/Pr)^{1/3} \tag{2-31}$$

In this expression, Nu is the Nusselt number, Pr the Prandtl number, and Sc the Schmidt number for the bulk gas-vapor mixture.

The total heat flux q (units of J/m^2-s) consists of two components, one for convective heat transport across the boundary layer, q_c, and one for the heat transported by the mass flux, q_m, and is approximated by

$$q^{(0)} = q_c^{(0)} + q_m^{(0)} \tag{2-32}$$

where

$$q_c^{(0)} = h_c(T_{bulk} - T_{wall}) \tag{2-33}$$

for which the heat transfer coefficient for convective conduction is related to the Nusselt number by

$$h_c = Nu(k/L) \tag{2-34}$$

Here, k is the thermal conductivity of the gas-vapor mixture.

The second component of the total heat flux, accounting for the heat transported by the mass flux, is approximated as

$$q_m^{(0)} = J^{(0)}H_{\ell v}^{(0)} = J^{(0)}[H_v(T_{bulk}) - H_\ell(T_{wall})] \tag{2-35}$$

where $H_{\ell v}^{(0)}$ is defined as the difference between the bulk vapor specific enthalpy and the specific enthalpy of the liquid at the wall temperature.

Several standard correlations are available in CONTAIN for determining Nu in either forced or natural convection regimes. For laminar natural convection,

$$Nu = 0.27(GrPr)^{1/4} \tag{2-36}$$

For turbulent natural convection,

$$Nu = 0.13(GrPr)^{1/3} \tag{2-37}$$

For forced convection,

$$Nu = 0.037\left(Re^{4/5}Pr^{1/3}\right) \tag{2-38}$$

In these equations, Gr is the Grashof number, and Re is the Reynolds number. The larger of the natural or forced convection Nusselt numbers is always used in modeling the heat transfer.

The forced convection correlation is only used when the keyword FORCED appears in the input for the CONDENSE block, and the option requires the specification of a time-dependent gas surface velocity or its equivalent for each structure. As alternatives, the user may specify time-dependent Reynolds numbers or Nusselt numbers associated with each structure. The two surfaces of any structure located entirely within a given cell are assumed to see the same convective heat transfer conditions.

For the other two correlations, only one input variable is required. This is the characteristic length for the Grashof number, "chrl", specified for the structure. Note, however, that there is actually very little dependence of the heat transfer coefficient on this characteristic length. For laminar natural convection, the dependence is to the -1/4 power of length, while for turbulent natural convection, there is no dependence at all.

Note that convection and condensation heat transfer to the surface of a lower cell pool are also treated according to the above equations if

CONDENSE has been specified. The pool is treated as a floor with a characteristic length equal to the square root of the pool area and a "wall" temperature equal to the pool temperature. The first order corrections discussed below, however, are not applied.

Equations (2-28) through (2-38) together specify the first approximations to the mass and heat fluxes to structures. The next step is to correct the treatment for the effects of the changing condensate layer depth by including the next term in the series expansion in $(T_i - T_{wall})$. The first-order Taylor series expansion of $P_{sat}(T_i)$ about its value at T_{wall} is

$$P_{vi} = P_{sat}(T_i) = P_{sat}(T_{wall}) + [dP_{sat}(T)/dT]_{T_{wall}}(T_i - T_{wall}) \quad (2\text{-}39)$$

The corrected mass flux can now be written as

$$J^{(1)} = J^{(0)} - B(\Delta T)/H_{\ell v}^{(0)} \quad (2\text{-}40)$$

where the correction term B is given by

$$B = K_g M[dP_{sat}(T)/dT]_{T_{wall}} H_{\ell v}^{(0)} \quad (2\text{-}41)$$

and ΔT by

$$\Delta T = T_i - T_{wall} \quad (2\text{-}42)$$

Similarly, $H_{\ell v}$, q_m, and q_c are expanded to first order in ΔT. The heat flux to the film surface is equated to the heat flux through the liquid

film and paint layers (using an effective heat transfer coefficient h_{eff} given by the inverse of the total series resistance):

$$q^{(1)} = q_m^{(1)} + q_c^{(1)} = h_{eff}\Delta T \tag{2-43}$$

Equation (2-43) can be solved to obtain

$$\Delta T = \frac{q^{(0)}}{h_c + h_{eff} + J^{(0)}c_p + B} \tag{2-44}$$

where c_p is the specific heat of the liquid at the temperature T_{wall}. The corrected fluxes are then obtained by substituting Equation (2-44) for ΔT into Equations (2-40) and (2-43).

Realistic treatment of accumulated condensate is important because the condensate constitutes a reservoir of coolant that is available for evaporation when the atmosphere dries out. The resistance of the paint or oxide layer is fixed by the code at 5×10^{-4} m^2K/W, while that of the condensate layer is calculated from the thermal conductivity of the water and the film depth. The film depth is initially zero, and increases with problem time according to a simple model for the accumulated condensate mass on each exposed surface. The maximum film depth "flmax" is an input variable with a default of 5.0×10^{-4} m. When the accumulated volume of condensate on any surface exceeds the product of the surface area and "flmax", the excess condensate is not allowed to accumulate on the surface, but is instead assumed to drain into the pool of the overflow cell.

By default the overflow cell is the cell in which the structure is defined, but this can be changed to any other cell with the cell OVERFLOW option discussed in Section 3.3.1.11. (This overflow cell is also the destination cell for aerosol mesh losses.) If no pool has been specified in input for the overflow cell, or if the overflow cell is specified to be zero, the mass of the condensate runoff is lost from the problem.

Aerosol deposition is very sensitive to whether the atmosphere is saturated or superheated, because moisture in the atmosphere can condense on aerosols and affect their settling characteristics. Therefore, it is important to have a relatively realistic model not only for the coolant that is available from the pool or sump surfaces, but also for the limited reservoir of condensate that resides on structures and is available for evaporation. In choosing a value or performing sensitivity analyses on the parameter "flmax", the analyst should remember that the effect of the film on heat transfer to the surface is unlikely to be very significant, but the effect on the degree of atmospheric superheat could be quite large. Therefore, the most relevant consideration is probably the question of what volume of condensate should be allowed to accumulate (in puddles and droplets as well as in films) on a large exposed surface area and be available for evaporation. The question of how thick a condensate layer might be on a hypothetical wall for the purpose of heat transfer calculations is generally of secondary importance.

Note that aerosols deposited on structure surfaces, with the possible exception of coolant aerosols, remain on the surface. If CONDENSE has been specified, coolant aerosols are incorporated into the condensate film, which may drain if conditions warrant. Fission products may be carried with the draining liquid, according to the transport efficiency factors defined in the FPLIQUID input block and discussed in Section 2.2.5.5.

2.3.1.5 Thermal Radiation. When high gas temperatures occur (e.g., during a combustion event) in a compartment, gas radiation may become a significant heat transfer mechanism. The heat transfer is affected by the large quantities of water vapor that are typically present in containment, due to its strong emission bands and the optical depth attainable in typical containments. In addition to steam, carbon monoxide and carbon dioxide may be present as the result of core-concrete interactions and may also contribute to the optical properties of the atmosphere. Aerosols contribute to the scattering and absorptivity of the atmosphere, and therefore their effects should also be considered in the radiative process.

Two different methods are available through the RAD-HEAT input block to calculate radiative heat transfer within a cell. The user can activate either a net enclosure model, through the keyword ENCLOS, or a simpler model, through either of the keywords GASWAL or GEOBL. The simple GASWAL model treats the radiative heat transfer between the atmosphere and the structures in the cell and between the atmosphere and the uppermost lower cell layer. The GASWAL model allows radiative heat transfer from the atmosphere to both the inner and outer surfaces of a structure if they are within the cell. A separate model consistent with the GASWAL model but specified through structure input treats the direct radiative exchange between the uppermost lower cell layer and the inner surface of structures. Finally, the net enclosure method (ENCLOS) self-consistently treats radiative heat transfer among all structures and the lower cell, between the atmosphere and structures, and between the atmosphere and lower cell, but only the inner surfaces of structures within the cell are allowed to participate.

Both models make use of gas radiation properties that account for the absorptivity of aerosols and the emissivity of H_2O, CO_2, and CO. For those cases where only water vapor is present, a Cess-Lian correlation may be specified with the CESS keyword.[Ces76] If this option is chosen, CO and CO_2 (if present) are assumed to be transparent and therefore do not contribute to the total gas mixture emittance. When either of the latter two species is present, the default CONTAIN model, based on the method developed by Modak, is recommended.[Mod79]

In the next sections, the models for gas and aerosol optical properties will be described, followed by a discussion of the two radiative heat transfer methods. The simpler options for radiative heat transfer are provided for those cases in which a relatively simple treatment is adequate. It is the responsibility of the user to assess the appropriateness of the simpler treatments when they are used for a particular application.

2.3.1.5.1 Radiative Properties of H_2O, CO_2, and CO Mixtures. The characterization of the energy transfer for a participating gas medium requires the determination of the gas emittance. This quantity is a

function of the gas composition, pressure, temperature, and the average optical depth of the gas. The average optical depth is also referred to as the mean path, or beam, length.

The emissivity ϵ_g of a gas mixture is calculated from the emissivities of the individual CO, CO_2, and H_2O species with a correction for the overlapping of absorption bands from different species.

The emissivity of each species has been obtained by summing over its spectral absorption bands.[Edw73] In the parameter space of interest for nuclear reactor containments, the spectral emissivities and the experimental results agree to within 5%. In the approximate method adopted here, the species' spectral emissivities are approximated by curve fits, and the overlap correction is taken to be a temperature-dependent form of Leckner's correction $\Delta\epsilon_{cw}$.[Lec72]

The species' emissivities (ϵ_{CO2}, ϵ_{CO}, or ϵ_{H2O}) are fit to functions of partial pressure P, pressure-pathlength PL, and temperature T by the expression

$$\ln \epsilon = \sum_{i=0}^{2} T_i(x) \sum_{j=0}^{3} T_j(y) \sum_{k=0}^{3} c_{ijk} T_k(z) \qquad (2\text{-}45)$$

In the above expression,

$$x = p_1 + \frac{\ln P}{p_2}$$

$$y = [\ell_1 + \ln PL]/\ell_2 \qquad (2\text{-}46)$$

$$z = [T - t_1]/t_2;$$

c_{ijk} denotes a set of 48 coefficients for CO_2, CO, and H_2O, derived from experimental data and spectral calculations; p_1, p_2, ℓ_1, ℓ_2, t_1, and t_2

are Gauss-Chebyshev approximation parameters for partial pressure, pressure-pathlength, and temperature; and $T_n(x)$ is a Chebyshev polynomial of order n and argument x.

The gas mixture emissivity ϵ_g is computed from

$$\epsilon_g = \epsilon_{CO} + \epsilon_{CO2} + \epsilon_{H2O} - \Delta\epsilon_{cw} \tag{2-47}$$

where ϵ_{CO}, ϵ_{CO2}, and ϵ_{H2O} are the emissivities of CO, CO_2, and H_2O, respectively, and $\Delta\epsilon_{cw}$ is the overlap correction factor for CO_2 and H_2O. The overlap correction $\Delta\epsilon_{cw}$ accounts for the 2.7- and 15-μm overlapping bands of CO_2 and H_2O. The overlap correction originally suggested by Leckner has been modified to include the temperature variation of $\Delta\epsilon_{cw}$: [Edw73]

$$\Delta\epsilon_{cw} = \left| \frac{\zeta}{(10.7 + 101\zeta)} - \frac{\zeta^{10.4}}{111.7} \right| \times$$

$$\{\log_{10}[101.3(P_{CO2} + P_{H2O})L]\}^{2.76} F(T) \tag{2-48}$$

$$\text{for } (P_{CO2} + P_{H2O})L \geq 1.013 \times 10^4 \text{ Pa-m}$$

$$\text{and } \zeta \geq 0.01; \text{ and}$$

$$\Delta\epsilon_{cw} = 0, \quad \text{otherwise.}$$

The parameter ζ is defined by

$$\zeta = P_{H2O}/(P_{H2O} + P_{CO2}) \tag{2-49}$$

and F(T) is given by

$$F(T) = -1.0204 \times 10^{-6}T^2 + 2.2449 \times 10^{-3}T - 0.23469 \tag{2-50}$$

2.3.1.5.2 Aerosol Opacity. The emissivity ϵ_m of the gas-aerosol mixture is given by

$$\epsilon_m = \epsilon_s + \epsilon_g - \epsilon_s\epsilon_g \tag{2-51}$$

With ϵ_g defined in the preceding section, it remains to determine ϵ_s, the aerosol emissivity that the aerosols would have in the absence of optically active gas species.

The method of Felske and Tien is used to obtain ϵ_s.[Fel73] This method is applicable to absorbing particles that are small enough to produce negligible scattering. In this limit, the spectral absorption coefficient k_λ is proportional to λ^{-1}, the inverse wavelength. Thus,

$$k_\lambda = \beta f_v/\lambda \tag{2-52}$$

where f_v is the aerosol concentration by volume (m^3 aerosol/m^3 gas), and β is a constant of proportionality. The expression used for the aerosol emissivity is

$$\epsilon_s = 1 - \frac{15}{\pi^4}\psi^{(3)}(1 + k_{\lambda m}LT\lambda_m/C_2) \tag{2-53}$$

where $\psi^{(3)}$ = pentagamma function,

L = beam length of the path,

$k_{\lambda m}$ = absorption coefficient at the reference wavelength,

T = gas temperature,

λ_m = reference wavelength at which $k_{\lambda m}$ applies, and

C_2 = second Planck constant.

For this implementation, λ_m is chosen to be 0.94 μm, a value representative of infrared radiation. Note that $k_{\lambda m}\lambda_m$ in Equation (2-53) is independent of wavelength according to Equation (2-52).

There are two methods provided for evaluating $k_{\lambda m}$. The first is selected by the ABSORB option in the RAD-HEAT input block. In this option, a constant value may be specified for $k_{\lambda m}$. This value will be independent of total aerosol mass concentration in the problem.

The second method is more mechanistic in that it couples the aerosol cloud emissivity calculation to the aerosol mass loading. A formula for the aerosol cloud absorption coefficient derived by Pilat and Ensor is used to obtain the value of $k_{\lambda m}$.[Pil70] Thus

$$k_{\lambda m} = 4000 \text{ "kmx" } C_a \qquad (2\text{-}54)$$

where C_a is the total aerosol mass concentration (in kg/m^3) computed by the code, and "kmx" is a constant of proportionality specified through the KMX option of the RAD-HEAT input block. In the limit of zero aerosol suspended mass, this correlation gives zero absorption. The constant of proportionality is provided to allow the user to account for the effects of wavelength, index of refraction, particle size distribution and aerosol particle material density, as explained in Reference Pil70. A value of "kmx" = 1 corresponds approximately to soot-like particles with a density of 2000 kg/m^3.[Pil70] Note that since $f_v = C_a/\rho_a$, where ρ_a is the aerosol particle material density, a value of "kmx" of $\beta/(4000\rho_a\lambda_m)$ will result in $k_{\lambda m} = \beta f_v/\lambda_m$.

2.3.1.5.3 Steam Emittance (Cess-Lian). If the CESS keyword is chosen in the RAD-HEAT input block, an analytic correlation developed by Cess and Lian is used to calculate the steam/air emissivity and absorptivity.[Ces76] In this model, data from Hottel emittance charts [Hot67] have been fitted to an equivalent single-band exponential form, which requires significantly less computation time than that for a wide band exponential model.

The Cess-Lian equations are

$$\epsilon_{H2O} = a_0\left[- \exp\left(-a_1\sqrt{X} \right)\right] \tag{2-55}$$

$$X = P_{H2O}L \left[\frac{300}{T_g}\right] \left[\frac{P + \left(5\sqrt{\frac{300}{T_g}} + 0.5\right) P_{H2O}}{(101325)^2}\right] \tag{2-56}$$

where ϵ_{H2O} = steam emissivity,
a_0, a_1 = coefficients determined from Table 2-3,
P_{H2O} = steam partial pressure,
L = beam length,
T_g = gas temperature, and
P = total gas pressure.

Table 2-3
Coefficients for the Cess-Lian Correlation

T (K)	a_0 (dimensionless)	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

2.3.1.5.4 Atmosphere-Structure Radiative Heat Transfer (Simple Models). Simple models for the radiative transfer between the upper cell atmosphere and heat transfer structures, between the atmosphere and the uppermost lower cell layer, and between the uppermost lower cell layer and heat transfer structures are available. In contrast to the net enclosure (ENCLOS) model, in the simple models, secondary reflections between surfaces are treated only in an approximate fashion. The simple model for radiative heat transfer between the upper cell atmosphere and structure and lower cell surfaces is invoked by specifying either GASWAL or GEOBL in the RAD-HEAT input block. The simple model for direct radiative exchange between the lower cell and heat transfer structures is invoked by specifying the "vufac" parameter in the structure input block (see Section 3.3.1.3).

The net radiative heat transfer flux q between the gas-aerosol mixture at temperature T_g and a black enclosure at temperature T_w is determined from

$$q = \sigma\left[\epsilon_m T_g^4 - \alpha_m(T_w)T_w^4\right] \qquad (2\text{-}57)$$

where the emissivity ϵ_m of the gas-aerosol mixture (hereafter referred to as the "gas") is obtained from correlations evaluated at the gas temperature T_g, and the gas absorptivity α_m is obtained from the same correlations at the surface temperature T_w. Note that the gas absorptivity is usually not equal to the gas emissivity if T_g and T_w are different.

If the enclosure is gray rather than black, some of the radiation striking it is reflected back into the gas and to other parts of the enclosure. Multiplication of Equation (2-57) by the surface emissivity ϵ_s allows for proper reduction of the primary beams (gas-to-surface or surface-to-gas), but secondary reflections can at best be incorporated into an effective surface emissivity ϵ' in the simple model.[Bau78] The emissivity corrected for secondary reflections, ϵ', lies between ϵ_s and 1. In practice, it may be sufficiently accurate to use an effective emissivity ϵ', which is equal to $(\epsilon_s + 1)/2$. The effective emissivity ϵ' depends primarily on the surface properties, but depends also on the gas

properties and beam lengths. Expressions for ϵ' and their limitations can be found in Reference Bau78.

Equation (2-57) is modified empirically to give the expression used for the heat flux between the gas and structures and between the gas and the lower cell in the GASWAL or GEOBL options:

$$q = \sigma\epsilon' \left[\epsilon_m T_g^4 - \alpha_m(T_w)T_w^4\right] \qquad (2\text{-}58)$$

The user must supply the values of ϵ' for dry structure or lower cell surfaces through the EMSVT keyword. If the surface has a water film, a value appropriate for water ($\epsilon' = 0.94$) is automatically used in the code.

The gas absorptivity α_m is calculated from either the Cess-Lian correlation or the Modak model by using Kirchhoff's law of radiation, which states that spectral emissivity for the emission of radiation at temperature T is equal to the spectral absorptivity for radiation coming from a blackbody at the same temperature T. This law may be considered valid whether or not thermal equilibrium prevails. Its proper application greatly simplifies the calculation of radiative transfer.

Equation (2-58) does not consider direct radiative exchange between the lower cell and structures. However, direct radiative exchange between the uppermost lower cell layer surface and the inner surfaces of heat transfer structures is modeled separately if "vufac" is specified in the input for heat transfer structures (see Section 3.3.1.3). This input parameter, as defined below, is the fraction of the blackbody radiant energy leaving the layer that is intercepted and absorbed by a given structure. The direct exchange model includes the attentuating effects of the intervening atmosphere if the GASWAL or GEOBL option has been invoked. However, the direct exchange model can be invoked even if one of the former options is not. In that case, the atmosphere has no effect on the radiative exchange.

The energy transfer rate due to direct radiative exchange between the layer surface and a given structure is calculated using the equation

$$Q_{rad} = \left[1 - \alpha_m(T_{surf})\right] A_p C \left[T^4_{surf} - T^4_{struc}\right] \qquad (2\text{-}59)$$

where α_m = gas absorptivity. (This is set to zero if the GASWAL model is not invoked.)

T_{surf} = layer surface temperature,

A_p = surface area of layer,

C = product of Stefan-Boltzmann constant and user-specified parameter "vufac", and

T_{struc} = inner surface temperature of structure.

The "vufac" parameter is a function of the emissivities of the radiating bodies and their geometrical relationships. For gray bodies, "vufac" can be defined as

$$\frac{1}{vufac} = \frac{1}{\bar{F}_{ps}} + \left[\frac{1}{\epsilon_p} - 1\right] + \left[A_p/A_s\right]\left[\frac{1}{\epsilon_s} - 1\right] \qquad (2\text{-}60)$$

where $\bar{F}_{ps}$ = standard view factor. (It is the fraction of the radiation from the layer surface directed into the solid angle subtended by the structure and is available in tabulated and graphical form in most heat transfer texts and handbooks.)

ϵ_p = emissivity of layer surface,

ϵ_s = emissivity of the structure surface, and

A_s = area of the inner surface of the structure.

Because of the possibility of confusion, the user should note again that direct radiative exchange between the lower cell and the structures through an intervening gas is modeled only if the "vufac" parameters are specified in the structure input. The attenuating effects of the gas on the direct exchange are taken into account only if either the GASWAL or GEOBL options is also used. Also, neither Equation (2-58) nor Equation

(2-59) is used if the next model to be discussed, the net enclosure model, is invoked.

2.3.1.5.5 Net Enclosure Radiative Heat Transfer (ENCLOS Option). The net enclosure model in CONTAIN is a treatment of radiative transfer involving a participating gas-aerosol mixture and the surrounding structures that takes secondary reflections into account automatically. It is based on a formulation for diffuse gray surfaces from Reference Sie81 (see the derivation in Reference Ber85). Since the method as implemented requires the gas in the enclosure to be isothermal, only one cell is modeled at a time. When a participating medium is not present in the cell (i.e., when steam, CO, CO_2, and aerosols are absent), the radiation model reduces to the surface radiative exchange problem with a transparent nonattenuating gas medium.

The net radiation flux density q_i to the i-th surface with area A_i is the difference between the incoming radiation flux density Ξ_i and the outgoing radiation flux density, or radiosity, Ψ_i.

$$q_i = \frac{Q_i}{A_i} = \Xi_i - \Psi_i \qquad (2\text{-}61)$$

Since the outgoing flux is the sum of the reflected flux and the blackbody flux multiplied by the emissivity ϵ_i of the surface, the following equation is obtained from Kirchhoff's law:

$$q_i = \frac{\epsilon_i}{1-\epsilon_i} (\Psi_i - B_i) \qquad (2\text{-}62)$$

where q_i = net heat flux to the i-th surface,
ϵ_i = emissivity of the surface,
$B_i = \sigma T_i^4$ = blackbody flux emitted from the surface,
σ = Stefan-Boltzmann constant, and
T_i = surface temperature.

The radiosities are determined by solving the following system of simultaneous equations

$$\Psi_i - (1 - \epsilon_i) \sum_{j=1}^{N} F_{ij}[1 - \epsilon_{mji}]\Psi_j$$

$$= \epsilon_i B_i + (1 - \epsilon_i) \sum_{j=1}^{N} F_{ij}\epsilon_{mji}B_g \qquad (2\text{-}63)$$

where N = number of surfaces,

F_{ij} = view factor from surface i to surface j (i.e., the fraction of radiation from i directed toward j),

$B_g = \sigma T_g^4$ = Planck blackbody flux for the gas, where T_g is the gas temperature, and

ϵ_{mij} = emissivity of the gas that is a function of the beam length to the receiving surface.

The dry surface emissivities, view factors, and characteristic beam lengths between surfaces are provided by the user. Whenever a water film is present on surfaces, the emissivity for that surface is automatically equated to the emissivity of water, which is set to 0.94. Since the surface and gas temperatures are known, a network of equations for the radiative heat transfer among the surfaces can be constructed, and the resulting linear system of equations is solved to give the net heat flux to each surface. These equations are solved with a standard linear equation solver. Note that if the gas is transparent, then the last term of the right hand side and the gaseous emission terms of the left hand side of Equation (2-63) vanish, yielding equations which are independent of the gas temperature and composition:

$$\Psi_i = \epsilon_i B_i + (1 - \epsilon_i)G_i \qquad (2\text{-}64)$$

where $G_i = \sum_{j=1}^{N} F_{ij}\Psi_j$ is the irradiance for surface i, which is composed of radiation coming from the other surfaces.

2.3.1.6 Heat Transfer Control Options. The code allows the user to deactivate the heat transfer across certain interfaces on a cell-by-cell basis. The heat transfer that can be deactivated corresponds to:

- heat transfer between the atmosphere and all structures, including convection, condensation, and radiative heat transfer,
- heat transfer between the first node in the lower cell model and the basemat,
- heat transfer between different layers in the lower cell, excluding the atmosphere layer,
- heat transfer between the uppermost solid or liquid layer in the lower cell and the atmosphere above it, including convection, condensation, and radiative heat transfer,
- radiative heat transfer between the uppermost layer in the lower cell and all structures and between the atmosphere and all structures.

The user can control these heat transfer processes by setting specified flags to ON or OFF. The default for all flags is ON. If a flag is set to OFF, the corresponding heat transfer is set to zero.

This optional heat transfer control option is useful for simulating adiabatic or insulated conditions. It also provides a means by which the user can check the effectiveness of various heat transfer mechanisms.

2.3.1.7 Hydrogen and Carbon Monoxide Combustion. The treatment of hydrogen and carbon monoxide combustion is derived directly from the HECTR code developed at Sandia National Laboratories for analyzing hydrogen behavior in containment.[Cam86] The burn model initiates combustion when threshold parameters are exceeded and the time is within the window during which burns are allowed. The user may define the burn window to account for the presence or absence of ignition sources (e.g., igniters, sparks from electrical equipment, etc.). The burn continues

for a time that is based on either an internally calculated or a user-specified flame speed, and the burn can propagate to adjacent cells if conditions are favorable.

The molar concentrations required for ignition of a mixture containing more than one combustible gas are related to the concentration required for a mixture with a single combustible gas through Le Chatelier's formula. That formula is expressed here in terms of the initial mole fractions X_{CO} and X_{H2} of carbon monoxide and hydrogen, respectively:

$$X_{H2} + BX_{CO} \geq X_C^{crit} \qquad (2\text{-}65)$$

where X_C^{crit} is the threshold (or critical) mole fraction for hydrogen. Values for B are derived from empirical values of the threshold for the two limiting cases with only one combustible. Values of X_C^{crit} and the associated values of B for spontaneous ignition, and for downward, upward, and horizontal propagation are given in Table 2-4. Table 2-4 also gives the threshold mole fraction of oxygen X_O^{crit} for ignition and the threshold for the sum X_S^{crit} of the mole fractions of carbon dioxide and water vapor for inerting. For the default values in Table 2-4, a burn is spontaneously initiated if the effective combustible mole fraction is above 7%, the oxygen mole fraction is above 5%, and the sum of the carbon dioxide and water vapor mole fractions below 55%. For sensitivity studies, the various concentration limits can be changed through input to the code, as described in Section 3.3.1.7. Note that the concentration limits specified for propagation apply to the adjacent cells, not the cell in which the burn originates.

All of the energy from the burn is deposited as heat into the cell atmosphere. In this respect, the CONTAIN treatment differs from that of HECTR, which calculates the relative amounts thermalized in the atmosphere and radiated directly to heat transfer structures without first being thermalized. The latter energy is not reflected in the gas temperature and thus does not contribute to the pressurization. Experience

Table 2-4

Default Values of Concentration Thresholds**

Condition	B	$X_C^{crit\dagger}$	$X_O^{crit\dagger}$	$X_S^{crit\dagger\dagger}$
Spontaneous Ignition	0.541	0.07*	0.05	0.55
Downward Propagation	0.600	0.09	0.05	0.55
Horizontal Propagation	0.435	0.06	0.05	0.55
Upward Propagation	0.328	0.041	0.05	0.55

* With this setting and burns activated, the cell would spontaneously ignite before downward propagation would occur

** X_C^{crit} is the threshold for $X_{H2} + B*X_{CO}$, X_O^{crit} the threshold for X_{O2}, and X_S^{crit} the threshold for $X_{CO2} + X_{H2O}$

† Threshold for ignition
†† Threshold for inerting

with HECTR, however, indicates that relatively little energy from hydrogen burns is radiated directly to the structure surfaces. (Radiation of the thermalized energy is, of course, a major heat transfer mechanism during and after burns, and this process is modeled as discussed in Section 2.3.1.4.)

The H-BURN input block must be specified for a cell in which hydrogen and carbon monoxide burns are to be considered. Besides the parameters specified in Table 2-4, a number of other parameters controlling the burn can be specified by the user in the H-BURN input. The cell burn time "burnt" can be specified by the user or, alternatively, is internally calculated; in the latter calculation, a cell characteristic length "chrl" is divided by the flame speed. The default for "chrl" is calculated by taking the cube root of the volume. The flame speed "flam" can be specified by the user or, alternatively, is internally calculated; that calculation uses an experimentally derived correlation that depends on initial combustible gas, oxygen, and steam concentrations. The fraction of initial combustible "cfrmng" left following a burn can be

specified by the user or, alternatively, is internally calculated from a correlation based on the initial concentration. The final combustible concentration may never be reached if the burn is oxygen limited. By default, a burn is considered to be oxygen limited when the oxygen mole fraction falls below a value "mormng", which by default is 0.005. The appropriate amount of hydrogen and carbon monoxide is burned in each timestep, based on the remaining concentrations, the final combustible gas concentrations desired, and the remaining burn time.

In most situations, the user should allow the code to calculate the values of "burnt", "flam", and "cfrmng". The user should have a knowledge of the correlations used and reasons for overriding them before specifying alternative values. When these values are calculated, they are calculated for each burn based on the conditions existing at the start of the burn. When specified, they are held constant throughout the run. Note that the fact that the flame speed or burn time is not altered during the course of a burn could result in errors if significant amounts of gases, including combustible gases, are introduced during a burn. Also, note that the flame speed is not used if the burn time is specified.

It is possible for a burn to propagate from one cell to an adjacent cell if a connecting flow path is present and the combustible gas, oxygen, and water vapor concentrations in the adjacent cell allow propagation. The interconnections between the cells must be defined in the FLOWS or ENGVENT input blocks. (Propagation through BWR suppression pool vents is not allowed.) The criteria in Table 2-4 for the propagation of a burn to another cell depend on whether that cell is located above, along side of, or below the originating cell. The relative locations of the cells are specified through the elevation variable "elev", which has a default value of zero. These elevations, given in the H-BURN input block, should not be confused with the elevations given in the FLOWS input block, which govern natural convection. For horizontal propagation to occur between two cells, their "elev" values must be identical. If the "elev" value for cell i is greater than the value for cell j, propagation from cell j to cell i is upward, and propagation from cell i to cell j is downward. The time delay factor "kprop", $0 \leq$ "kprop" ≤ 1, delays the propagation of

a burn to an adjoining cell by the amount "kprop" multiplied by the total burn time in the cell from which the burn propagates. The default for "kprop" is 0.5.

Figure 2-13 illustrates the use of the "chrl" and "kprop" variables. A flame that starts in cell 1 has the ability to propagate to cell 2 if the proper conditions exist in cell 2. The "chrl" for cell 1 should be envisioned as the length of the cell in the flame direction, which in this illustration is X. As the cells are drawn, it will take half of the total burn time in cell 1 for the flame to reach the passage way to cell 2, which corresponds to the default "kprop" value of 0.5. In the event of a relatively long passageway, the passage length could also be taken into account by increasing the value of "kprop". If there is more than one downstream cell, an average value of "kprop" should be used.

When conditions for a burn are satisfied, the burn does not start immediately but is delayed until the start of the next system timestep. (This could cause larger burns than warranted if the system timestep is very

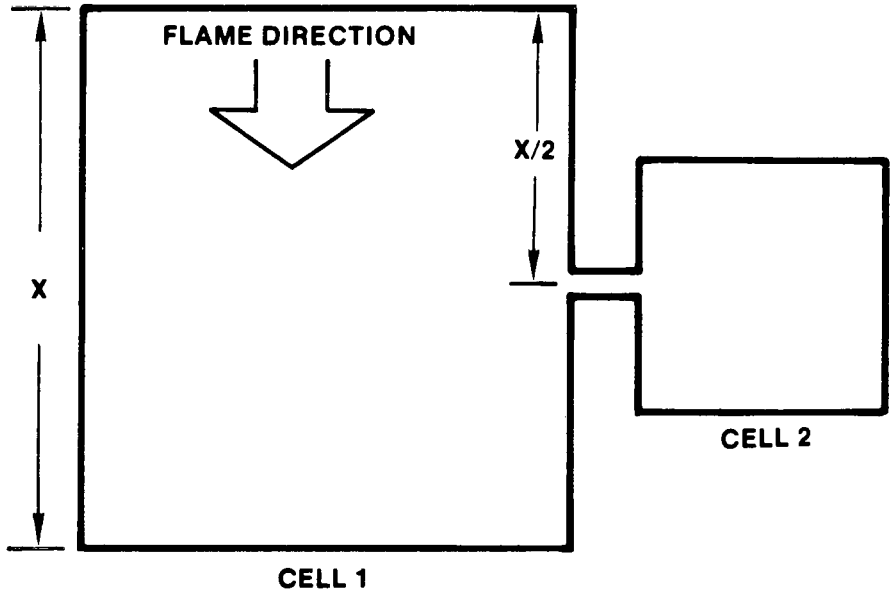

Figure 2-13. Flame Propagation Diagram

large.) That system timestep and following ones are set to the mimimum of all of the timesteps calculated internally for cells in which burns are in progress or have just finished. The internal timestep for a cell by default is set to one-tenth of the burn time for a period corresponding to twice the burn time. Burns within a given cell cannot be reinitiated until twice the burn time has elapsed following ignition in that cell. The user may adjust the timestep during the burn through the TSFRAC keyword in the TIMES input block and set the edit frequency through the EDMULT keyword (see Section 3.2.6).

A message indicating that a burn has started is written to the event summary and main output files at the time a burn starts.

2.3.1.8 Aerosol Initial Conditions and User-Specified Sources. At the global level, the keyword AEROSOL is used to specify the global aerosol characteristics, which are the same for all cells. The same keyword is used at the cell level to specify initial suspended masses and sources of aerosols. For the latter, the general format for source tables is used; however, because aerosol materials are assumed to have negligible specific heat, one need not specify a temperature or enthalpy for an aerosol material. The specific format to be followed for aerosols is discussed in Section 3.3.1.8.

The size distribution of aerosols initially present or introduced into a cell is assumed to be lognormal. The distribution is given by the "amean" and "avar" parameters specified in the global AEROSOL block. (These correspond to the spherical-equivalent mass median diameter and the natural logarithm of the geometric standard deviation with respect to diameter, respectively.) Each aerosol component or species may have a different distribution. Aerosol dynamics will in general alter the lognormal distributions as time progresses.

2.3.1.9 User-Specified Fission Product Sources. Fission product mass sources are specified at the cell level under the FISSION keyword, which must be immediately followed by the keyword SOURCE. For sources of fission products, the general format for source tables is used. However, because fission products are assumed to have negligible specific heat,

one need not specify a temperature or enthalpy for fission products. The specific format of fission product source tables is discussed in Section 3.3.1.9.

The linear chain decomposition of decay processes may result in more than one occurrence of the same fission product within the set of linear chains. The location within the chains to which the source table mass is to be assigned is specified by the fission product name and, if that is not unique, by the number of the linear chain. It is the user's responsibility to distribute a given fission product properly among the linear chains in which it occurs. As with the initial masses, a fission product should be distributed according to the branching ratio of the fission product in the chain in question.

Fission product mass specified through a source table is placed on the host specified through the HOST keyword. This keyword must be followed by a valid host number. Host number 1 is the atmosphere gas, and hosts number 2 to 1+"nac" represent the "nac" aerosol component hosts. After 1+"nac", there are two hosts for each cell structure (the inner surface host followed by outer surface host for each structure). These are followed by one host for each lower cell layer (beginning at the bottom), including the atmosphere layer, if a lower cell is specified. Finally, the last two hosts are the DUMMY host and waste holding location. Since large host numbers are not uncommon in cells with multiple structures, extreme care should be taken in specifying host numbers for fission product sources on nonairborne hosts. Input decks with nonairborne fission product sources written for versions prior to CONTAIN 1.1 should also be closely checked since host numbers greater than 1+"nac" have different meanings prior to and after CONTAIN 1.1. If a host is not specified, the host by default will be the atmosphere gas (the first host).

Note that the effects of decay on the masses specified in a source table are not modeled until the mass is introduced into the cell. It is the user's responsibility to provide source tables that reflect the radionuclide distribution at the time of introduction into the cell.

As noted in Section 2.2.5.2, fission products are treated as being massless in terms of their impact on aerosol dynamics. For fission products that are associated with aerosols and have sufficient mass to influence aerosol behavior significantly, or for fission products that are themselves aerosols, mass effects can be simulated. Means of accounting for fission product mass effects are discussed in Section 5.3.

2.3.2 Lower Cell Models

Overview

CONTAIN includes models for a number of processes that can take place in the lower cell. These include decay heating, core-concrete interactions, coolant pool behavior (including boiling), and heat and mass transfer between the lower and upper cells. Many of the models are relatively simple, yet the availability of numerous user options and user-specifiable parameters adds much flexibility to the calculation.

The nature of the material covered in each subsection of Section 2.3.2 should be reasonably apparent from the abbreviated model descriptions of Section 1.4.5, together with the titles of the subsections themselves; hence, separate overviews have not been provided for each subsection.

The lower cell models provide sources of energy, gases, fission products, and aerosols to the upper cell models. If the user can provide these sources by means of source tables as described in Section 2.3.1, lower cell modeling may not be required for problems in which only upper cell properties are of interest. However, liquid water removed from the upper cell atmosphere by any process can be lost from a problem if a lower cell model with a pool is not specified.

The lower cell system of models differs from the upper cell system primarily in that it deals with liquid and solid layers, as opposed to a gaseous atmosphere. Many of the lower cell capabilities are designed to be used as parametric models of the physical phenomena that can take place in the reactor cavity. In part, this approach is due to the high degree of uncertainty concerning phenomena involving core debris and its interactions with the coolant and concrete in the reactor cavity. Although recent experimental research has yielded improved understanding, for example, in the area of core-concrete interactions (CCI), much remains to be learned. Most of the lower cell models are intended to be a

vehicle for implementing our understanding of these phenomena and, at the same time, to be a means for the analyst to explore various alternative hypotheses concerning the disposition and interactions of the debris and coolant. The CORCON and VANESA models have been included as the best mechanistic treatments currently available for the simulation of CCI and ex-vessel aerosol production. But these models are also subject to improvement and revision as new experimental results become available.

An example of a configuration that can be analyzed by the lower cell models without invoking CORCON/VANESA is depicted in Figure 2-14. The various layers shown interact with each other primarily through heat conduction. Five layers are defined in this case, including the atmosphere layer, the coolant pool, two debris layers, and the concrete floor. (The atmosphere layer is simply an interface to the upper cell model.) The debris layers shown in Figure 2-14 are considered intermediate layers, and the user can specify an arbitrary number of them and give them arbitrary names. The composition of the layers may be specified through initial conditions provided by the user and/or through material source tables, if the composition is time-dependent.

If CORCON is not invoked, heat transfer and temperature predictions in the lower cell are made with an implicit one-dimensional finite difference conduction model. This model treats the layers in the lower cell as a coupled thermal system. This thermal system can include the basemat below the first layer, a nodalized concrete layer, multiple intermediate debris layers, a coolant pool, and the atmosphere layer. Special provisions are made to properly handle the heating of a subcooled pool, the transition to saturation, and the transport of energy to a boiling pool. Each layer is thermally coupled to adjacent layers by interlayer heat transfer coefficients as described in Section 2.3.2.7. These interlayer heat transfer coefficients are by default internally calculated but may be overridden by the user through the HT-COEF option (see Section 2.3.2.7.3). If CORCON is specified, the conduction model is operative prior to the start time for the CORCON calculations and after CORCON finishes, but not while CORCON is active. Moreover, the conduction model assumes that core debris is absent prior to the start time and is present after CORCON finishes, as discussed in Section 2.3.2.4.

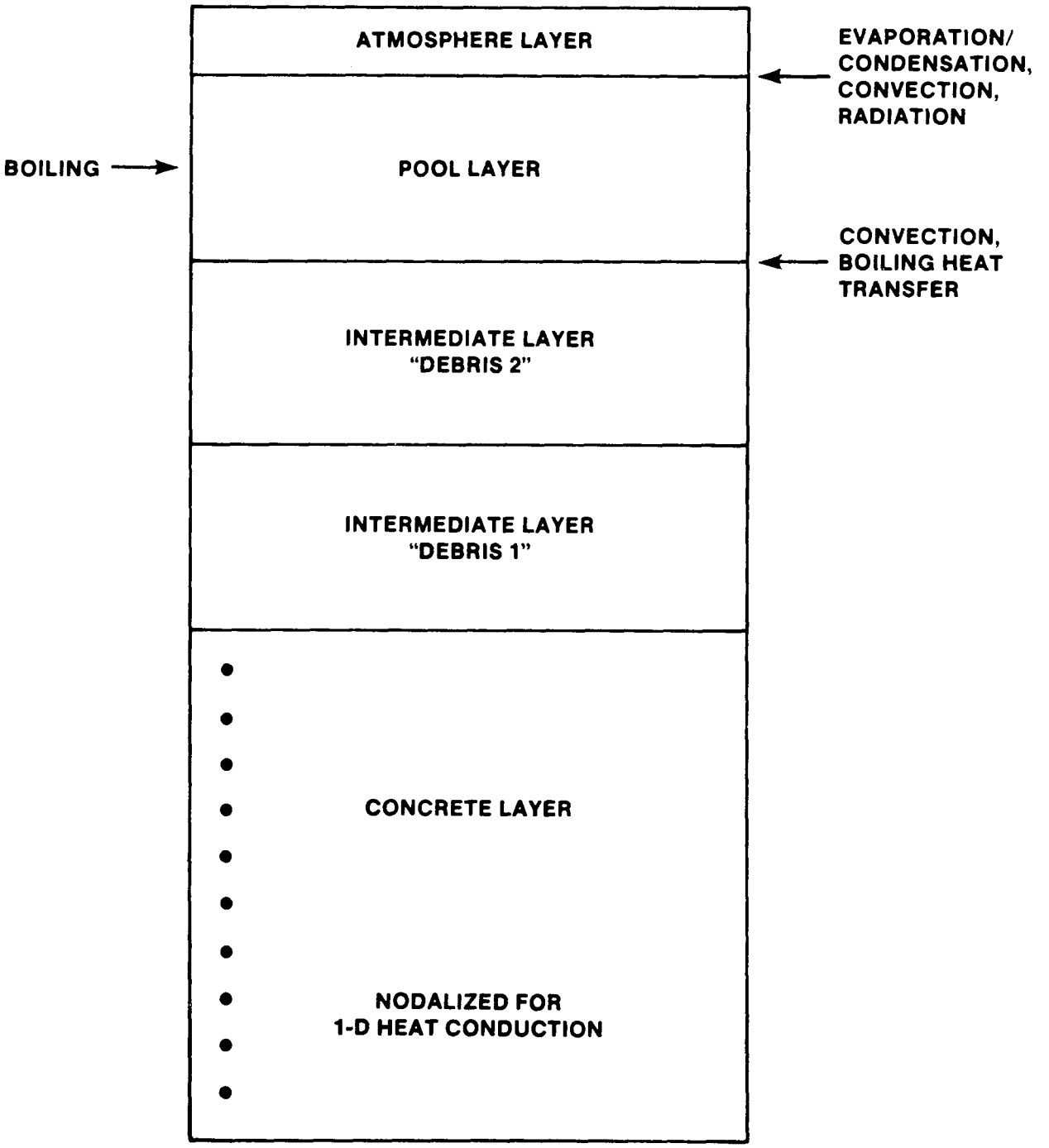

Figure 2-14. Sample Configuration for Lower Cell Conduction Modeling

The mass transfer processes allowed in the lower cell in conjunction with the conduction model are limited. Coolant may condense on the pool surface or evaporate from it if CONDENSE has been specified. Pool boiling is modeled if BOIL is specified in the pool PHYSICS input block as discussed in Section 2.3.2.5.1. The gases bubbling through the pool (e.g., due to the operation of safety relief valves in a BWR) are either partly or completely equilibrated with the pool depending on conditions, as discussed in Section 2.3.2.5.2. Humidification of the gas in the bubbles through evaporation of coolant from the bubble wall is modeled if the BOIL keyword is specified. Coolant liquid can be transferred into the pool directly through the operation of ESFs, aerosol deposition, and the draining of condensate films on heat transfer structures. Finally, the masses in any layer can often be modified through source tables in a manner which simulates a mass transfer process.

Various options for volumetric heating of the lower cell layers in conjunction with the conduction model are available. The first is the decay heating from fission products that the user has explicitly specified to be in the problem (see Section 2.2.5.4). The second is the Q-VOL option discussed in Section 2.3.2.10, which allows the user to specify tables for the volumetric heating rate as a function of time for any layer. The third is the DECAY-HT makeup decay power option discussed in Section 2.3.2.2. DECAY-HT allows the user to introduce makeup decay power to lower cell layers so that the overall decay heating in the problem follows the ANSI-standard curve. Note that DECAY-HT may also be used for the CORCON layers, but only if material source tables for the CORCON layers are not used.

The flexibility of the lower cell input allows the user to simulate a variety of processes through the conduction model. Not only can the number of intermediate layers and their composition be specified by the user, but also the default interlayer heat transfer coefficients can be overridden by user-defined functions of time, temperature, or the temperature difference between two layers. This flexibility allows the simulation of phenomena that are not explicitly modeled, such as steam spikes

resulting from fuel-coolant mixing, or even vapor explosions. How this can be done will be shown in Section 2.3.2.7.3.

However, it often is only in the reactor cavity that complex processes involving debris need to be analyzed. In many cases, intermediate layers need not be specified, and the required lower cell model may reduce to a simple coolant pool that can evaporate, boil, or be condensed upon, that can transfer heat to the basemat by simple heat conduction, and that can serve as a repository for condensate or containment sprays.

If the user has specified that the CORCON model is to be used in simulating the effects of CCI, the physical processes occurring within the core debris and below it are modeled by CORCON. CONTAIN's lower cell layer architecture is used to specify and initialize the CORCON problem and to report results. CORCON has been integrated into CONTAIN so that it receives feedback from the upper cell atmosphere or the coolant pool, but aside from this connection, CORCON runs quite independently from CONTAIN. The CORCON calculation acts much like a generator of external sources to the upper cell models of CONTAIN.

Figure 2-15 presents examples of the use of the CORCON model in two different situations. Shown are configurations both with and without a coolant pool. A single CONTAIN intermediate layer is used to initialize and report on the three possible CORCON internal layers. The name of this intermediate layer will always be "CORCON".

The three CORCON internal layers are associated automatically with three nodes of the CONTAIN intermediate layer. (Normally, only one node is available for each intermediate layer.) The intermediate layer input is used to initialize the CORCON internal layers.

If CORCON has been specified, the use of material source tables, heat transfer coefficient options, and volumetric heating options for the intermediate and concrete layers is either modified or restricted. For a pool layer, these options still function as they would without CORCON. For the intermediate and concrete layers, however, these options are ignored during the time CORCON is active, with the following exceptions:

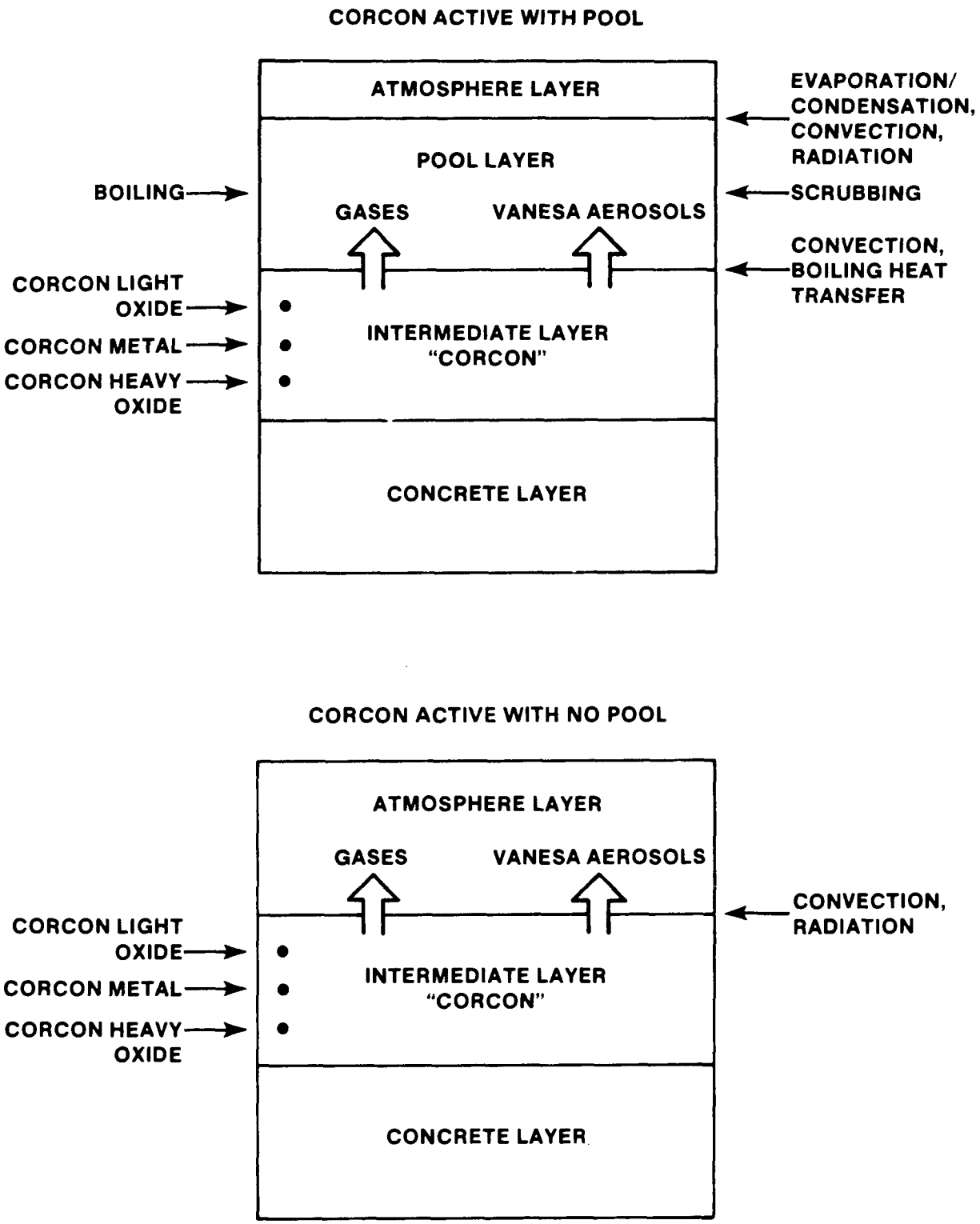

Figure 2-15. Examples of Lower Cell Configurations for CORCON With and Without a Pool Layer

(1) material source tables may still be used to add material to CORCON, as described in Section 2.3.2.3.2; (2) the HT-TRAN heat transfer control option may be used to turn off heat transfer from CORCON to the upper cell atmosphere in the sense discussed in the next paragraph; and (3) the DECAY-HT makeup decay power option may be used to override the CORCON internal decay power calculation as discussed in Section 2.3.2.2.

CORCON and VANESA interact with the upper cell in several ways. Gases produced by CCI modeled in CORCON are introduced directly into the atmosphere unless a coolant pool is present above the CORCON layers. In the latter case, the gas bubbles are assumed to equilibrate with the pool as they rise through the pool, as discussed in Section 2.3.2.5.2. The hot upper surface of the core debris interacts with either the pool or the upper cell atmosphere and heat transfer structures. This interaction can be disabled through the HT-TRAN heat transfer control options (see Section 2.3.1.6), so that neither the pool or the upper cell "see" any heat radiated from the core debris. CORCON, however, will still assume surroundings at the appropriate temperature are present and will radiate heat accordingly. With the interaction turned off, this heat is simply lost from the problem.

Aerosols produced by the VANESA model may be scrubbed by an overlying coolant pool if the scrubbing model is turned on through the SCRUB input block. If scrubbing is not modeled, the aerosols and fission products directly enter the atmosphere regardless of the presence of a pool. The VANESA input format allows the user complete flexibility in assigning the VANESA constituents to specific aerosol components and fission products. VANESA constituents may not be assigned directly to nonairborne hosts; however, this assignment may be made through use of the fission product targeted release formalism.

2.3.2.1 Layer Properties. The material properties in the lower cell required by the conduction model are based on the temperature and composition of each node in a lower cell layer. Note that the concrete layer is the only layer treated by the conduction model that can be comprised of more than one node. The densities, heat capacities, and thermal conductivities of the various materials in a node are determined from the

CONTAIN material property routines. The mixture density of a node is defined as a mass-weighted average of the densities of the materials present. The mixture heat capacity is similarly a mass-weighted average of the component heat capacities. The mixture thermal conductivity is defined as a volume-weighted average of the component conductivities. Unlike those for upper cell heat transfer structures, the lower cell node thicknesses are calculated by the code. The total node mass, area, and mixture density are used to define the node thickness to be used in the conduction model.

When the CORCON model is active, the property functions and tables in CORCON are used in the calculations.

2.3.2.2 Makeup Decay Power. It would be very tedious to specify explicitly all the fission products that contribute to the total reactor decay heat after shutdown. Therefore, a model has been developed that allows the user to specify explicitly only those fission products which are of interest with respect to transport within and release from containment, yet allows the proper amount of decay heat to be present in the problem. The model calculates the decay heat not represented by the explicitly specified fission products and allows the user to distribute that decay heat among the various lower cell layers in the problem. (The decay heat not carried by explicitly specified fission products is referred to as "makeup power.") The model bases the total decay heat on the ANSI standard ANSI/ANS-5.1-1979, which assumes LWR characteristics.[Ame79] It is activated by specifying DECAY-HT in the lower cell input block for those lower cells in which makeup power is desired.

Makeup decay power can be specified for any number of cells. In the DECAY-HT input for cell i, a portion $P_{i,0}$ of the operating power is specified together with the parameters for the ANSI decay power model for that cell. The sum of all such operating powers P_T should correspond to the nominal power at which the reactor operated prior to shutdown, unless not all the core debris is explicitly in the problem. In the makeup decay power modeling, the heating from all of the explicitly specified fission products in all cells is summed up to give the total explicit decay power at each system timestep. A fraction, $P_{i,0}/P_T$, of this

explicit decay power is compared to the value of the ANSI decay power $P_i(t)$ for that cell. For the vast majority of cases, that fraction of the explicit decay power will be smaller than the ANSI decay power $P_i(t)$. The makeup decay power for cell i is obtained by subtracting the former from the latter.

If positive, the makeup power is allocated among the lower cell layers according to the layer distribution fractions specified by the user. All layers can accept this makeup power (including the atmosphere interface layer between the lower cell and the upper cell atmosphere).

In the event that the makeup power turns out to be negative, the code will set it to zero. This condition may arise through a physical inconsistency introduced by the user or in a situation in which a large fraction of the core debris is not explicitly in the problem or is modeled in a manner that does not use the lower cell or explicit fission products (e.g., a significant part of the debris may be assumed to be retained in the reactor coolant system). In the latter situation, if the user wishes to use the makeup decay power model, the decay power from the missing debris should be made part of the DECAY-HT input. (It could be placed in a lower cell that is purposely isolated from the rest of the problem.)

If CORCON is not invoked, the distribution among the layers in a given lower cell is handled as follows. Within the DECAY-HT input, the layer distribution keyword DIST-PWR is followed by a list of fractions, "dpwr", the sum of which should be less than or equal to one. These fractions define how much of the makeup power will be placed into each of the lower cell layers specified; the first fraction in the list is associated with the first or bottommost layer, the second with the next layer up, and so forth. The last fraction refers to the atmosphere interface layer. The user should note that the makeup power assigned to the atmosphere layer is associated with the lower cell interface with the upper cell and not with the atmosphere originally in the cell. In a multicell problem the assigned makeup power thus does not flow with the atmosphere into another cell but remains fixed in the original cell.

If the CORCON model is used along with the makeup power model, provision has been made to normalize the CORCON internally calculated rate of decay heating to the makeup power value. In this case, the total amount of decay heating in all CORCON layers is adjusted at each CORCON timestep to be equal to the makeup power assigned to the representative CORCON intermediate layer. Note that the DECAY-HT option should not be used with CORCON if core debris is added to CORCON through source tables.

The makeup power model performs a normalization (if possible) over the layers, such that all the power calculated by the makeup power model will be placed in the nonnull lower cell layers. If a layer has zero mass, the energy of that layer will be split up and distributed among the remaining layers with nonzero mass. If the "dpwr" fractions are not specified at all for a given cell or are all specified to be zero, the total makeup power for that cell will be calculated as it normally would but the power will not be distributed to the layers. If CORCON is being used in conjunction with the makeup power model, such input will also result in turning off the decay heat source to CORCON.

2.3.2.3 Concrete Layer. If CORCON is not invoked, the concrete layer is nodalized and heat transfer predictions are made with the heat conduction model. The Q-VOL volumetric heating option and the DECAY-HT makeup decay power option, if specified, are utilized in the layer and heating by explicitly specified fission products is taken into account. If CORCON is invoked, the concrete layer is primarily used as a vehicle for supplying CORCON initial conditions and for reporting the results of the independent CORCON calculation. Volumetric heating and heat conduction in the concrete and intermediate layers are not taken into account by CONTAIN while CORCON is active. However, during the periods that CORCON is not active, the concrete layer is included in heat conduction modeling. The mass of the concrete layer will be that given by the "cmass" variable and the material assumed present will be the CONTAIN CONC material. The volumetric heating options enumerated above are also taken into account during these periods.

2.3.2.3.1 Nodalization for Conduction Heat Transfer. In the heat conduction model, the concrete layer is nodalized and thermally coupled to

the remaining layers in the lower cell. The concrete layer is the only layer that may be nodalized by the user, with all other layers consisting of a single node. By default the concrete layer will initially consist of five equal size nodes; however, the number of nodes may be increased by specifying a value greater than five for "jconc" in the cell level CONTROL block. The number of nodes in a concrete layer may not be decreased below the default value of five. Node thicknesses are automatically adjusted throughout the calculation based on the mass present and the temperature-dependent densities of the material in the node.

When used with the conduction model, the concrete layer will normally consist of CONC material from the CONTAIN material library. However, since the layer composition for use with the conduction model may be specified by the user for non-CORCON problems, other materials could be specified as well in those problems. However, the material used with the conduction model in CORCON problems, during the periods CORCON is inactive, is restricted to be the CONC material. It should be noted that specifying the CORCON concrete types discussed in Section 2.3.2.3.4 has no effect on the properties of the CONC material itself. However, the properties of CONC may be altered through the user-defined materials option.

2.3.2.3.2 Core-Concrete Interactions. CONTAIN uses an embedded version of CORCON-MOD2 for CCI modeling. This code comprises a detailed mechanistic model of the physical phenomena that are postulated to occur when core debris comes in contact with the concrete of a reactor cavity. The reader is referred to the CORCON-MOD2 User's Manual for details on the models and assumptions contained in the code.[Col84] Only a brief overview of the code's capabilities will be presented here.

CORCON models the thermal attack on concrete by a molten pool of metal and oxides. The pool is postulated to form after core materials melt through the reactor vessel bottom head in the advanced stages of a severe reactor accident. The CCI are driven by the decay heat of radionuclides in the core debris and the heat from chemical reactions. The heat so generated escapes the core debris pool via the top surface or along the interfaces with the concrete, and a quasi-steady state is soon achieved

in which heat loss nearly balances heat generation. The heat lost to the concrete may be sufficient to decompose it, generating gases (H_2O and CO_2) and oxide products. The gases are strongly oxidizing at the temperatures of the core debris pool and react with metals in the debris.

Two models for computing chemical reactions have been provided in the version of CORCON incorporated into CONTAIN. The default model is an ideal solution model, which is the model available in the most recent (MOD 2.03.00) stand-alone version of CORCON. The second model available in CONTAIN's version of CORCON is a mechanical mixture model. The latter is the only chemistry model available in versions of CORCON prior to MOD 2.03.00. The difference between the two models is the treatment of the activities of the constituents of the metal layer. In the ideal solution model, the activities are set equal to the constituent mole fractions rather than unity, as done in the mechanical mixture approach. The user may override the default and select the CORCON chemistry package to be used.

Hydrogen and carbon monoxide gases may be produced by chemical reactions between oxidizing gases from concrete ablation and reactive metals in the melt. These gases can exit the core debris both from the surface and in a film along the side. Being combustible, such gases constitute one of the primary threats to containment associated with CCI.

The thermal response of the concrete is complex, involving the efflux of both free and chemically bound water and other gases. Because CORCON is concerned with modeling a quasi-steady state, transient concrete response is not treated, and a constant temperature profile in the concrete is assumed. The CONTAIN conduction model is therefore not used when CORCON is active.

CORCON treats the core debris as being separated into as many as three layers of oxides and metals. These layers do not have to be homogenous; axial and radial crusts are allowed to form and melt in each of the layers. The initial inventory of oxides is usually more dense than the metals and thus forms a heavy oxide layer at the bottom of the debris pool below the metal layer. As the interaction proceeds, a light oxide

layer forms above the metal layer. This light oxide layer consists of the oxide products created by the ablation of concrete and the chemical reactions between the gases from the ablation and metallic melt components. This three-layer configuration lasts until the heavy oxides are diluted by the concrete products from ablation and the lower layer becomes less dense than the metal layer. At this point, CORCON predicts a "layer flip," and the heavy and light oxide layers are merged into a single oxide layer above the metals.

Heat transfer between the CORCON layers and from the core debris to the concrete is modeled in CORCON. The latter heat transfer occurs only during periods of ablation. Should the melt interface temperature fall below the concrete ablation temperature, CORCON assumes the interface is adiabatic and heat transfer across it ceases. The cavity ablation is followed in two dimensions, assuming axisymmetric conditions. The consequences of any interactions of the upper surface of the core debris with either a coolant pool or the upper cell atmosphere are handled by CONTAIN.

Provision has been made for the addition of materials to the CORCON system in a time-dependent manner. User-specified material source tables can be defined in the representative CORCON intermediate layer to specify mass addition rates and temperatures of CORCON materials as functions of time. The material added will also be reflected in the VANESA inventories (if it is active) and also in the CORCON decay heat computation. Metal species will be added to the CORCON metal layer, and oxide species will initially enter the upper light oxide layer. If this latter addition results in a light oxide layer density greater than the metal layer, an "inverse layer flip" will occur, and the contents of the light oxide layer will be transported to the heavy oxide layer.

Fission products are also added to the CORCON inventories whenever UO_2 is included among the materials being added to CORCON. The reason for this association is that CORCON computes the radionuclide inventory based on the user-specified mass of UO_2 in the core debris and the values of the retention factors for fission products. The fission products added in association with the additional UO_2 may thus affect the decay heat

computation. The added fission products will also be used to modify the VANESA inventories.

Note that while changes in CORCON can affect VANESA, the converse is not true. Radionuclides which VANESA calculates as being released from the core debris are not removed from the CORCON inventories of fission products. Such a treatment awaits work being done by the CORCON/VANESA development group to produce an integrated version of the two models.

CORCON's models are, in some cases, very detailed and involved. Although rapid progress is being made in their validation with respect to experiments, some phenomenological uncertainty remains. Questions now being resolved concern the mechanism of heat transfer to the concrete and the effective heat transfer coefficient that applies to this process. Another issue that is still unresolved is the correctness of the assumption of an initially layered pool with heavy oxides on the bottom, which results in subsequent layer flip. Also being examined is CORCON's treatment of the carburization reaction. In this treatment, CO_2 gas is reduced to CO and carbon by reaction with zirconium metal until the zirconium is exhausted. The carbon is then rapidly oxidized to CO until it is also exhausted. The onset of carbon oxidation is marked by a rapid increase in evolved gas flux and an increase in the molten pool void fraction.

Despite these uncertainties, CORCON is the best available tool for analysis of CCI. Work is still being done on the CORCON model, and, as improvements are made, they will be implemented in future versions of CONTAIN.

2.3.2.3.3 Radionuclide and Aerosol Release During CCI. During CCI, there can be substantial release of radionuclides from the melt as well as generation of nonradioactive aerosol species. These processes are calculated in the VANESA module which, like CORCON, was developed independently of the CONTAIN project and is documented in some detail elsewhere.[Pow86] Hence, only a brief description of the model will be given here.

In VANESA, radionuclides are released and aerosols generated by two processes, mechanical aerosol generation and vaporization. Mechanical aerosol generation results from the dispersal of small droplets of melt when gas bubbles rising through the melt burst upon reaching the surface. The composition of the particles is assumed to be that of the light oxide layer which, in VANESA, is always assumed to overlie the metallic layer. In the installed version of VANESA, the user may specify the size and number of particles generated by each bubble and also the bubble size, if the default values are not satisfactory. The values of these parameters are assumed to be constant throughout the calculation.

In most scenarios, the vaporization release is more important than mechanical aerosol generation, and the vaporization release is treated in a much more mechanistic fashion. Each species within the melt represents an element or group of elements presumed to have similar physical and chemical properties. At the start of the calculation, each melt species is assigned to either the metallic or the oxidic layer, depending upon the species' chemical characteristics; in most cases, this assignment remains fixed throughout the calculation. For each potential vapor species (typically 4 to 10 vapor species are considered for each melt species treated), vapor pressures are computed using equilibrium thermochemistry. The user has no control over the treatment of vapor species and provides no input concerning them. Once the vapor pressures have been calculated, the rates of vaporization into the gas bubbles rising through the melt are calculated, taking into account mass transfer rate limitations in both the melt and the gas phase (usually, the mass transfer rate limitations do not control the vaporization rates). All vapor species representing a given melt species are converted into a standard assay form for the corresponding aerosol species and combined before reporting the release rates. No inferences can be drawn as to the actual chemical form of either the vapor species or the aerosol species from the standardized assay form used in the VANESA aerosol report; i.e., only the elemental (and isotopic) composition of the aerosol may be inferred.

In developing VANESA, several simplifying assumptions were required in order to cope with the limited available information and to keep the calculation tractable. In calculating vapor pressures, both the metallic

layer and the oxidic layer of the melt are treated as being ideal solutions. Furthermore, the oxygen potential of the oxidic layer is assumed to be the same as that calculated for the metallic layer. (Here, the oxygen potential may be represented by the ratio $P(H_2O)/P(H_2)$ calculated to be in equilibrium with the melt, where P represents the partial pressure.) This assumption is equivalent to the assumption that oxygen transport between the oxidic and metallic phases is sufficiently rapid to compensate for various processes that would otherwise increase the oxygen potential of the oxidic layer. This assumption can be very important to the results obtained, because many important radionuclides are assumed to be present as their oxides in the oxidic layer, while the equilibrium $P(H_2O)/P(H_2)$ ratio calculated for the metallic phase is typically very small (10^{-5} to 10^{-3}) when substantial zirconium or carbon is present in the metallic phase. Under these conditions, the dominant vaporization reactions typically involve reduction of the molten oxidic species to lower valent vapor species, e.g.:

$$SrO(m) + H_2 \text{ -----> } Sr(g) + H_2O \qquad (2\text{-}66)$$

$$La_2O_3(m) + H_2 \text{ -----> } 2LaO(g) + H_2O \qquad (2\text{-}67)$$

where the 'm' and 'g' in parentheses refer to species in the melt and in the gas phase, respectively. The vapor pressures of the lower valent species associated with Equations (2-66) and (2-67) will vary as $[P(H_2O)/P(H_2)]^{-1}$ and $[P(H_2O)/P(H_2)]^{-1/2}$, respectively.

The VANESA model represents a major advance in sophistication over earlier models for releases during CCI. Nonetheless, important uncertainties do remain. These include some complexities associated with carbon chemistry discussed in Reference Pow86, limitations to the available thermochemical data base for many of the species treated, inadequacies of the ideal solution assumption, uncertainties concerning the actual speciation in the melt (e.g., the molecularity and the oxidation state of the species in the melt), and the assumption of equal oxygen potential for the metallic and oxidic phases. The latter two subjects are discussed in

Reference Wil88. Little quantitative study has been made of the impact of these uncertainties, but they are known to be potentially large (having order-of-magnitude effects) in some instances. As an aid to users interested in studying some of these uncertainties, options have been installed in the CONTAIN version of VANESA that permit the user to investigate the consequences of a very limited subset of alternative assumptions about the melt speciation and oxidic-phase oxygen potential.

Three such options are available:

- Molecularity Uncertainty. For odd-valent oxidic species, VANESA uses a bimolecular representation of the melt species, e.g., La_2O_3 and Nb_2O_5. This representation typically yields vaporization rates varying approximately as the square root of X, where X is the mole fraction of the species in the melt. If the MOLEC keyword is specified, monomolecular representations for lanthanum and niobium, $LaO_{1.5}$ and $NbO_{2.5}$, will be used. This typically yields vaporization rates varying approximately as X. Since $X \ll 1$ for radionuclides, the difference can be significant. Similar questions apply to cesium and several nonradioactive species, but the MOLEC option is implemented only for lanthanum and niobium.

- Oxidation State Uncertainty. VANESA treats cerium and niobium in the melt as always being present as Ce(IV) and Nb(V) oxides in the oxidic phase. If the STABLE keyword is specified, the possible existence of Ce(III) oxide and niobium metal (in the metallic phase) is also considered, and the actual calculation will be based upon whichever species is the more stable thermodynamically for the particular conditions of temperature and oxygen potential existing at the time. In considering Ce(III) oxide in the melt, the monomolecular representation of La(III) oxide is used as a stand-in. The STABLE option is implemented only for cerium and niobium, although similar uncertainties apply to the release of several nonradioactive aerosol species.

- Oxygen Potential Uncertainties. If the OXPOT keyword is specified and followed by a value of the variable "vnoxpt", $0 \leq$ "vnoxpt" ≤ 1, the vaporization of species assumed to reside in the oxidic layer will be calculated assuming an oxygen potential given by

$$Y = (1.0 - \text{"vnoxpt"})\ Y(\text{met}) + (\text{"vnoxpt"})\ Y(\text{ox}) \qquad (2\text{-}68)$$

  where $Y = \ell n[P(H_2O)/P(H_2)]$ and Y(met) and Y(ox) are, respectively, the values appropriate for the metallic layer and the oxidic layer if the layers did not interact at all;

i.e., if there were no oxygen transport between them. The assumption that $Y(ox) = \ell n(0.5)$ is also made. A value of "vnoxpt" = 0 yields the standard calculation and is the default value. All species, radioactive and nonradioactive, residing in the oxide layer are treated under this option, while species in the metallic layer are unaffected.

The three options are mutually compatible. Specification of either or both of the first two options can only reduce the calculated releases. Specification of the third, with "vnoxpt" > 0, can either increase or decrease releases, although decreases are expected when reactions of the type given in Equation (2-67) dominate the release process. It is extremely important to remember that these options treat only a small subset of the many uncertainties involved, and several of the other uncertainties have the potential to increase releases as well as decrease them.

Above all, it must be emphasized that the use of the above options is only recommended as an aid to investigating uncertainties associated with CCI releases. The options are not present in the released versions of VANESA, and results obtained using them can claim no support from the VANESA verification and validation programs. Such results must not be cited as being "VANESA results" without careful qualification explaining the option(s) used.

2.3.2.3.4 Concrete Type Definitions. Three predefined concrete types are available for analysis of CCI. These types are basaltic concrete (specified through the keyword BASALT), limestone/common-sand concrete (LIME), and limestone concrete (GENERIC). The concrete type specifications for the CORCON and VANESA models serve separate functions and therefore may be different.

For the CORCON model the concrete type is specified with the COMPOS keyword. The properties and compositions of the three predefined concrete types are listed in Table 2-5 in terms of the values of the associated input parameters. In addition the user may specify an arbitrary CORCON concrete type through the keyword OTHER, followed by the appropriate values of the input parameters, as described in Section 3.3.2.3.

Table 2-5

Properties of CORCON Predefined Solid Concrete Types

Species	Input Variable	Basaltic (BASALT)	Limestone/ Common Sand (LIME)	Limestone (GENERIC)
			Mass Fraction	
SiO_2	fsio2	0.5484	0.3580	0.0360
TiO_2	ftio2	0.0105	0.0018	0.0012
MnO	fmno	0.0	0.0003	0.0001
MgO	fmgo	0.0616	0.0048	0.0567
CaO	fcao	0.0882	0.3130	0.4540
Na_2O	fna2o	0.0180	0.00082	0.00078
K_2O	fk2o	0.0539	0.0122	0.0068
Fe_2O_3	ffe2o3	0.0626	0.0144	0.0120
Al_2O_3	fal2o3	0.0832	0.0360	0.0160
Cr_2O_3	fcr2o3	0.0	0.00014	0.00004
CO_2	fco2	0.0150	0.21154	0.35698
H_2O (e)	fh2oe	0.0386	0.0270	0.0394
H_2O (b)	fh2ob	0.0200	0.0200	0.0200
Ablation Temperature tabl (K)		1575.0	1575.0	1575.0
Heat of fusion efusn (J/kg)		1.811×10^6	1.199×10^6	1.199×10^6
Solidus temperature tsolct (K)		1350.0	1420.0	1690.0
Liquidus temperature tliqct (K)		1650.0	1670.0	1875.0
Density rhoc (kg/m^3)		2340.0	2340.0	2340.0
Emissivity ew		0.8	0.8	0.8

(e) - Evaporable water
(b) - Chemically bound water

For the VANESA model the concrete type is specified with the CONCCOMP keyword. The compositions of the three predefined concrete types refer to melted concrete and are given in Table 2-6. In addition, the user may specify an arbitrary concrete type through the keyword OTHER, followed by the appropriate mass fractions as described in Section 3.3.2.3.

The predefined concrete compositions do not include any allowance for steel rebar, which can be on the order of 20% of the concrete mass. The user can specify a rebar mass fraction by means of the REBAR keyword in both the CORCON and VANESA input.

The specific concrete types and the REBAR option described above apply only to the CORCON and VANESA models and do not pertain to the heat conduction model. In the heat conduction model, the CONC material in the CONTAIN material library is typically used, even if one of the above concrete types is specified. This material is unaffected by the above concrete type definitions. Since the concrete layer composition for the conduction model is specified by the user when CORCON is not invoked, the layer properties may be adjusted by including other materials in the concrete layer besides CONC. For example, the presence of steel rebar in the concrete may be simulated by including the appropriate amount of steel in the concrete layer. The properties of the CONC material may also be specified through the user-defined materials option.

2.3.2.4 Intermediate Layers. Recall that there are four types of layers in the lower cell model: the atmosphere layer, the concrete layer, the intermediate layers, and the coolant pool layer. Only one concrete layer, pool layer, and atmosphere layer can exist in any cell. If CORCON is not invoked, there can be any number of intermediate layers. All of the above layers can participate in the conduction heat transfer model. However, if CORCON is invoked, only one intermediate layer may be present. It is used to initialize the CORCON internal layers and to report results. This layer, named CORCON, will have 3 nodes, one for each possible CORCON internal layer. The mass appearing in these nodes will be associated with special material names. These material names are LCCHOX for the heavy oxide layer, LCCMET for the metal layer, and LCCLOX for the light oxide layer. These material names are also used in the

Table 2-6

Mass Fractions of VANESA Predefined Melted Concrete Types

Species	Input Variable	Basaltic (BASALT)	Limestone/ Common Sand (LIME)	Limestone (GENERIC)
CaO	fcao	0.1640	0.4299	0.8752
Al_2O_3	fal2o3	0.0908	0.0487	0.0295
SiO_2	fsio2	0.5984	0.4843	0.0617
Na_2O	fna2o	0.0197	0.0011	0.0014
K_2O	fk2o	0.0588	0.0165	0.0117
FeO	ffeo	0.0683	0.0195	0.0205

plot file. The user need not specify these names in the MATERIAL list of the global COMPOUND block since they are included by default when CORCON is invoked.

When CORCON is not invoked, the main physical phenomenon analyzed in the intermediate layers is heat transfer by conduction. Mass transfer within the intermediate layers is not modeled, and the composition of these layers can be changed only through source tables.

If CORCON is invoked, volumetric heating of the CORCON intermediate layer, due to heating by explicitly specified fission products or as specified through Q-VOL tables, will not be taken into account prior to or during the time CORCON is active. Fission product heating of core debris layers is calculated in CORCON through its own decay heat models or, alternatively, specified through the DECAY-HT option (see Section 2.3.2.2). Mass sources to the CORCON internal layers can be specified through use of time-dependent material source tables (see Section 2.3.2.8).

Prior to the start of the CORCON calculations, the CORCON layer is treated as a null layer. Should the CONTAIN calculation continue beyond the time that the CORCON calculations are completed, the representative CORCON intermediate layer will become an active lower cell layer with a

single node composed of UO2 and FE. The layer mass will be equal to the summed final masses of the CORCON layers with UO2 representing CORCON's internal oxide layers and FE representing the internal metal layer. After the CORCON calculations are completed, this intermediate layer is included in heat conduction modeling, along with the concrete layer and pool layer, if any. The purpose of providing an active intermediate layer is to allow a smooth transition in the heating of the containment when the CORCON calculations are completed.

2.3.2.5 Pool Layer. The coolant pool layer is a key aspect of the lower cell model. It is a repository for coolant from sprays, fan coolers, ice condensers, aerosol deposition, and condensation on structures. Condensation onto or evaporation from the pool surface can also occur according to the CONDENSE model described in Section 2.3.1.4. The pool is also the only layer in which boiling can occur. The pool layer can also be a source of coolant for various ESFs. Aerosols and fission products produced from CORCON/VANESA or introduced through the SRV model can be scrubbed by the pool.

If the boiling model is not activated, the pool is treated like other nodes in the conduction model. If boiling is activated, the pool is still considered thermally coupled to the other lower cell nodes; however, any energy that would raise the pool above saturation is kept separate and passed to either the semi-implicit or fully implicit pool boiling routine to determine the boiling rate. This energy is determined by iteration if the conduction routine returns a pool temperature above the saturation temperature. The pool boiling routine assumes that water is the pool material for LWRs and that sodium is the pool material for LMRs. Thus, if boiling is activated, only coolant material may be present in the pool. Unlike the concrete and intermediate layers, volumetric heat sources to the pool layer are taken into account regardless of whether CORCON is active or not.

2.3.2.5.1 Coolant Boiling Model. Two pool boiling models are included in CONTAIN; one is used with the explicit gas flow solver and the other with the implicit gas flow solver. In either model, the pool is assumed to be well mixed and at a uniform temperature. Heat can be added to the

pool either through a boundary characterized by a heat transfer coefficient, or volumetrically through decay of explicitly specified fission products, the DECAY-HT makeup decay power option, the Q-VOL option, or coolant source tables. The coolant specific internal energy is calculated each timestep, taking mass and energy changes into account. If the calculated specific energy exceeds the saturated liquid specific energy, then a boiling rate is calculated that will keep it at the saturation value. Checks are made in both models to account for the boiloff of the pool inventory within a timestep.

When the explicit flow solver is used, the boiling rate is calculated every cell timestep in a semi-implicit, self-consistent manner. Heat and mass sources to both the pool and atmosphere are considered explicitly. Mass and energy flows to adjacent cells driven by pressure differences are estimated semi-implicitly so that their effect upon boiling may be taken into account. Coolant mass and energy entering the cell atmosphere as a result of boiling can, in the next system timestep, affect the mass and energy flows to or from other cells.

When the implicit flow solver is used, pool boiling is calculated fully implicitly with respect to pressure, in conjunction with the implicit flow solution. Heat and mass sources to the pool are accumulated every cell timestep. They are then used to calculate a continuous boiling rate during the system timestep in which the sources are accumulated. Because of the fully implicit treatment, the pressurization due to the coolant mass and energy entering the atmosphere as a result of boiling is consistent with both the pool saturation temperature and the mass and energy flows to and from other cells.

2.3.2.5.2 Equilibration of CORCON Gases With the Pool. Gases from CORCON due to CCI that pass through an overlying coolant pool are assumed to come to temperature equilibrium with the pool. If BOIL is specified in the pool PHYSICS input, coolant vapor in the gas bubbles is assumed not only to come to temperature equilibrium, but also to equilibrate with the pool vapor pressure, unless the amount of vapor evolved from the bubble wall to achieve equilibrium is too large. Complete pressure equilibrium is assumed unless the molar ratio of vapor to noncondensables

exceeds 5 at the pool top surface. In that case, pressure equilibration is restricted to yield a ratio which is the larger of 5 or the ratio present for the gases and vapor as they are introduced to the pool. The factor of 5 is introduced to minimize numerical problems due to the explicit nature of the vapor evolution calculation. It may unrealistically inhibit vaporization in some cases when the pool is close to saturation. In such cases, however, the pool will be brought to saturation in a shormount of time, and vaporization will proceed through normal boiling. If BOIL is not specified, the coolant vapor in the gas bubbling through the pool is assumed to condense completely in the pool.

2.3.2.5.3 Pool Scrubbing of VANESA Aerosols. If a coolant pool layer is specified along with CORCON/VANESA, aerosols generated by the VANESA model may be scrubbed in the pool with the same modified Fuchs' model that is present in the stand-alone VANESA code. To activate this model (referred to in CONTAIN as SCRUB), the SCRUB block must appear in the VANESA input. The full pool depth is used as the scrubbing depth. The user may specify the initial bubble diameter "bsizi", which is defaulted to 1.0 cm, in the SCRUB input block. A second parameter "vrovr", described in the VANESA manual as essentially the ratio of bubble gas circulation velocity to rise velocity, may be used to incorporate effects due to bubble swarming and nonsphericity.[Pow86] The default value is 1.

The SCRUB model determines an overall decontamination factor for each aerosol size class. The processes of sedimentation, impaction, and diffusion to the surface of a bubble are modeled. It is assumed that the bubble is filled with ideal gas and expands as it rises through an isothermal pool. The gas temperature is assumed to be the pool temperature. The effects on aerosols of the evaporation of liquid into the bubble as it rises are not modeled. (Note that vapor evolution <u>is</u> modeled with respect to the material inventory of the rising gas bubbles, as discussed in the previous section.) Decontamination factors ranging from 1 to 10^5 are possible. If SCRUB is not specified, the decontamination factors will be set to unity.

The aerosols that are scrubbed out are deposited in the pool, with the remainder passing to the upper cell atmosphere. Fission products hosted

by the aerosol materials that are scrubbed out are also deposited in the pool.

2.3.2.6 Atmosphere Layer. No physical modeling is carried out for the atmosphere layer. This layer serves merely as a collector of mass and energy which are generated by other layers and are to be passed to the upper cell.

2.3.2.7 Heat Transfer. The correlations for heat transfer coefficients used in the lower cell model are presented in this section. The section consists of three parts: the first presents and briefly discusses the correlations; the second discusses which correlation is used in a given situation; the third discusses user-specified correlations.

2.3.2.7.1 Heat Transfer Correlations. Several predefined heat transfer correlations are provided in the lower cell for modeling heat transport across a layer interface.

The first three correlations apply to natural convective heat transfer conditions. The first two apply to hot liquid layers cooled from the top, and cool liquid (or gas) layers heated from the bottom. The third correlation applies to cool liquid layers heated from the top, and hot liquid (or gas) layers cooled from the bottom.

- The first correlation deals with natural convective heat transfer under laminar flow conditions. This is a variation of the McAdams correlation, [Mca54] the form of which was taken from Blottner's work.[Blo79] In this correlation, the Nusselt number is a function of the Rayleigh number (the product of the Prandtl number and the Grashof number):

$$Nu = 0.54(PrGr)^{1/4} \tag{2-69}$$

- The next correlation models natural convective heat transfer under turbulent flow conditions. This correlation is again a form of the McAdams relation [Mca54] and is given by

$$Nu = 0.14(PrGr)^{1/3} \tag{2-70}$$

- Natural convective heat transfer for cool liquid layers heated from the top, and hot liquid (or gas) layers cooled from the bottom, is modeled with a correlation given in Blottner.[Blo79] This correlation applies to both laminar and turbulent flow regimes and is given by

$$Nu = 0.067(PrGr)^{1/3} \qquad (2\text{-}71)$$

The next two correlations deal with heat transfer coefficients for boiling coolant pools.

- The heat transfer correlation for sodium pools in the case of an LMR is based on the Rosenhow model of liquid metal boiling. The reader is referred to Reference Dwy76, p. 243, for a discussion of the correlation.

- The heat transfer correlation for boiling water pools is based on a full boiling curve computed from expressions and correlations taken from the CORCON code. Due to the number and complexity of the expressions and correlations, the reader is referred to the CORCON-MOD2 User's Manual.[Col84]

The final expression gives the effective heat transfer coefficient for solid layers. It is actually not a correlation but a definition used in place of a correlation at the outer surfaces of solid layers.

- The following heat transfer coefficient is used at the surface of solid layers. Solid layers are assumed to be in perfect contact with adjacent layers; therefore, the effective heat transfer coefficient between the center of the node, where the temperature is defined, and the node surface is simply a function of the thermal conductivity, k, and the characteristic length, L, of the node at the surface of the layer. This coefficient is also used between the bottommost layer and the basemat if the lowest layer is solid. The heat transfer coefficient is given by

$$h = 2k/L \qquad (2\text{-}72)$$

2.3.2.7.2 Boundary Heat Transfer Correlations. In the conduction heat transfer model, an overall heat transfer coefficient is required to model

the heat transfer across a layer interface. Such a heat transfer coefficient lumps together processes occurring on both sides of the interface. An overall heat transfer coefficient that models the boundary layer effects on both sides of an interface is defined by

$$h_{eff} = \frac{1}{(1/h_{\ell} + 1/h_{u})} \tag{2-73}$$

In this formula, h_{ℓ} is the coefficient for the layer below the interface and h_{u} is the coefficient for the layer above the interface.

At each interface, the partial heat transfer coefficients h_{ℓ} and h_{u} are evaluated using correlations appropriate to the layers involved. Thus, if a layer is composed predominantly of solid material, the partial coefficient is determined by Equation (2-72). The conductivity is defined to be that of the dominant material, and the characteristic length is defined to be the thickness of the layer. If a layer is predominantly gas or liquid, a natural convection heat transfer correlation is employed to determine the partial coefficient. If such a layer is below the interface and is hotter than the layer above it, or above the interface and cooler than the one below it, then the natural convection, laminar flow correlation given by Equation (2-69) is used if the Rayleigh number $Ra = PrGr < 10^7$. If $Ra > 10^7$, the turbulent flow correlation given by Equation (2-70) is used. In other situations with gas or liquid layers, the correlation used is that of Equation (2-71).

Treatment of the interface adjacent to the pool layer poses a number of unique requirements. If sodium pool boiling is being considered, the Rosenhow boiling correlation discussed in Section 2.3.2.7.1 is used, while if the coolant is water, the CORCON correlations are used.

User-specified heat transfer coefficients will override the overall effective heat transfer coefficients and not the partial heat transfer coefficients. There are two ways the user may specify coefficients. The first utilizes the HT-COEF table option for the heat transfer coefficient, discussed in the next section. When conditions fall within the

range of the table, the overall heat transfer coefficient is set equal to a value obtained from the user-defined tables. The other way involves the use of the HT-TRAN control option, discussed in Section 2.3.1.6. It can be used to turn off heat transfer between layers, from the basemat to the first layer, and from the uppermost lower cell layer to the upper cell. Another HT-TRAN option will disable radiation heat transfer in the problem.

2.3.2.7.3 User-Specified Heat Transfer Correlations. One of the features of the lower cell model is that it provides the analyst sufficient flexibility to explore the consequences of adopting various alternative hypotheses regarding the disposition of debris and water and regarding heat transfer among the different materials. There are two ways in which this flexibility is exercised: (1) The number and composition of the layers can be specified by the user; (2) through the HT-COEF option, the user can override the default heat transfer correlations described in Section 2.3.2.7.1 by specifying any correlation that is a function of layer temperature, time, or temperature difference for use between any two adjacent layers or the basemat and the lowest layer. That correlation is specified in tabular form.

In the HT-COEF option, there are two quantities that need to be defined: The first (the independent variable) is time, layer temperature, or interlayer temperature difference; the second (the dependent variable) is the heat transfer coefficient. If temperature is the independent variable, it is the temperature of the layer for which the table is specified. If a temperature difference is the independent variable, the difference refers to the bottom temperature of the layer above minus the top temperature of the layer for which the table is specified. In most cases the bottom and top temperatures are the same as the layer average temperature. The only exceptions are nodalized layers, i.e., the concrete layer.

The user may also override the default heat transfer coefficient between the first nonnull layer in the lower cell and the basemat substructure. This is done by specifying BAS-MAT, as opposed to another layer name, in the HT-COEF input for a layer.

An important use of user-specified heat transfer coefficients may be to model an enhanced heat transfer area. Because the CONTAIN calculation is based on the nominal area of the layer, the analyst wishing to consider a significantly enhanced area, as when molten fuel is in the form of droplets suspended in the coolant layer, must increase the effective heat transfer coefficient. This can be done by multiplying the nominal heat transfer coefficient by the ratio of the true area to the nominal area. The ratio might be several thousand in the case of fragmented fuel. An example of the use of the table option to simulate a steam spike due to a fuel-coolant interaction is given in Section 6.3. Other uses of this option for enhanced-area calculations might include the simulation of a debris bed or the simulation of direct heat transfer between the atmosphere and fine, particulate debris produced by high pressure ejection of molten fuel.

Heat transfer between layers can be set to zero through the use of the table option, but there is a simpler method. This involves the use of the keyword HT-TRAN, followed by five flags. This capability is discussed in Sections 2.3.1.6 and 3.3.1.6.

2.3.2.8 Lower Cell Material Source Tables. Material sources can be introduced into lower cell layers through user-specified source tables. In the case of sources specified for the representative CORCON intermediate layer only temperature tables will be accepted. This is due to CORCON's own unique method of referencing its internal enthalpy values.

2.3.2.9 Lower Cell Layer Processing. A simplified overview of the processing that occurs each time step in the CONTAIN lower cell modules is given here. First, any radiant energy exchange between the uppermost layer and the atmosphere is taken into account. The actual radiant heat flux is computed by the upper cell radiation controller. External mass and energy sources are then added to the appropriate layers and new equilibrium conditions are found. These external sources can include sources from mechanistic upper cell models (e.g., sprays) and user-defined material source tables. The pool condensation/evaporation model is then processed if the CONDENSE option is used (see Section 2.3.1.4.1) and a pool is present. If CORCON has not been invoked, the interlayer

heat transfer coefficients are then determined and the conduction model is called. In the absence of the CONDENSE option, the conduction model accounts for convective heat transfer from the topmost layer to the atmosphere. Volumetric heating of the layers (e.g., by explicitly specified fission products, through the DECAY-HT option, and through user-specified Q-VOL tables) is also incorporated in the conduction solution. If a coolant pool is present, any energy that would raise the pool above saturation in the conduction solution is kept separate and passed to the pool boiling routine. This energy is determined by iteration whenever the conduction solution returns a pool temperature above the saturation temperature. If CORCON is active, the conduction module is skipped since CORCON assumes a steady state temperature profile in the concrete and models the heat transfer in the melt layers independently of CONTAIN.

At this point, the physical models that are specifically associated with an individual layer are called, starting with the bottom layer. If the CORCON/VANESA model is used, it is called when the concrete layer is processed. There are presently no physical models specific to the intermediate layers; however, interfacing between the CORCON arrays and CONTAIN arrays is carried out when the representative CORCON intermediate layer is processed. When the pool layer is processed, either semi-implicit pool boiling or energy accounting for the fully implicit pool boiling model is performed. If CORCON is active, the effects of volumetric heating of the pool are taken into account, since the conduction routine which normally incorporates such effects is not called. If CORCON is active and CONDENSE has not been specified, the effects of convective heat transfer between the pool and the atmosphere are also taken into account when the pool layer is processed.

After the completion of individual layer processing, sources accumulated in the various lower cell modules are gathered together for eventual transfer to the upper cell. If a pool is present, the gas equilibration and VANESA pool scrubbing models are also invoked at this time. Any aerosol and fission product sources produced by VANESA that are not scrubbed out are transferred to the atmosphere.

2.3.2.10 Lower Cell Volumetric Heating Option. Energy sources may be introduced to the lower cell layers by means of the Q-VOL table option available for each layer. (Energy may also be introduced through material source tables, as discussed in Section 2.3.2.8 or the DECAY-HT makeup power option discussed in Section 2.3.2.2.) The values entered in the Q-VOL tables refer to rate of energy addition to the entire layer in units of watts. If the layer has multiple nodes, this power is partitioned among the nodes with a mass weighting. During the periods that CORCON is active, the specified energy addition is ignored in all layers except the pool.

2.3.3 Engineered Safety Systems

Overview

> Mechanistic models for three major engineered safety features (ESFs) are included: containment sprays, fan coolers, and ice condensers. Thermal hydraulic effects and the removal of aerosols (and associated fission products) from the atmosphere are modeled, as is removal of gaseous iodine species for spray and fan cooler systems (but not ice condensers). Various individual engineered components (tanks, heat exchangers, pumps, valves, pipes, orifices, and pool overflows) are also modeled. Restrictions on the allowed combinations of systems and components are discussed in the appropriate subsections.

As a hypothetical severe accident progresses, the structural integrity of the containment building, the final barrier to fission product release, may be challenged. Virtually all nuclear power plants include ESFs designed to reduce pressure, temperature, and fission product concentrations and thus to reduce the threat to containment integrity and limit fission product release. CONTAIN has models for three major ESFs for LWR analyses: containment sprays, fan coolers, and ice condensers. Associated with these models is a framework for construction of a liquid transport system which can provide sources and sinks of coolant for the ESFs. The liquid transport system can also function independently of the major ESF models.

In general, the ESF models are mechanistic in nature, so that their range of applicability is greater than would be possible with more empirical models. The current engineered safety systems are suited primarily for application to LWRs. The spray, fan cooler, and ice condenser systems are applicable only to LWRs. However, the liquid transfer systems can be used for LMRs.

The arrangements of some of the engineered system components used with an ESF are illustrated by the containment spray system of an LWR, shown in Figure 2-16. After initiation of the spray, water from the refueling water storage tank (RWST) is pumped through nozzles located near the top of the containment dome. The resulting fine spray produces rapid steam condensation, a drop in temperature, and reduction of fission product concentrations in the atmosphere. Upon reaching the floor, the spray water drains into the cavity sump. When the water in the RWST is exhausted, recirculated water from the sump is pumped through a cooling heat exchanger and then to the spray nozzles. The CONTAIN ESF framework allows a detailed description of such a system, or alternatively, the user may simply specify the mass flow rate and temperature versus time through the spray system.

The removal of aerosols and fission products from the atmosphere through the operation of engineered safety features is modeled. Except in the case of sprays, the only fission products considered in this modeling are those attached to aerosols. For sprays, however, the removal of molecular iodine and gaseous organic iodides is also modeled. The removed aerosols and fission products are conveyed, along with the effluent from operation of the ESF, to cell "iclout".

The optional FPLIQUID global input block can be specified (see Section 2.2.5.5) to allow the liquid transport system to carry fission products from one pool to another. Such fission product transport between pools occurs only in conjunction with single engineered system components, such as a pipe, that are connected between pools. Such transport does not occur, for example, when the spray system is operated in a recirculation mode between two different pools. Only those fission products with nonzero values of "fpliq" will be transported to the destination pool.

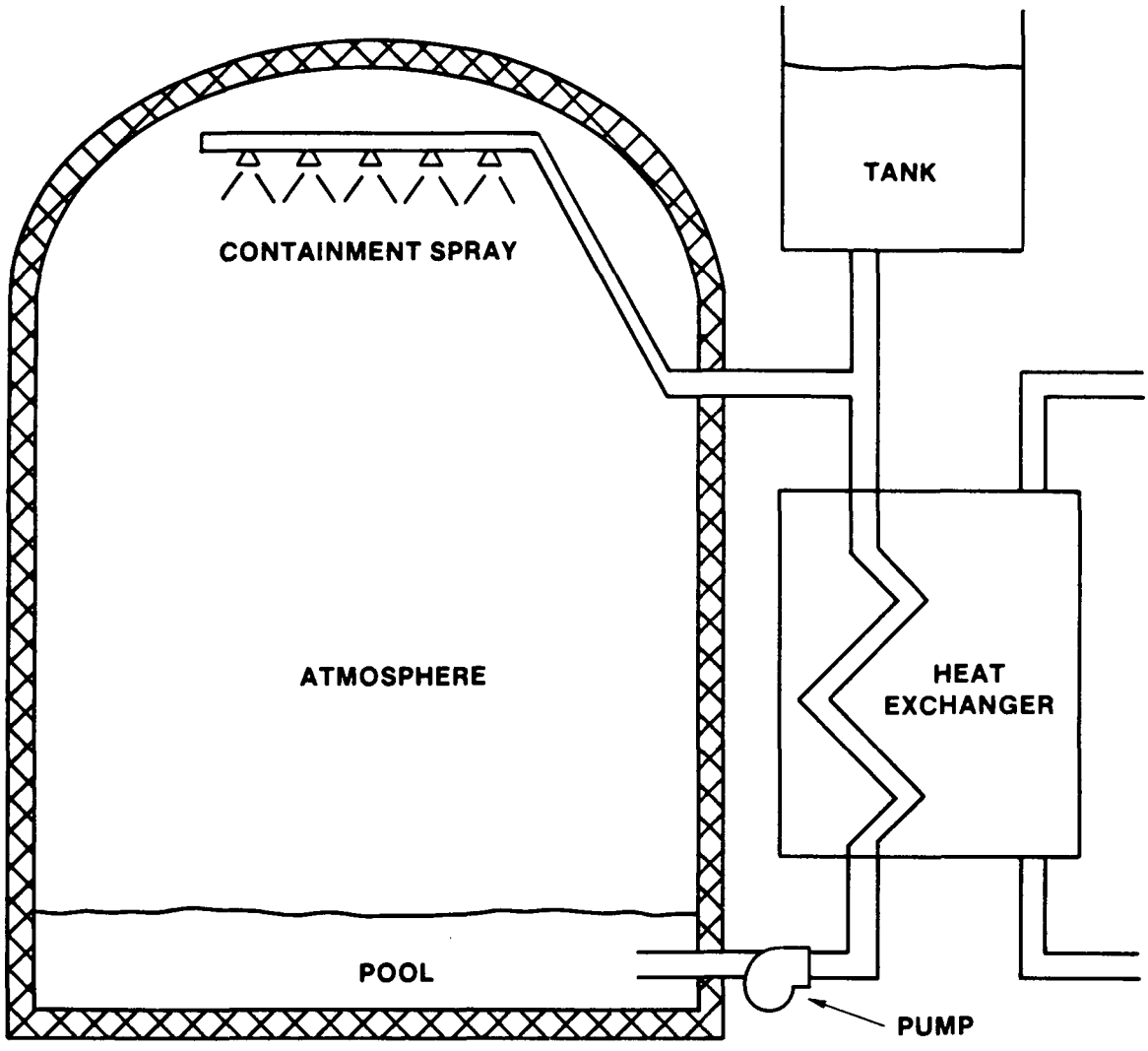

Figure 2-16. Containment Spray System With Recirculation

The fraction of fission products transferred with the liquid is equal to the fraction of liquid transferred from a pool times "fpliq".

2.3.3.1 External Engineered System Source. An engineered systems source table may be used to provide a time-dependent source of coolant at a specified temperature or enthalpy to an ESF. Because of the nature of the systems modeled, the only allowed source material is water. This option otherwise is specified much like the other source tables in CONTAIN. It is activated by the keyword SOURCE. For further details on this source table, see Section 3.3.3.1.

2.3.3.2 Containment Spray. The containment spray system is a nearly universal safety feature in LWRs. This system provides a high pressure, finely divided water spray to the containment atmosphere. Heat transfer to and steam condensation on the droplets provide a rapid reduction in temperature, pressure, and fission product concentration. The sprayed water collects in a sump at the bottom of the containment. Generally, the initial spray water is from the RWST. When that source is exhausted, water is pumped from the sump, through a heat exchanger, and to the spray nozzles. A model has been developed that determines the heat transfer between the droplets and atmosphere and the associated condensation of steam onto or evaporation of the droplets. The removal of iodine and aerosols from the atmosphere due to the spray is calculated.

The calculation involves the simultaneous integration of the equations for drop height, mass, and energy. The spray is assumed to have a single droplet diameter, which has a default of 0.001 m if a value is not specified. The assumption is made that the droplets fall at a terminal velocity that depends upon droplet diameter. The diameter may increase or decrease as the spray falls through the atmosphere; thus it is a dynamic variable. The heat transfer and mass transfer to the spray as it falls are calculated. The model for these processes is basically the same as that for heat transfer structures described in Section 2.3.1.4. The Nusselt number correlation used is that of Ranz and Marshall for forced convection around a spherical droplet.[Ran52] The rate of evaporation of, or condensation on, a spray droplet is controlled by the diffusion of water vapor through the gas boundary layer at the surface of

the drop and is driven by the difference in water vapor pressure between the atmosphere and the droplet surface.

The spray calculation begins with the determination of the number of droplets n introduced in a cell timestep. The equations for drop height, mass, and energy are solved for the entire fall of a single droplet. The fall height is an input parameter which is defaulted to the cell height. The resulting transfers of mass and energy between the droplet and the atmosphere are then multiplied by the number of droplets. Note that the effects on the atmosphere due to a given spray drop are assumed to be instantaneous and not spread out over its fall time. This assumption is normally not of concern if the atmosphere conditions are not calculated to change rapidly over the droplet fall time.

Spray droplets that reach the bottom of the cell contribute their mass and energy to the lower cell pool, if present, in the cell to which the engineered system effluent is directed. That cell is specified by the user as cell "iclout", which by default is the cell in which the spray is defined. If no lower cell pool is specified for that cell, the water is lost from the problem. For most situations that call for the use of containment sprays, one would expect a liquid pool to form as a result of spray droplets reaching the floor. Therefore, it is recommended that the user include a lower cell model with a pool in cell "iclout".

The explicit coupling between the spray model and the atmospheric thermal-hydraulics can lead to oscillations in the atmospheric temperature and pressure when the system timestep is too large. Though often small in amplitude, these oscillations can be detrimental; e.g., they can cause the saturation ratio to oscillate back and forth across unity, which can in turn cause spurious condensation on the aerosols and artificial enhancement of aerosol scavenging by the sprays. The best means of testing for this condition is to check the saturation ratio (written at every long and short edit) for oscillatory behavior. The only safe procedure is to reduce the system timestep until the oscillations go away, unless the user can establish that they cause no harmful effects in the particular calculation at hand. The maximum stable timestep decreases somewhat with increasing spray flow rate and, more

noticeably, with decreasing spray drop size. The increase in computer time from reducing the system timestep may be partially recovered by reducing the number of cell timesteps per system timestep (i.e., increasing "ctmfr"; see Section 3.2.6).

For the purpose of discussing the depletion of airborne fission products by containment spray washout, they may be divided into the following groups:[Lew77]

- Noble gases,
- Elemental iodine (I_2),
- Methyl iodide (CH_3I) and other gaseous organic compounds of iodine, and
- Aerosol particles.

The noble gases are inert and are not affected by the spray system. Iodine is the only other element that is likely to be in gaseous form in compartments with sprays operating. It may be present either elementally (I_2), in which case it is very reactive, or as methyl iodide, CH_3I, which is gaseous but much less reactive. All remaining fission products will likely be liquid or solid under spray conditions and, if airborne, will be in the form of aerosols.

The initial removal of molecular iodine by containment sprays is experimentally observed to be a relatively rapid process that slows down abruptly as equilibrium is approached between competing absorption and desorption mechanisms.[Hil71] No attempt is made to model the observed late time desorption of iodine within the spray model, because the experimentally observed desorption probably occurs from reservoirs (such as walls) that should be modeled outside of the spray model itself. Additives have been adopted in PWR spray systems to enhance the rate and extent of removal of iodine. The most common spray additive is sodium hydroxide.

The depletion rate for iodine is defined as the product of an absorption efficiency and the fraction of the compartment volume swept by spray per

unit time. The efficiency is calculated from the diffusion rate of iodine through both a gas-side and a liquid-side boundary layer at the surface of a droplet. It is assumed that the drop interior is well mixed. The liquid-side boundary layer is based on a stagnant film model, which is somewhat crude but provides a simple way to treat the problem. The input parameter "sppci2" is the partition coefficient used to calculate the elemental iodine absorption efficiency. The partition coefficient depends on the amount and type of additive used. A value of 5000 for "sppci2" is the default. A good source of recommended values for this parameter for a wide variety of spray additives is provided in Reference Gri82. Depletion rates for the organic compounds of iodine (e.g., methyl iodide) have not been well established. A partition coefficient for organic iodides, "sppcmi", has been provided to allow the user to model the removal rate for such relatively inert species. A value of zero for "sppcmi" is the default. The depletion rate for elemental iodine will be applied to those fission products with names beginning with MOLI...; and that for organic iodides to those with names beginning with ORGI....

The depletion rate for airborne aerosols is again defined as the product of a collection efficiency and the fraction of the cell volume swept out by spray per unit time. The collection efficiency is integrated over the fall of a droplet, taking into account the droplet size and temperature, aerosol size, and containment conditions. Collection mechanisms considered in deriving the efficiency are Brownian diffusion, thermophoresis, diffusiophoresis, interception, and impaction. No additional input parameters beyond the ones specified in the global AEROSOL block are necessary for control of aerosol washout.

The aerosols and fission products removed by sprays, including the fission products attached to the aerosols, are all deposited into the pool, if present, of cell "iclout". If a pool is not defined in that cell, the removed aerosols and fission products will be divided up among floor structures in that cell according to surface area. A waste holding array will be used in case neither of these locations is available.

The containment spray must be used in either one of two engineered system combinations. For the simplest system, the spray is paired with an engineered system source table, and the spray is active as long as the source is finite. A more elaborate system may be initiated using a containment pressure setpoint given by the input parameter "spstpr". In the latter system, the user must include a tank to supply an initial amount of fresh water to the spray train (see Section 2.3.3.5). When the tank is empty, a pump provides recirculated water, which goes through a heat exchanger and then to the spray trains. Failure of recirculation may be simulated by specifying zero flow for the pump or by drawing water from a source cell "iclin" that contains no pool. Sample input for this system is given in Section 3.3.3.2.

2.3.3.3 Fan Cooler. Fan coolers are included in large dry PWR containments both to provide nonemergency cooling and to augment the steam removal capabilities of the water sprays in the event of a severe accident. If operable during a severe accident, they could be important in reducing pressure and temperature.

The coolers consist of banks of finned, service-water-cooled coils across which large capacity fans pull the containment atmosphere. Each unit has several parallel coolant paths, each routing water back and forth across the path of the circulated atmosphere. The coils are horizontal, with the coolant entering at the back and leaving at the front, as depicted in Figure 2-17. The geometry is, therefore, that of a cross-flow heat exchanger with counterflow, i.e., the atmosphere inlet side corresponds to the coolant outlet side. For large dry PWRs, the coolers are designed to work under normal conditions, as well as under accident conditions. Typical design-basis-accident temperatures are roughly 400 to 420 K, with a saturated atmosphere, and pressures ranging between 0.3 and 0.6 MPa. The heat removal capability is in the range of 2×10^7 to 4×10^7 W. BWR and subatmospheric containments generally include fan coolers that are designed only for normal operating conditions, but the performance of such coolers may still be important following an accident.

CONTAIN has two fan cooler models. The simpler of the two models is the fan cooler model developed for the MARCH code.[Woo83] This model is

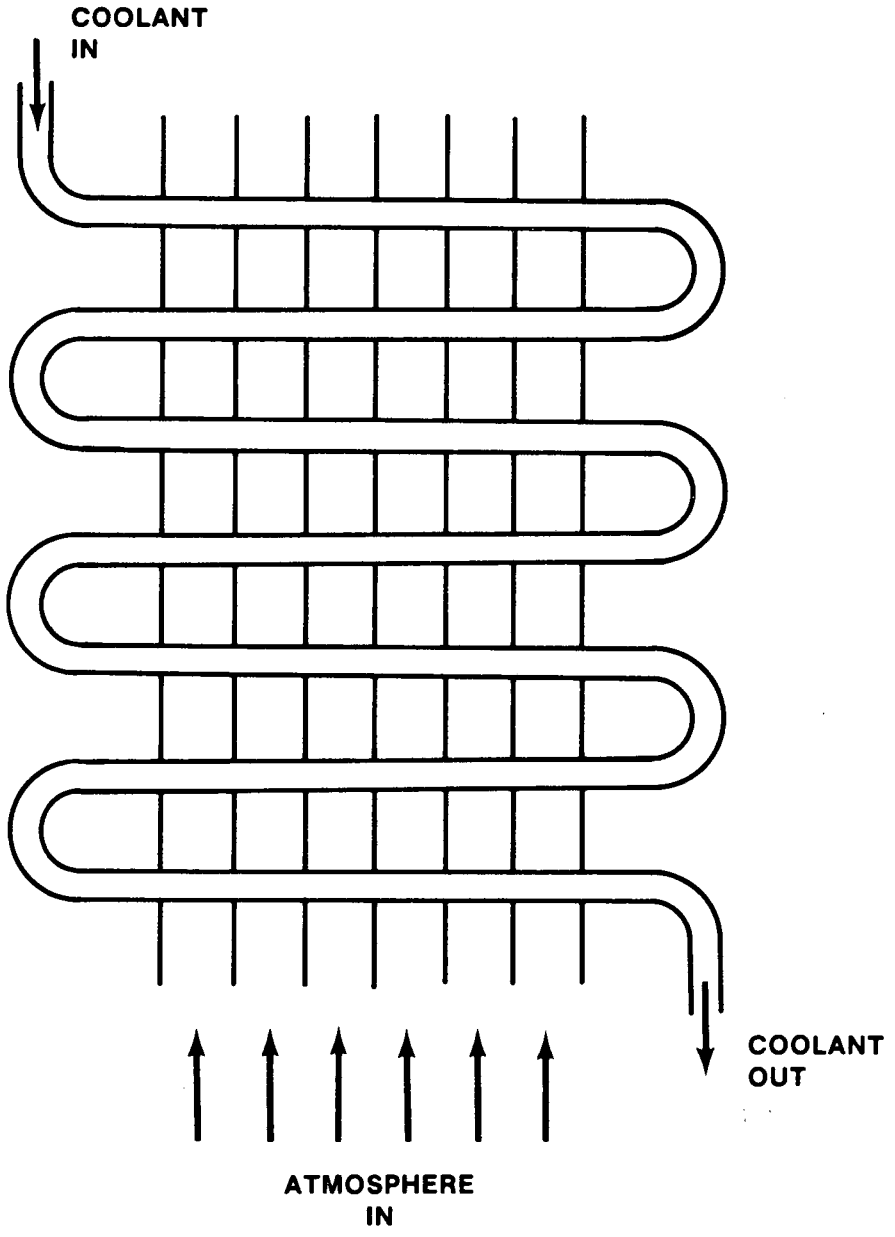

Figure 2-17. Simplified Fan Cooler Geometry

activated by the keyword MARCH. The user input for this model includes the design cooling capacity "fcqr", the associated design inlet gas temperature "fctpir", the coolant inlet temperature "fctcli", and the coolant mass flow rate "fcclmd". A correlation for the effective heat transfer coefficient h as a function of steam vapor fraction has been derived from the capacity curves for saturated conditions presented in the Oconee Power Reactor Final Safety Analysis Report. The heat transfer coefficient h for design conditions is used along with the rated capacity to calculate an effective heat transfer area. A cooling capacity for prevailing conditions is then calculated using this area and a heat transfer coefficient corresponding to the prevailing containment vapor fraction. The default values of input parameters are those characteristic of the fan coolers in the Zion nuclear power plant.[Zio00]

The MARCH model is simple and fast, and when used with the Zion fan cooler characteristics, reproduces the Zion published capacity curve with reasonable accuracy. It does not address the effect of noncondensable gases other than air or superheated atmospheres. Also, no fission product or aerosol depletion is calculated for this model. If these effects are not expected to be important, this model is recommended because it is much simpler to use and faster than the alternative condensation model described below.

The more mechanistic fan cooler model, activated by the keyword CONDENSE, is based upon the heat transfer formulation (described in Section 2.3.1.4) that is used elsewhere in CONTAIN. The model uses condensation and convective heat transfer coefficients that depend on the cell atmospheric conditions. The Nusselt number used to determine the heat and mass transfer coefficients is a Reynolds-Prandtl correlation for flow over horizontal tubes.[Hol68] The Reynolds number is based upon the coil outside diameter "fcclod" and a stream velocity based upon the air/steam flow rate and the cooler frontal area "fcflar". The effective heat transfer area per row is the input parameter "fcefar". For most applications, this parameter will not be available from cooler design data. Rough calculations based upon typical cooler fin and tube designs and prior experience indicate that a value of about ten times the cooler frontal area is appropriate. A constant heat transfer coefficient

"fchntr", is used for heat transfer between the gas/condensate-film interface and the coolant. An approximate value for this parameter found reasonable in parametric comparisons with published cooler capacity curves is 1000 W/m^2-K, which is also the default value.

The calculation is carried out iteratively. The steam/air mixture inlet conditions and flow rate, given by the input parameter "fcwin", are known. The cooling water exit temperature is first estimated from the MARCH model and the input cooler capacity "fcqr". The temperature change of the cooling water due to convective and condensation heat transfer in the last row of coils is calculated for the estimated cooling water exit temperature. (Recall that the last row of coils seen by the cooling water is the first row seen by the incoming air/steam mixture.) The water temperature and the air/steam mixture conditions are updated prior to repeating the calculation for the next row. The process is repeated for successive rows until the water inlet temperature and exhaust gas temperature have been determined. The water inlet temperature is compared to the specified value "fctcli". If there is a significant difference, the calculation is repeated with a revised estimate for the coolant outlet temperature. The process is continued until there is sufficient agreement between the calculated and specified coolant inlet temperatures. Because the total heat transferred is relatively insensitive to changes in cooling water temperature, convergence is rapid.

The two input parameters that cannot be easily characterized, the effective heat transfer area and the heat transfer coefficient between the gas/condensate-film interface and the coolant, present difficulties for the user of this model. The values recommended above for these parameters will provide reasonable results for typical fan cooler designs. If accurate simulation of a cooler is important, however, the user should vary the values chosen so that the published cooler capacity is obtained. Note that the default values for input parameters are suitable for the Zion plant.

Aerosol deposition driven by diffusiophoresis may be significant across a fan cooler. Deposition by this process is calculated when the condensation model is active. Any deposited aerosols and fission products hosted

by these aerosols are routed to cell "iclout" along with the condensate. The repository in which the aerosols and fission products are placed in cell "iclout" is determined in the same manner as for aerosols and fission products collected by sprays.

2.3.3.4 Ice Condenser. The ice condenser containment system is an innovation by Westinghouse Electric Corporation designed to suppress the pressure rise within a containment arising from a LOCA. The design incorporates a large volume of subcooled ice that acts as a low temperature, passive heat sink. A typical ice condenser is shown in Figure 2-18. The only significant flow path from the lower compartment housing the reactor vessel to the upper compartment is through the ice compartment. The ice, in granulated form, is contained in perforated metal buckets approximately 0.3 m in diameter, stacked about 15 m high. There are 24 annular modules, occupying approximately 300° of the containment periphery. Although the ice containers are perforated, most of the flow is around the outside of the buckets, so little or no entrainment of ice or condensate occurs. Because the ice is a highly efficient heat sink, nearly all of the steam is condensed. As long as a significant amount of ice remains in the ice condenser, the peak pressure is determined largely by the accumulation of noncondensable gases in the upper compartment.

Under blowdown conditions, the doors opening into and out of the ice compartment are held closed by spring and gravity forces, respectively. These doors may be simulated by using pressure criteria to open the flow paths representing the doors, or, if the user wishes to simulate the actual spring or gravity-controlled motion of the doors, the flow area may be specified as a function of the pressure difference across it using one of the flow path table options described in Section 2.2.3.

Heat transfer to and condensation on the ice is treated by the convection/condensation heat transfer model that is used elsewhere in CONTAIN (see Section 2.3.1.4). Because the ice is contained in buckets, the cross-sectional area is assumed not to change as the ice melts. The ice is modeled as a cylindrical heat sink structure; the length and hence the heat transfer area decrease as heat is absorbed and the ice is melted. The condensate and melted ice are diverted to cell "iclout".

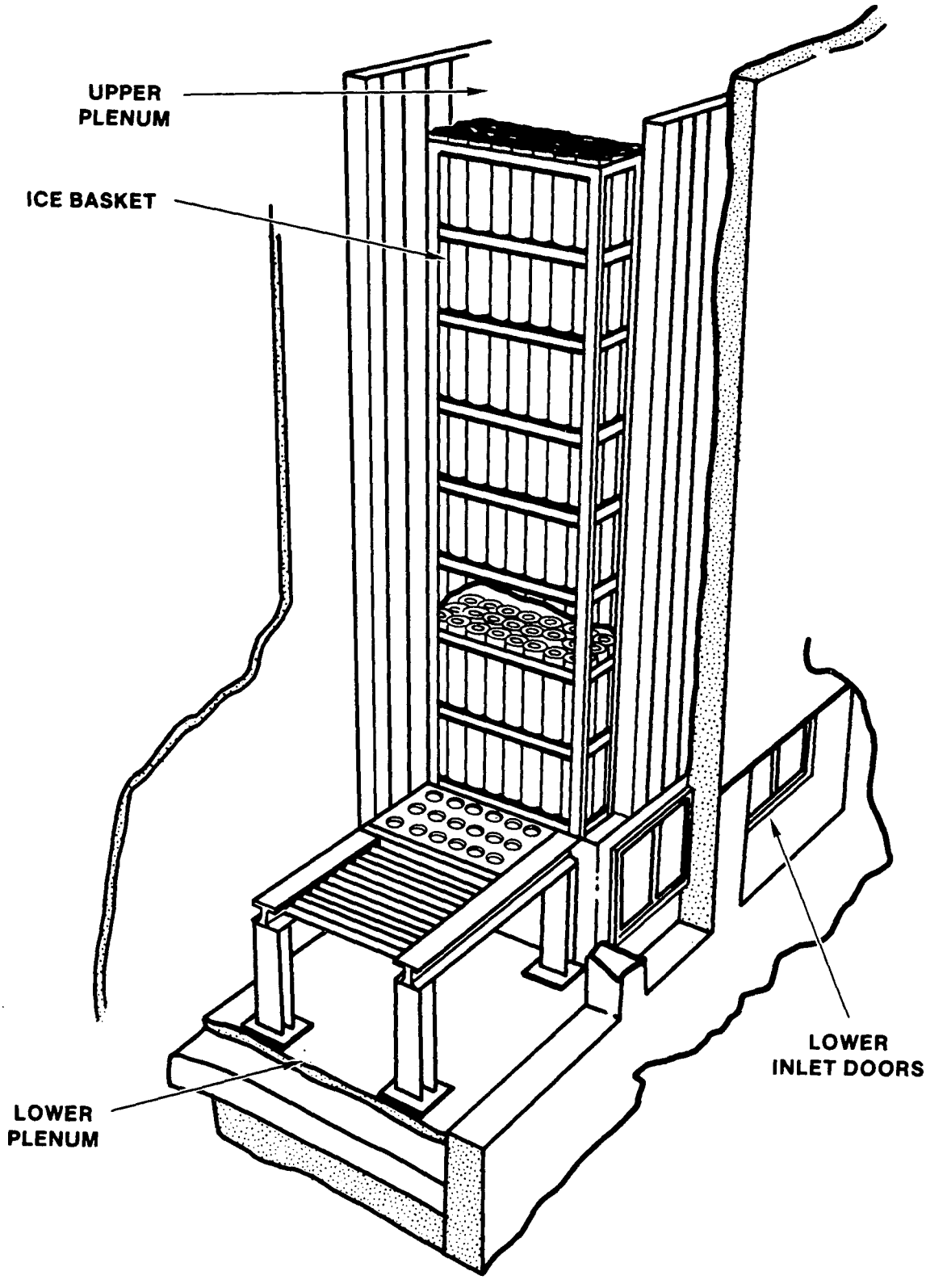

Figure 2-18. Simplified Diagram of an Ice Condenser

Because heat is also transferred from the incoming steam/air mixture to the stream of condensate and melt falling from the baskets, the performance of an ice condenser system depends to some extent upon the temperature "citlex" of this effluent. This temperature is difficult to calculate mechanistically and is therefore an input parameter.

Most of the input parameters for the ice condenser model are design data that may be taken directly from plant safety analysis reports. These parameters include the initial height of the ice column "hitici", initial ice mass "tmsici", initial ice temperature "citici", and cross-sectional area "ciarfl" available for flow through the ice compartment.

Others require some discretion on the part of the user. Among these are the melt/condensate temperature "citlex" and the initial total surface area available for heat transfer "arhtin". The effluent temperature is dependent upon the flow rate through the compartment, and tests have produced values between 335 and 373 K. In an ice condenser plant, there is initially over 7×10^5 m^2 of ice surface potentially available for heat transfer. However, a reasonable assumption is that the available area is that of the outside of the baskets, or about 10^4 m^2. The final input parameter "icllp" is the number of the cell directly below, or upstream, of the ice compartment. This may be the lower plenum or the lower compartment, depending upon the noding scheme.

As noted above, the heat transfer to and steam condensation on the ice is treated in a manner similar to that found in other modules of CONTAIN. Differences in the ice condenser treatment include a film resistance corresponding to a fixed 0.5 mm water film and neglect of the unlikely possibility of evaporation. Conduction within the ice is also neglected. Heat and mass transfer from the gas flowing through the ice condenser is assumed to melt ice as long as ice remains. Once the ice has been exhausted, heat and mass transfer to the ice basket structures is not considered unless they are modeled separately as heat transfer structures.

The ice condenser provides conditions under which significant removal of suspended aerosols from the atmosphere can occur. An aerosol depletion

model treating sedimentation, impaction/interception, Brownian diffusion, diffusiophoresis, and thermophoresis is included. The model is based on Reference Win83b, with minor modifications to make it consistent with other CONTAIN models. Aerosol depletion is calculated even in the absence of ice, because it is believed the large surface areas represented by the ice baskets would be effective in removing particulates. This model includes only effects attributable to the ice and ice basket structures. The walls, floors, and ceiling of the ice compartment should be modeled separately as structures (see Sections 2.3.1.3 and 3.3.1.3).

The aerosols and associated fission products that are removed from the atmosphere are placed into the pool, if present, in cell "iclout". If a pool is not present in the "iclout" cell, the aerosols and fission products will be distributed among floor structures, if present. Otherwise waste holding locations will be used. This treatment assumes that the aerosols and fission products are immediately carried from the ice compartment along with the effluent. One consequence is that fission product decay heating does not contribute to the melting of the ice.

Care should be taken in interpreting results of ice condenser calculations, because few experimental or calculational results are available for comparison.

2.3.3.5 Storage Tank. A storage tank component is provided to allow an initial amount of fresh water to supply the containment spray. (See Section 2.3.3.2.) Three input parameters are required following the keyword TANK: the first, "tnkmas", is the initial mass of water available for the spray; "tnktem" is the temperature of the water, and "tnkflo" is the mass flow rate at which water is delivered to the spray.

2.3.3.6 Pump. The pump component may be used in one of two types of systems: when used by itself in a system, it controls the flow of coolant liquid from the pool of one cell to that of another. The flow is directed from cell "iclin" to cell "iclout". When used in conjunction with a containment spray, it controls the flow of recirculated water from a pool to the sprays. When it is used in this mode, the recirculation flow does not start until the storage tank supply is exhausted. The user

must specify "pmpmdt", the pump flow rate. A sample input is shown in Section 3.3.3.2.

2.3.3.7 Orifice. The orifice component is used only by itself in a single-component system to control the transfer of coolant liquid from a pool in cell "iclin" to that of cell "iclout". The flow is pressure- and gravity-driven, with the driving pressure calculated from the gas pressures and the elevation difference "delev" between the bottoms of the pools in the two cells. (The flow is assumed to occur between the bottoms of the pools. Thus, the flow connection cannot be uncovered and the flow interrupted while there is still water in the donor pool.) The flow is assumed to be incompressible and to occur at the steady-state rate. A flow resistance characteristic of an orifice[Flo79] is used. Input parameters that describe the geometry of the orifice are "orifid", the orifice minimum diameter, and "orifdr", which is the ratio of "orifid" to the free stream diameter. No defaults are provided for these parameters. Figure 2-19 illustrates the geometry of a liquid redistribution network utilizing an orifice, a pipe, or a valve.

2.3.3.8 Pipe. The pipe component is used like the orifice (see Section 2.3.3.7), except that the flow resistance is characteristic of pipe flow rather than orifice flow.[Flo79] The geometry of the pipe is described by input parameters defining the pipe length "pipel", the inside diameter "pipeid", and a total loss factor "pipekf", equal to the sum of the Moody friction factor, entrance and exit loss factors, and any other form loss factors.

2.3.3.9 Valve. The valve component is used only by itself in a single-component system to control transfer of coolant liquid from the pool of cell "iclin" to that of cell "iclout". Two types of control are available. If the keyword PRESSURE is specified, the flow path becomes in effect a rupture disk. When the difference in hydraulic head between cell "iclin" and cell "iclout" exceeds the input pressure "valopp", the flow path is opened, and the flow is characterized by the flow area "valvar" and a flow loss coefficient "valvkf", equal to the sum of the Moody friction factor, any form loss factors, and entrance and exit loss factors. Alternatively, the keyword TIMES indicates that the valve is to

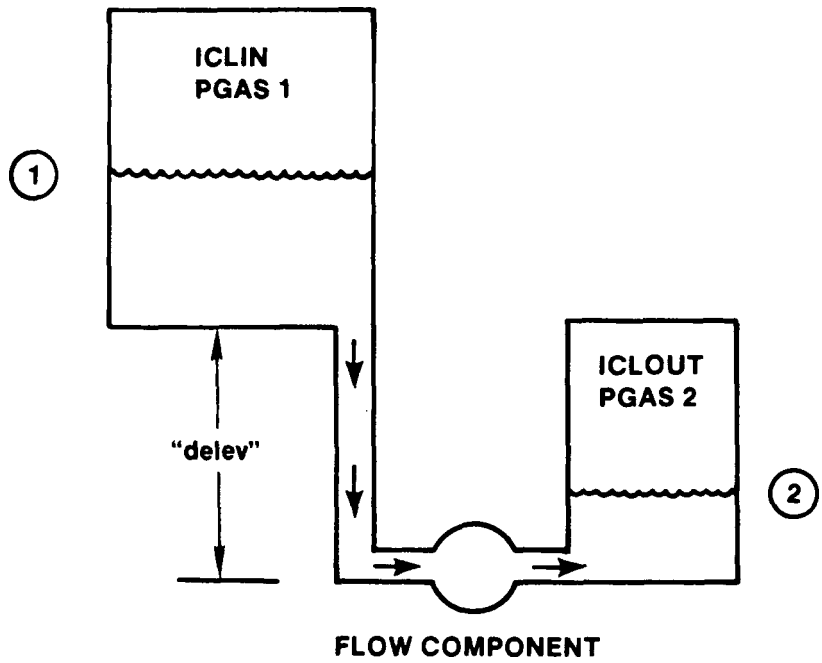

Figure 2-19. Liquid Redistribution Network

open and close at five user-specified times. The times are alternating opening and closing times. The valve is assumed to be initially closed and the first time specified is an opening time; thus, if the valve is to be initially open, the first entry in the array should be the problem start time. No defaults are available for valve input parameters.

2.3.3.10 Heat Exchanger. A heat exchanger is available as a component in a containment spray system to provide cooling of the recirculated water. There is only one combination of components in which a heat exchanger can appear, i.e., along with a spray, tank, and pump. An example of such a system is given in Section 3.3.3.2. Any one of five

heat exchanger models may be chosen. These correspond to (1) a single-pass shell and U-tube geometry, (2) a cross-flow geometry with hot-side tubes and cold-side shell, (3) a counterflow geometry, (4) a parallel flow geometry, and (5) a nonmechanistic model with a constant user-specified hot-leg temperature drop.

The first four models are based on the heat exchanger efficiency formulations of Kays and London.[Kay64] The important quantity to model for a heat exchanger is the hot-leg outlet temperature. In this formulation it is expressed as a function of an efficiency parameter, the inlet hot- and cold-leg temperatures, the cold-leg mass flow rate, and the product of the hot-leg flow rate and the cold-leg liquid isobaric heat capacity. The hot-leg flow rate and temperature are determined from the pump capacity and pool thermal conditions, respectively. The cold leg flow rate and temperature are input parameters "hxclmd" and "hxticl". The efficiency depends upon the heat exchanger type, effective surface area, and the overall heat transfer coefficient, which correspond to the input parameters "nhxtyp", "hxarea", and "hxcoef", respectively. Expressions for the overall efficiency are given in Reference Kay64. Input for the last model simply consists of "hxdelt", which is the temperature drop across the hot leg. Because heat exchanger designs vary greatly, no default parameters are provided.

2.3.3.11 Engineered Systems Overflow. The engineered systems OVERFLOW keyword initiates input of data for the pool overflow model. (This keyword should not be confused with the cell OVERFLOW keyword which defines the overflow cell for condensation runoff and aerosol mesh losses.) Three required variables, "iclfrm", "iclto", and "flovht", indicate the overflow cell number, the destination cell number, and the height relative to the bottom of the pool at which overflow occurs, respectively. In the pool overflow model, all coolant above height "flovht" in cell "iclfrm" is diverted to "iclto" during each timestep in which the condition is met. Note that the water level of the destination pool must be below the overflow height for the pool overflow model to work properly. Overflow may be included along with any allowable combination of components making up an engineered system or it may

constitute the sole component in a system. Its presence should be reflected in the number of components "numcom".

2.3.4 Safety Relief Valve Discharge Model

Overview

> A model for the scrubbing of gas, aerosol, and fission product sources which are introduced at the bottom of a pool, as in the operation of the safety relief valves in the BWR containment, is discussed.

In a BWR, SRV discharge lines leading from the reactor vessel terminate in the wetwell pool and are used under both normal and accident conditions for relieving excess pressure buildup. The SRVs are activated manually or upon reaching a pressure set point. A gas flow distribution device or quencher (typically with T- or X- shape) is attached to the end of these lines for efficiently condensing steam and dispersing the gas through the wetwell pool in a swarm of very small bubbles.

The model for scrubbing gas, aerosol, and fission products from SRVs is activated in CONTAIN through the use of the SRVSOR keyword. Source tables are used to describe the rates of introduction of the various materials into the pool. Although the model is intended primarily for modeling the SRVs, it could be used in any situation in which gas, aerosol, and fission product sources are introduced into a pool. One restriction on the fission product sources is that the fission products must be hosted by the aerosol source; one cannot introduce a gaseous fission product to be scrubbed by the pool. (There is also no gaseous fission product scrubbing model for the suppression pool vent model discussed in Section 2.2.3.4.2.) Fission products hosted by aerosols that are scrubbed out in the pool are also considered to be removed by the pool. A new feature of SRV aerosol sources is that the lognormal size distribution parameters for the aerosol source may now be specified in the source table as a function of time. If given, these values are used for the aerosol source instead of the global size distribution parameters defined for the aerosol component. (See Section 2.2.4 for a definition of these parameters.)

Noncondensable gaseous SRV sources which pass through a pool are assumed to come to temperature equilibrium with the pool. If BOIL has been specified in the pool PHYSICS input block, coolant vapor in the bubbles is assumed not only to come to temperature equilibrium, but also to equilibrate with the pool vapor pressure, unless the amount of vapor evolved from the bubble wall to achieve equilibrium is too large. Complete pressure equilibrium is assumed unless the exit molar ratio of vapor to noncondensables exceeds 5. In that case, pressure equilibration is restricted to yield a ratio which is the larger of 5 or the ratio present for the gases and vapor as they are introduced to the pool. The factor of 5 is introduced to minimize numerical problems with the explicit vaporization calculation done in the SRV model. It may unrealistically inhibit vaporization in some cases when the pool is close to saturation. In such cases, however, the pool will be brought to saturation in a short amount of time, and vaporization will proceed through normal boiling. If BOIL has not been specified, the coolant vapor in the incoming gas is assumed to condense at the bottom of the pool. Vapor evolution is not considered. Note that all nonaerosol liquid and solid material sources, if specified, are completely trapped in the pool.

For an LWR, the scrubbing of SRV aerosol sources may be described using either the SCRUB model or the SPARC model. These two scrubbing models are described in more detail in Section 2.2.3.4.2 in connection with the suppression pool vent flow path model. For an LMR, the SCRUB model may be used, but the SPARC model may not be used because of explicit reference to the properties of water in the latter.

The effectiveness of pool scrubbing can change as the pool depth changes. The SRV discharge is assumed to be at the elevation above pool bottom specified by the ELESRV keyword. If the pool level drops below the discharge level, no scrubbing will occur.

The user should take care to ensure that the gas, aerosol, and fission product source tables are consistent. For example, a finite aerosol source rate would not make sense unless there is a supporting gas source rate to convey the aerosols into the pool. A finite fission product

source rate also would not make sense unless the supporting aerosol source rate for the component hosting the fission product is nonzero.

However, if the supporting gas source rate for aerosols is zero and the discharge level is below the pool surface, the aerosols will be scrubbed with the maximum decontamination factor of 10^5. If the rate is zero and the discharge level is above the surface, the aerosols will be introduced directly into the atmosphere without scrubbing. The user should note that the maximum decontamination factor will also result if the gas flow consists entirely of coolant vapor, as this flow will condense completely in the pool. If a fission product is hosted by a particular aerosol component and the source mass rate for that component is zero during a given period, the fission product source mass introduced during this period will be placed in the pool if the discharge is submerged and directly on the airborne aerosol component if the discharge is not submerged.

3. INPUT DESCRIPTION

The input needed to run CONTAIN and to use its various options is described in this section. The overall format for the input file is first discussed, followed by the specific data requirements. In general, the structure of input to CONTAIN is quite flexible. Certain restrictions on the ordering of the main input blocks are identified below, but these are quite limited.

It is important for the user to understand an important principle concerning input: if a keyword is left out of the input, the model associated with it is not activated, even if this means physically unrealistic results. Leaving CONDENSE out of the input, for example, results in no condensation heat transfer in the problem. Also, leaving FLOWS or THERMO out of the input will result in cell thermal-hydraulic conditions and gas inventories that do not change with time.

The ordering of the data block descriptions closely parallels the ordering of the discussions in Section 2 of the physical models in CONTAIN. This approach allows the new user to understand the input parameters by referring to the corresponding subsections in Section 2 (e.g., refer to 2.3.1.3 for explanation of 3.3.1.3) and at the same time keeps Section 3 as concise as possible for the experienced user.

3.1 General Input Format and Structure

CONTAIN has a large number of models and features, and as a consequence, a complete cataloging of input options and instructions might be somewhat overwhelming at first sight. To maintain a clear perspective, the input format will be shown in three successive levels of detail: first, an outline of the input file structure; second, summaries of the global input and cell input sections; and third (in Sections 3.2 and following), detailed instructions for each input option.

Figure 3-1 shows an outline of the input file structure. Note that there are several sections of the input. A short machine control section, initiated by the specification of the type of computer to be used, must be given first. This section may also specify a number of output files and the type of memory allocation scheme to be used. The global input, initiated by the word CONTROL, must be given next. This section has blocks of information common to all cells, including standard CONTAIN material names, the names of any user-defined materials, information on fission products and their properties, and information that defines interactions among cells. A number of cell input sections, initiated by the keyword CELL, must follow the global input. There is one such section for each cell in the problem. Each section has blocks of information required by the various physical models used in individual cells. Finally, the file is terminated by the keyword EOF.

The machine control input usually consists of only one keyword--the machine name. However, in this input block, a number of options are also available for specifying the memory allocation method used and for assigning plot files and the user-defined output file. Because these

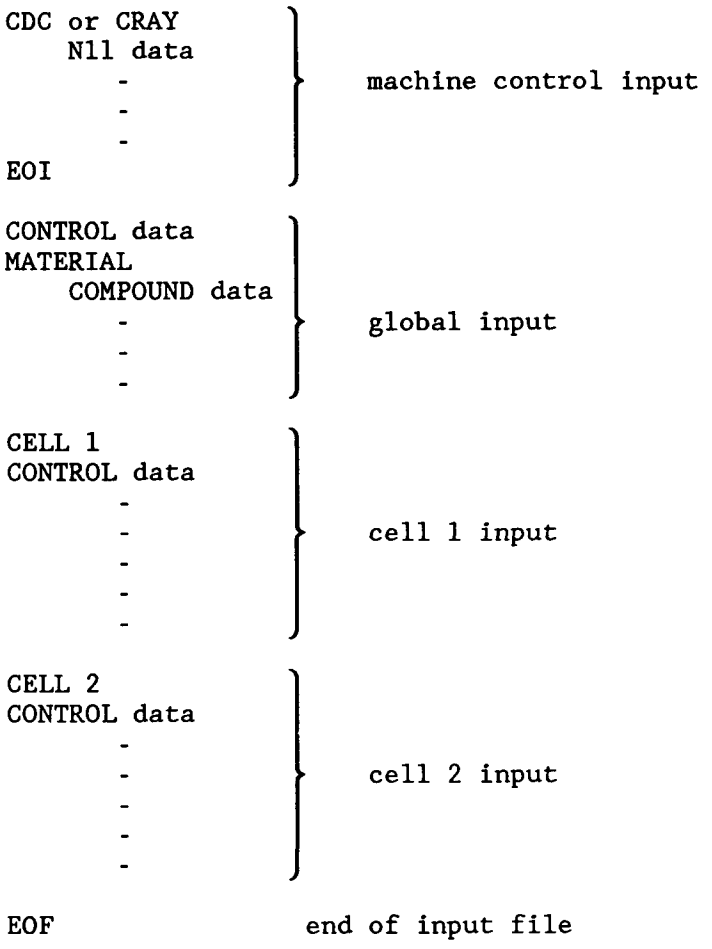

Figure 3-1. CONTAIN Input File Structure

features have more to do with hardware than with the code itself, details are left to Appendix B.

Global and cell level input sections are shown in summary form at the next level of detail in Figures 3-2 and 3-3, respectively. Each keyword and parameter will be explained in detail below. Parentheses ( ), square brackets [ ], the symbol &&, and the curly brackets { } have special meanings which will also be explained below. The purpose of the figures is to illustrate the overall pattern of the global and cell sections of input.

As shown in Figure 3-2, the first blocks of information required in the global input group specify control information, materials, and fission products. The data in these blocks enable the code to allocate the total amount of global data storage space required. Thus, the first two blocks of data in the global input must be the CONTROL and MATERIAL blocks, in that order. In the MATERIAL block, the keyword MATERIAL should be followed immediately by the COMPOUND subblock and then by the USERDEF, FP-NAMES, or AERNAMES subblocks, if used.

```
CONTROL
    NCELLS=ncells NTITL=ntitl NTZONE=ntzone NFCE=nfce
    NCHAIN=nchain NSECTN=nsectn NAC=nac NENGV=nengv
    NUMTBG=numtbg MAXTBG=maxtbg NTGT=ntgt NWDUDM=nwdudm
EOI
MATERIAL
    COMPOUND (names)
    USERDEF  (names)
    FP-NAMES (names)
    AERNAMES (names)
TITLE
    (a number of full lines)
TIMES cput tstart (timinc edtdto tstop)
    (KEYWORD=value)
EOI
SHORTEDT kshort
LONGEDT klong
DEBUG=n (names) routml routm2
THERMAL
FLOWS
    IMPLICIT=nimpli (KEYWORD) (KEYWORD(i,j)=value)
ENGVENT
    (data)
SPVENT
    (data)
EOI
AEROSOL (KEYWORD) (KEYWORD=value) (mapaer amean avar)
FISSION
    (NFPCHN=nfpchn FPNAME=(data) HFLIFE=(data)
    FGPPWR=data)
EOI
USERDAT
    (name phase
    MOLEW=molew RHO=nrho (temp density)
    COND=ncond (temp conduct) ...
    EOI)
EOI
FPLIQUID
    (fpname=data)
EOI
&& output control options
PRFLOW
PRSPRAY
PRLOW-CL
PRHEAT
PRAER
PRFISS
PR-USERO
PRENGSYS
&& end of global input
```

Figure 3-2. Summary of Global Level Input

The subsequent data consists of global blocks of data. These may occur in any order (provided they precede the cell level input). In Figure 3-2, each left-justified keyword with the exception of EOI denotes the beginning of a different main input block. The left-justified EOI (end of information) keyword simply denotes the end of the main block above it. With the exception of the reactor-type option, if a block is not specified, then the corresponding model or option is not invoked. The physical models that require global input information are the fission product model, the intercell gas flow model, and the aerosol model.

Figure 3-3 shows the structure of the cell level input for one cell. The first block of information for each cell specifies the information needed to determine the total storage required by this cell. Thus, the CONTROL block must immediately follow the CELL input line. Also, the GEOMETRY block should precede any block with physical parameters since the cell volume is often needed to calculate physical conditions.

The order of the subsequent main blocks of information is again arbitrary. Most, but not all, main blocks are shown in Figure 3-3 with the same format used in Figure 3-2. If a block for a given model is omitted in a cell, then that model is not used in that particular cell.

In the following sections, the third and final level of detail, the definition of the main input blocks, will be provided. A number of alternative input formats are available for certain blocks and are described in Appendix D. These formats will generally be of little interest since the standard formats will provide the same or more options. The alternative formats are obsolete but are still supported in the interest of maintaining upward compatibility with old input decks.

The rest of this section is organized to be roughly parallel with the model descriptions in Section 2. For example, Section 3.2.2 describes the input for intercell flow, and Section 2.2.2 describes the models for the thermodynamics and intercell flow calculation. Because Section 2 has additional detailed discussion, some of the definitions and explanations in Section 3 will be quite brief.

In order to understand the following input instructions, the reader must be familiar with a number of conventions, both in the input dataset format itself and in the instructions for writing the input. The input data consist of keywords, which are indicated in the following by upper case letters, and values for variables, which are indicated by lower case alpha-numeric groups. (In the text, variables are enclosed in quotation marks to avoid confusion.) Appropriate values for some of the variables are character constants (i.e., names), while other values are integers or floating point numbers. In CONTAIN the convention is followed that all keywords and names must have 8 or fewer characters. The input data are specified in a free field format with the exception of titles, which reserve a number of entire lines of 80 or fewer characters. Acceptable and equivalent separators for keywords and values are a blank space, a comma, an opening parenthesis, a closing parenthesis, a new line (carriage return), or an equal sign. Any number of keywords and values can be present on a line of input, up to a maximum of 80 characters per line. Each data block can be continued on as many lines as desired; however, an individual keyword or value cannot be continued from one line to the next. At any position on an input line a comment (which will not affect

```
CELL 1  && beginning of input for cell 1
CONTROL NHTM=nhtm MXSLAB=mxslab NSOPL=nsopl NSPPL=nsppl
    NSOATM=nsoatm NSPATM=nspatm NSOSPR=nsospr NSPSPR=nspspr
    NSOAER=nsoaer NSPAER=nspaer JCONC=jconc JINT=jint JPOOL=jpool
    NUMTBC=numtbc MAXTBC=maxtbc NRAYCC=nray NVFPSM=nvfp
    NSOSAT=nsosat NSPSAT=nspsat NSOSAE=nsosae NSPSAE=nspsae
    NSOSFP=nsosfp NSPSFP=nspsfp NAENSY=naensy
EOI
TITLE
    (one line)
GEOMETRY volume height
ATMOS nma pgas tgas (gas frac)
    SOURCE data
STRUC
    (NAME=data TYPE=data SHAPE=data NSLAB=data CHRLEN=data
    TUNIF=data COMPOUND=(data) X=(data)
    EOI)
CONDENSE
    FORCED nmtb (table data)
    STR-COND (data)
HT-TRAN (htflags)
H-BURN
    (KEYWORD=data)
EOI
OVERFLOW novcel
FPM-CELL
    (HOST=hname (data)) TARGET (data) EOI
EOI
FISSION SOURCE (data)
AEROSOL=naero (mat mass) SOURCE data
LOW-CELL
    GEOMETRY carea
    DECAY-HT data EOI
    CONCRETE (data)
        TEMP data
        COMPOS (data)
        PHYSICS
            Q-VOL (table data) EOI
            HT-COEF (table data) EOI
            SOURCE (data)
            CORCON (data) EOI
            VANESA (data) EOI
        EOI
    EOI
    INTERM
        LAY-NAM data
        TEMP data
        COMPOS (data)
```

Figure 3-3. Summary of Cell Level Input

```
        PHYSICS
            Q-VOL (table data) EOI
            HT-COEF (table data) EOI
            SOURCE (data)
            DKPOWER (data) EOI
        EOI
    EOI
    POOL (data)
        TEMP data
        COMPOS (data)
        PHYSICS
            Q-VOL (table data) EOI
            HT-COEF (table data) EOI
            SOURCE (data)
            BOIL
        EOI
    EOI
    BC txl
EOI
ENGINEER onmsys numcom iclin iclout delev
    SOURCE data
   {SPRAY data EOI or
    FANCOOL data EOI or
    ICECOND data EOI}
    TANK data
    PUMP data
    ORIFICE data
    PIPE data
    VALVE data
    HEX data
    OVERFLOW data
EOI
SRVSOR (KEYWORD=value)
    AEROSOL SOURCE (data)
    FISSION SOURCE (data)
    ATMOS SOURCE (data)
EOI
EOF  && end of input file
```

Figure 3-3. Summary of Cell Level Input (continued)

the input processing) can be inserted after the pair of characters &&. A blank space must appear after the second &. The remainder of the input line may then contain comments of any sort. The use of && is very convenient for annotating input datasets with helpful comments, reminders, and brief descriptions of the problem. A few examples of the use of the comment symbol are shown in Figure 3-2.

Default values are available for many of the input variables; these are listed in the appropriate subsections. Default values are not provided for input variables which depend strongly on the nodalization selected by

the user. Thus, for example, the user must specify the configuration of cells to be used and all heat transfer structures in each cell.

In the descriptions of the input to follow, rows of asterisks are used to delimit the template for an input block. The template for an input block gives all of the available keywords and variables in a special format. That format does not have to be used in the input dataset itself, which is free field. However, the format defines completely the ordering requirements that must be taken into account within the input dataset and indicates to a large extent the option combinations available to the user in specifying models or modeling features.

The following notation is used in the templates:

- Upper case words are either keywords or character constants (i.e., names) that must be supplied literally in the input.
- Lower case words are considered variables which should be replaced by values which are either numbers or character strings. Lower case words representing a integer value follow the FORTRAN convention of starting with a letter between i and n, and the value should be specified as an integer. Lower case words representing character constants (i.e., names) should be replaced by the appropriate character constant (i.e., string). (Possible character constants are also capitalized in the following discussion.) Lower case words representing floating point values should be replaced by values in FORTRAN F or E format. (A decimal point must be present in numbers in the E format. For example, 1.E6 is acceptable but 1E6 is not.)
- Parentheses ( ) imply that the enclosed quantity or quantities should be repeated as necessary.
- Square brackets [ ] imply that the enclosed quantity is not always required.
- Quantities within a given set of curly brackets { } represent a number of alternatives, of which the user should select one. Each alternative is delimited by a curly bracket and a bold-face **or** or by two bold-face **or**'s, as indicated by the ellipses in **{...or...or...}**.

In the following discussions of the input blocks, the templates for each block are followed by descriptor blocks which describe each keyword and variable appearing in the template.

3.1.1. Ordering Requirements in Input Blocks

The input specified within a given input block cannot be in an arbitrary order but must satisfy two general requirements regarding the order of variables and the order of subblocks. Due in part to the fact that a variety of programming styles are represented in the input processing, these ordering requirements cannot be stated without lengthy definitions and considerable explanation. However, the system of input that is

represented is reasonably natural and flexible in use. Thus, the user should not feel compelled to dwell too long on the ordering requirements discussed below, especially if he or she is content simply to follow the basic order given in the template for that input block. To help the user with regard to the ordering requirements, caveats are usually given explicitly in the keyword or variable descriptor blocks when the order of specification of a subblock or variable is restricted in an way that is not obvious. Such restrictions are also completely defined by the template format according to the rules given below.

The ordering requirements within an input block are based on a heirarchy indicated in the template by the indentation level used to display a group of keywords and variables. A group of such items indented to the right relative to another group of items occupies a lower position in the heirarchy than that other group.

The first type of ordering requirement is related to the order of variables: a contiguous group of variables must be specified in the input in the order given in the template. A group of variables is considered contiguous if the variables are all at the same level in the heirarchy and are not separated by a keyword at any level. (Note that a contiguous group of variables may and often does consist of only one variable, especially one following a keyword.) Furthermore, a contiguous group of variables that immediately follows a keyword at the same level in the hierarchy must be specified immediately after that keyword. Most variables follow such a keyword. However, in some cases they do not. In such cases, the leading variable of the contiguous group has the same function as a keyword in defining ordering requirements. Such leading variables are often character variables representing the name of an option or material.

As an example, a keyword PVALUE that has "n" values of a variable "p" associated with it might be displayed in the template in the form:

PVALUE n (p)

where the parentheses imply that the enclosed item(s) should be repeated as necessary. This group of keywords and variables is considered to be at the same (the first) level in the heirarchy, since only one (the zero) level of indentation is used for the group. The variables are contiguous and follow a keyword in the template and thus must be specified in the order given immediately after the keyword. If there are four values 1.0, 2.0, 3.0, and 4.0 of "p" associated with PVALUE, the corresponding input would have the form:

PVALUE 4 1.0 2.0 3.0 4.0

The second type of ordering requirement involves subblocks of data. A subblock at a given level in the heirarchy is basically a contiguous group of keywords and variables at the given level or lower that is not separated by keywords or variables at a higher level. The subblock boundaries are not uniquely specified according to this definition. For present purposes additional rules are needed to make the division into subblocks at a given level unique. Because of the variety of ways that subblocks are recognized in the code, these rules are rather complex: (1) With the exception of an end-of-information (EOI) keyword, a keyword

or leading variable at the same level as the subblock marks the beginning of a new subblock, as does an indentation to a lower level than the subblock. If such a keyword or leading variable is present, it is considered included in the subblock it begins and also is considered to terminate the subblock at the same level immediately preceding it, if one exists. If such a keyword is present, it is called a leading keyword. An EOI keyword at a given level has a different effect: it terminates the preceding subblock at the same level and is considered included in the subblock it terminates. Note that a subblock can have at most one non-EOI keyword or leading variable at the same level as the subblock. Thus, at the lowest level in an input block, individual non-EOI keywords and leading variables each represent a different subblock.

A subblock thus can begin with a leading keyword or variable and end with an EOI. It can begin with a leading keyword or variable and end with the leading keyword or variable to the next subblock; it can begin with an indentation without a leading keyword and end with an EOI. (The EOI is the only keyword at the level of the subblock in the latter case.) From the above definitions, it follows that an EOI keyword, if present, will always be written at the same level of indentation as the subblock that it terminates. This consistent positioning of the EOI should be quite helpful in determining which subblock is terminated by each EOI when multiple subblock levels are present.

With the above definitions, it is now possible to give the ordering requirements for subblocks: (1) A subblock must be specified after the last keyword or leading variable that precedes it in the template and is at a higher level than the subblock. Similarly, the subblock must be specified before the next keyword or leading variable at a higher level. By induction, this rule constrains quantities within a subblock to be specified in the order given, with exceptions only as allowed by the second rule. (2) However, a contiguous group of subblocks at the same level may be specified in any order amongst themselves. A contiguous group of subblocks is defined as one that is not separated by a subblock at a higher level. (It is not possible to have subblocks at a given level separated by a subblock at a lower level since the subblock at the lower level is by definition included in one of the higher level sub-blocks.) Since at the lowest level, individual non-EOI keywords and leading variables each represent a subblock, the second rule implies that a contiguous group of such items at the lowest level can be specified in any order amongst themselves.

Two examples of the template format are given below. The first is:

```
**************************************************************************

KEY n (const)
    [OPTION1] {OPTION2 or OPTION3}
EOI

**************************************************************************
```

where "n" is defined as the number of values of "const" to follow the keyword KEY and OPTION1, OPTION2, and OPTION3 are the three options associated with the KEY block. In this example, KEY, "n", "const", and EOI are considered to be at the first level in the input hierarchy, and

OPTION1, OPTION2, and OPTION3 are considered to be at the second level. The "n" and "const" variables are required to immediately follow KEY in the input because of the ordering requirement for variables following keywords. OPTION1 is truly optional, as indicated by its square brackets. However, one of OPTION2 or OPTION3 must be selected, as indicated by the curly brackets. The option keywords selected are required to follow KEY, the last keyword preceding them at a higher level in the input hierarchy, and to precede EOI, the next keyword following them at a higher level. However, they are not required to follow KEY immediately as are "n" and "const". Since OPTION1, OPTION2, and OPTION3 are each considered subblocks at the lower level, they are not restricted in the order in which they may be specified with respect to each other. (However, the curly brackets indicate that only one of OPTION2 or OPTION3 can be specified.) The EOI terminates the subblock at the same level as the EOI, in this case the subblock beginning with KEY and not with OPTION1. In the input one might thus specify

```
KEY 3 1.0 2.0 3.0 OPTION2 OPTION1 EOI
```

if n is equal to 3, the three required values are 1.0, 2.0, and 3.0, and the indicated options have been invoked.

The second example is the template for heat transfer structures, which gives the format to be used for specifying all of the heat transfer structures in a cell. (Only the template format is discussed here. The meanings of the keywords and values are discussed in Section 3.3.1.3.)

```
**************************************************************************

STRUC
        (NAME=name    TYPE=type    SHAPE=shape
        NSLAB=nslab    CHRLEN=chrlen
        [SLAREA=slarea]    [CYLHT=cylht]
        [TOUTER=touter]    [IOUTER=iouter]
        [VUFAC=vufac]
        {TUNIF=tunif or TNODE=(tnode)}
        COMPOUND=(cname)
        X=(xvalue)
    EOI)

**************************************************************************
```

In this example three levels in the input heirarchy are represented. The keyword STRUC is at the first level, the EOI is at the second level, and all other quantities are at the third level. STRUC is the leading keyword for the subblock at the first level, which encompasses all the quantities shown. The subblock at the second level begins with NAME and ends with EOI. However, there is no leading keyword or variable for this subblock, which actually begins with an indentation. The reason for the lack of a leading quantity is that the pairs of quantities connected by the equal signs at the third level are accepted by the code in any order, and there is no quantity that should be given first. The freedom to specify these pairs in any order is indicated in the template by the fact they are each subblocks at the third level and, according to the above rules, may therefore be specified in any order. (The keyword STRUC is not the leading keyword for the subblock at the second level because it

is not repeated each time a new structure is specified; only the keywords beginning with NAME and ending with EOI are repeated. Note that the EOI does not terminate the entire block but each structure. Thus it is not placed at the first level. Also, the EOI should not be placed at the third level, because that would imply that it terminates one of the pairs of quantities, such as the "X = (xvalue)" input. However, according to the way the code is written, that is not its function. Thus, there is no ambiguity about where the EOI should be placed.)

3.2 Global Level Input

The global level input block provides data which either is required by a global model or is common to all cells in the system being modeled. The first two blocks of data in the global input must be the CONTROL and MATERIAL blocks, in that order. In the MATERIAL block, the keyword MATERIAL should be followed immediately by the COMPOUND subblock and then by the USERDEF, FP-NAMES, or AERNAMES subblocks, if used. Other main input blocks may occur in any order.

The global CONTROL block is used to specify the storage allocation associated with the global models.

```
**************************************************************************

CONTROL
    NCELLS=ncells [NTITL=ntitl] NTZONE=ntzone [NFCE=nfce]
    [NCHAIN=nchain] [NSECTN=nsectn] [NAC=nac] [NUMTBG=numtbg]
    [MAXTBG=maxtbg] [NTGT=ntgt] [NENGV=nengv] [NWDUDM=nwdudm]
EOI

**************************************************************************
```

In specifying this block, the keyword CONTROL is given first. It should be followed by the keyword and value pairs for each number the user wishes to specify. The pairs can be given in any order. Only the NCELLS and NTZONE pairs are required. The block must be terminated by an EOI.

CONTROL	keyword to begin specification of the global storage allocation.
NCELLS = ncells	number of cells.
NTITL = ntitl	number of title lines with a maximum of 80 characters per line. Default = 0.
NTZONE = ntzone	number of time zones.
NFCE = nfce	number of fission product chain elements. Default = 0.

NCHAIN = nchain — number of fission product linear chains. Default = 0.

NSECTN = nsectn — number of aerosol particle sections or sizes (20 is typical; maximum = number given by geometric constraint, Equation (2-15)). Default = 0.

NAC = nac — number of aerosol components. Maximum = 8. Default = 0.

NUMTBG = numtbg — number of global tables used. This number should be incremented by one for each table used in the AERTIM, VAR-AREA, and engineered vent table options (e.g., AREA-T). (Such tables are considered to be at the global level since these options are processed at that level.) Each such table specifies one dependent variable in terms of an independent variable. These tables should not be confused with source tables, which are always introduced with the keyword SOURCE (or, in one case, SRVSOR), or with user-defined material (USERDAT) tables. Default = 0.

MAXTBG = maxtbg — maximum number of points used in any global table. Default = 0.

NTGT = ntgt — a number that reserves space for the targeted release and acceptance model. The value of "ntgt" must be greater than or equal to the amount of space required to run the targeted release and acceptance model in all cells. (See Sections 2.2.5 and 3.3.1.10.) In most instances, "ntgt" is obtained by summing the number of FROM/TO pairs in all TARGET input blocks. However, since "ntgt" is actually defined as the number of targeted release equations, and because one FROM/TO pair may represent more than one targeted release equation, this method is not totally reliable. For example, if a fission product appears more than once in the linear chain decomposition, then its FROM/TO pairs must be counted once for every chain element that the fission product represents. (Note that such multiple occurrences may result if branching or merging chains are modeled.) Further guidelines are given in Section 3.3.1.10 for determining the value of "ntgt" when generic hosts such as ROOF, WALL, or FLOOR are used in the TARGET input. Default = 0.

NENGV = nengv — number of engineered vents in the problem. Default = 0.

NWDUDM = nwdudm — number of array locations reserved for the user-defined material (USERDAT) tables. This should be enough space to hold the pairs of temperature and property values defined in the USERDAT block for all user-defined materials. Such pairs of values are stored even if the TEMPS option is used. Default = 1000.

EOI — required keyword terminating the global CONTROL block.

Unless otherwise noted, there are no preset maximum values for the control variables. However, the amount of storage space needed increases rapidly as the values of control variables increase. There is a default total working storage limit specified in the code. If the set of control parameters requires more storage than allowed by that limit, a fatal input error will occur, and a message about how to update the code to allow more storage will be printed in the error file.

An additional global control keyword, NHM, is sometimes seen in older decks. This option is obsolete but still supported by the code; see Appendix D. Another format for the CONTROL block is available. This format is discussed in Appendix D. This alternative format may appear in input files developed for earlier versions of CONTAIN. While upward compatible, it is considered obsolete.

3.2.1 Material, Fission Product, and Aerosol Names

The material names block specifies the materials to be used in the problem. Four types of materials may be specified under the keywords COMPOUND, USERDEF, FP-NAMES, and AERNAMES, respectively.

```
**************************************************************************

MATERIAL
    COMPOUND   (names)
        [USERDEF   (unames)]
        [FP-NAMES  (fnames)]
        [AERNAMES  (anames)]

**************************************************************************
```

A library of material properties is provided in CONTAIN. A list of the materials included in this library is given in Table 2-1. Any number of materials from this table may be specified after the COMPOUND keyword. The user may also specify his own tabular values for properties of materials specified after the USERDEF keyword, as discussed in Section 3.2.8 on the USERDAT option. The names of all materials (excluding aerosols and fission products) to be used in any of the input blocks following the MATERIAL block must be included in either the COMPOUND or USERDEF input. Fission product names used in subsequent fission product input blocks must be specified after the FP-NAMES keyword. Aerosol names used in subsequent aerosol input blocks may either be taken from the materials specified after COMPOUND or from the names specified after the optional AERNAMES keyword. The COMPOUND keywords must immediately follow the MATERIAL keyword. The other keywords may be specified after COMPOUND as needed.

MATERIAL — keyword used to initiate the material block. This keyword must be the first keyword after the global control block.

COMPOUND — required keyword to initiate input of material names from the CONTAIN material library. This keyword must immediately follow the MATERIAL keyword.

names	names of materials taken from Table 2-1 to be used in any of the input following the MATERIAL block.
USERDEF	optional keyword to initiate input of the user-defined material names.
unames	names of materials which will use the properties tables defined later in the USERDAT input. The names included in this block are arbitrary, subject only to an eight character limitation. CONTAIN material names (see Table 2-1) may be used, in which case the internally defined properties will be overridden by any user-defined properties specified. However, USERDEF names which are CONTAIN material names must also be specified after COMPOUND.
FP-NAMES	optional keyword to initiate input of fission product names. The word FISSION may also be used to define fission product names for compatibility with older, existing input files. This obsolete keyword is described further in Appendix D.
fnames	names of fission products. Like user-defined material names, fission product names are arbitrary. A given name may appear more than once in the linear chain decomposition of fission product decay if branching or merging decays are present.
AERNAMES	optional keyword to initiate input of user-defined aerosol component names. Aerosol names may also be taken from the names specified after the COMPOUND keyword. Such names need not be declared after AERNAMES.
anames	user-defined aerosol component names. User-defined aerosol names are also arbitrary; however, aerosol names taken from the COMPOUND list should not be duplicated.

The user is cautioned that the MATERIAL block is terminated by any valid global keyword. As a consequence, user-defined material names, fission product names, and aerosol names should not match any of the global keywords allowed in CONTAIN input decks. This includes current and obsolete global keywords such as AEROSOL, FLOWS, TIMES, DUMMY, DEBUG, THERMAL, and TITLE.

3.2.1.1 User-Defined Material Definition. The materials specified in the USERDEF block of the MATERIAL input may be defined in this section. Provision is made for specification of the material properties as a function of temperature. The properties that may be defined are the density (except for gases), conductivity, viscosity, specific enthalpy and specific heat. The density may not be specified for gas phase user-defined materials due to the assumption of ideal gas behavior in CONTAIN.

The property values may be entered as explicit pairs of temperature and property values. Alternatively, the temperatures at which all properties are evaluated may be given first, with the TEMPS keyword input. This is then followed by groups of property values, with the number of property values being the same as the number of temperatures specified in TEMPS,

so that a one-to-one correspondence may be set up. The user may specify properties using a combination of these two methods. For example, the density and viscosity of a user-defined material may be specified with the RHO and VISC input blocks, which specify density and viscosity, respectively, along with the temperature, while the conductivity and enthalpy are specified with the CONDT and ENTHT blocks, which specify only conductivity and enthalpy, respectively. These blocks may be specified in any order but the TEMPS block must precede any block such as CONDT which specifies only property values and not temperature.

The user-defined material name may be a CONTAIN material name, taken from Table 2-1, provided it has also been specified after COMPOUND in the MATERIAL block. In this case, those properties specified in the tables described in this section will override the internal properties for that material. WARNING: THIS OPTION CAN HAVE SEVERE CONSEQUENCES ON THE ACCURACY AND RELIABILITY OF RESULTS, PARTICULARLY WHEN THE COOLANT VAPOR IS RESPECIFIED.

If the user-defined material name is not a CONTAIN material name, then all properties must be defined for that material with the exception of (1) the specific heat, which will by default be defined by differentiating the enthalpy table values, (2) the density for a gas material, which is not allowed, and (3) the viscosity for a solid material.

The keyword to begin this property specification section is USERDAT and the format of the input is described as follows.

```
**************************************************************************

USERDAT
    (name phase
        [MOLEW molew]
        {[RHO nrho (temp density)]
        [COND ncond (temp conduct)]
        [ENTH nenth (temp enthalpy)]
        [VISC nvisc (temp viscosity)]
        [SPH nsph (temp spheat)]
                  or
        TEMPS ntemp (temp)
            [{RHOT (density) or RHO nrho (temp density)}]
            [{CONDT (conduct) or COND ncond (temp conduct)}]
            [{ENTHT (enthalpy) or ENTH nenth (temp enthalpy)}]
            [{VISCT (viscosity) or VISC nvisc (temp viscosity)}]
            [{SPHT (spheat) or SPH nsph (temp spheat)}]}
    EOI)
EOI

**************************************************************************
```

USERDAT — keyword initiating user definition of materials.

name — required user-defined material name. Names given must also be specified after USERDEF in the MATERIAL block.

phase — required name of the material phase; may be one of the words GAS, LIQUID, SOLID.

MOLEW	keyword for specifying the molecular weight of the material. The molecular weight is required if "name" is not a CONTAIN material.
molew	molecular weight.

The following five keywords are used for specifying pairs of temperature-property values.

RHO	keyword for specifying density input. The density should not be specified for a gas but is required if "name" is not a CONTAIN material and the material is not a gas.
nrho	number of temperature-density pairs which follow.
temp	temperature value. (K)
density	density value. (kg/m^3)
COND	keyword for specifying thermal conductivity input. The thermal conductivity is required if "name" is not a CONTAIN material.
ncond	number of temperature-conductivity pairs which follow.
conduct	conductivity value. (W/m-K)
ENTH	keyword for specifying specific enthalpy input. The enthalpy is required if "name" is not a CONTAIN material.
nenth	number of temperature-enthalpy pairs which follow.
enthalpy	specific enthalpy value. (J/kg)
VISC	keyword for specifying viscosity input. The viscosity is required if "name" is not a CONTAIN material and the material is not a solid.
nvisc	number of temperature-viscosity pairs which follow.
viscosity	viscosity value. (kg/m-s)
SPH	keyword for specifying specific heat input. The specific heat is by default the derivative of the enthalpy table values for a non-CONTAIN material and the internal expression for a CONTAIN material.
nsph	number of temperature-specific heat pairs which follow.
spheat	specific heat value. (J/kg-K)
TEMPS	keyword for specifying a number of temperatures for the alternate format. This must precede any of the RHOT, CONDT, ENTHT, VISCT, or SPHT options.

ntemp — number of temperature values which follow. These temperatures will be paired with the values following the keywords RHOT, ENTHT, CONDT, SPHT, VISCT, which represent the density, enthalpy, conductivity, specific heat, and viscosity, respectively. Thus, "ntemp" property values should follow each of these keywords.

3.2.2 Reactor Type

Only one of two reactor types may be specified.

****

[{FAST **or** THERMAL}]

****

FAST — optional keyword to specify a sodium-cooled reactor.

THERMAL — optional keyword to specify a water-cooled reactor.

If neither keyword is specified, the default is THERMAL. The keyword for reactor type specifies the type of coolant (water or sodium) and sets flags that allow or prevent the activation of certain reactor-specific subroutines in a calculation.

3.2.3 Flow Options

The flow options specify intercell gas flow path characteristics, including those for the special BWR suppression pool vent flow path. The input is given in terms of three major input blocks: the FLOWS, ENGVENT, and SPVENT blocks. The FLOWS block describes the modeling options to be used with the regular flow paths and the solution method (implicit or explicit) to be used for the flows. It also activates atmosphere thermodynamics and mass accounting. (In problems without flow, one may also use the keyword THERMO instead of FLOWS to activate thermodynamics and mass accounting.) The ENGVENT block describes the modeling options to be used with the engineered vents. These include all of the options available for the regular flow paths and some others specific to engineered vents. The SPVENT block describes the liquid and gas flow characteristics and aerosol scrubbing parameters for use in the BWR suppression pool vent model.

Aerosols, fission products in the atmosphere, and other suspended materials will flow without slip with the gases through the flow paths, with two exceptions: (1) if FPCOSN or VCOSN is specified, aerosols will be allowed to settle through the flow path or vent, respectively; (2) if the flow is scrubbed in the suppression pool vent model, aerosols will become trapped in the pool. Fission products hosted by the aerosols will follow the aerosols in these two cases.

3.2.3.1 Flow Paths. The FLOWS block determines the method to be used to integrate the mass and energy equations for the cell atmospheres and also specifies the characteristics of the regular flow paths. If FLOWS or

THERMO, its equivalent for nonflow problems, is not specfied the cell atmosphere thermodynamic conditions or compositions will not be updated with time.

The flow model will be the inertial model and the integration method the Runge-Kutta method, unless the user specifies QUASI or IMPLICIT. QUASI selects the quasi-steady flow model for all flow paths and the Runge-Kutta method. IMPLICIT selects the implicit integration method, which is the generally recommended one. A number of code features, including the ENGVENT and SPVENT options, are available only with the implicit method. While the flow model used in general with the implicit method is the inertial model, a number of special flow options use a quasi-steady flow model. (Such usage is indicated in the discussion of those options.)

****

```
{FLOWS
    ([AREA,i,j=area] AVL,i,j=avl CFC,i,j=cfc [FLOW,i,j=flow]
    [TOPEN,i,j=topen] [TCLOSE,i,j=tclose] [DP,i,j=dp] [DP,j,i=dp]
    [PDAFLAG,i,j=pflag] [CFRFLAG,i,j=cflag]
    [VAR-AREA,i,j
        FLAG=iflag
        VAR-X=xname
        X=n (x)
        Y=n (y)
    EOI])
    [(IMPLICIT [nimpli]
    [DROPOUT] [PERROR=perror] [PIVOTMIN=pvtmin]
    ([CONTRACT,i,j=contr] [ELEVCL,i=elevcl] [ELEVFP,i,j=elevfp]
    [ELEVFP,j,i=elevfp] [FPCOSN,i,j=fpcosn]) or
    QUASI [DPREF=dpref] [REDUCE=nred])}]
or
THERMO}
```

****

The following keywords determine the characteristics of the regular flow paths. The keywords immediately below, with the exception of FLOWS itself, should all be followed by cell indices i and j representing the cells connected by the flow path and then by a numerical value for the variable represented by the keyword. Unless otherwise noted, only one permutation of the indices i and j need be specified. (Note that in the input, a comma is simply a field separator just like a blank, parenthesis, or equal sign.) Only the AVL keyword and the CFC keyword are always required for each regular flow path. If not explicitly stated, the quantities discussed in the descriptor blocks below refer to the numerical value to be given after the cell indices.

FLOWS — keyword to initiate the specification of regular flow paths. It also activates the atmosphere thermodynamics and mass and energy accounting calculations.

AREA,i,j = area — the (constant) cross-sectional area of flow path when open. (m^2)

AVL,i,j = avl — the ratio of effective flow path area to inertial length. The value corresponds to A_{ij}/L in Equation (2-3). (m)

CFC,i,j = cfc — the flow loss coefficient. This coefficient includes entrance, exit, and other discontinuity losses as well as frictional losses. The value corresponds to C_{FC} in Equation (2-3). (dimensionless)

CFRFLAG,i,j = cflag — flag that specifies that the "flow" value discussed below is a constant rate, as opposed to the initial flow rate. Specify 1 if the units of the specified "flow" value are kg/s, or -1 if the units are m^3/s. If CFRFLAG is not specified, the value specified for "flow" is interpreted as an initial flow rate rather than a constant flow rate.

FLOW,i,j = flow — a constant or initial flow rate. (CFRFLAG, discussed above, is a flag which indicates that the value specified for "flow" is a constant flow rate. If CFRFLAG is not specified, then the value for "flow" is taken to be an initial flow rate.) The value for "flow" should be positive if the flow is in the direction from cell i to cell j. Default = 0. (kg/s or m^3/s units are allowed if a constant flow rate is specified; kg/s only is allowed if an initial flow rate is specified.)

TOPEN,i,j = topen — the time to open the flow path. Default = -10^{30}. (s)

TCLOSE,i,j = tclose — the time to close the flow path. Default = 10^{30}. (s)

DP,i,j = dp — the positive definite pressure difference which opens the flow path. Once the flow path is open, it remains open even if the actual pressure difference drops below the opening value. DP,i,j determines the opening pressure difference when the pressure in cell i is greater than that in cell j. The value for DP,i,j does not have to be same as that for DP,i,j. It is assumed that the values are equal unless both DP,i,j and DP,j,i are specified. (Pa)

PDAFLAG,i,j = pflag — flag used with the area-versus-pressure option within the VAR-AREA table option. A value of 1 implies a reversible pressure-dependent area. A value of -1 implies an irreversible pressure-dependent area that can only stay the same or increase in size. Default = 1.

A flow path to be used in the calculation must be specified with a positive nonzero value of "avl" for all flow options; otherwise, that flow path will be ignored. A flow path may be either open or closed. If a flow path is open, the flow is calculated according to the cell pressure differences or set to a constant user-specified rate, set by the "flow" value and "cflag". "Avl" must be the area/length ratio for the flow path in the default and IMPLICIT flow options. The actual value of "avl" is ignored in the QUASI flow option. Note that an area specification is necessary for aerosol settling in the case of a user-specified constant flow rate even though it is not necessary for calculating the gas flow

rate. If the flow path is closed, no gas flow or aerosol settling through the flow path occurs. Note that, beginning with CONTAIN 1.1, constant (leakage) flow is no longer permitted for a closed path. In part, this is due to the fact that parallel paths, using the ENGVENT option discussed in the next section, are allowed and leakage can be modeled through a parallel path.

The logical state (open or closed) of a flow path can only be controlled by DP, TOPEN, or TCLOSE. Beginning with CONTAIN 1.1, the input value of "area" no longer affects this state. By default, a flow path is open. The state of the flow path is initially closed if DP is specified, or if TOPEN is specified without TCLOSE, or if both TOPEN and TCLOSE are specified with the value for "topen" less than that for "tclose". Once a flow path is open, the flow area can be controlled through the VAR-AREA option discussed below.

The VAR-AREA keyword allows the user to specify a global table for the flow area. The table keywords FLAG, VAR-Y, X, and Y are discussed in Section 3.5, as are the values associated with FLAG. Discussion of other keywords and values follow. (The word global implies that the table is stored at the global level in CONTAIN. Consequently the number of global tables "numtbg" and maximum global table size "maxtbg" specified in the global CONTROL block should take any tables specified in the following option into account.)

VAR-AREA,i,j — VAR-AREA initiates the input of a global table for specifying the flow area as a function of time or pressure difference. VAR-AREA should be followed by the indices i and j, which refer to the cells connected by the regular flow path which is to be governed by the table, and then by other table keywords.

VAR-X = xname — the name of the independent variable in the table. "Xname" can either be specified as TIME, which indicates that the "x" independent variable corresponds to time, or DELTA-P, which indicates that the "x" variable corresponds to a pressure difference. Note that for the DELTA-P option, the PDAFLAG keyword discussed above determines whether the area corresponding to the dependent variable "y" is reversible or irreversible.

n — number of points in the table.

x — the independent variable in the table. It corresponds to time if VAR-X=TIME is specified or to pressure difference if VAR-X=DELTA-P is specified. The "x" value for the DELTA-P table corresponds to ΔP_{ij} in Equation (2-8). The values must be monotonically increasing. Specify "n" values. Note that outside of the range of the independent variable of the table, the table is extrapolated. A constant value equal to the closest endpoint value is used in the extrapolation. (s or Pa)

y — the dependent variable in the table, which corresponds to area. Specify "n" values. (m^2)

An example of table input follows:

```
VAR-AREA,1,2                  && table for flow between cells 1 and 2
    FLAG=2                    && linear interpolation
    VAR-X=DELTA-P             && pressure difference is independent
                              && variable
    X=3 -1.E4 0. 1.E4         && three values of pressure difference
    Y=3 0. 0. 10.             && three values of area
EOI                           && table terminator
```

The following keywords are used only if IMPLICIT has been specified.

IMPLICIT — keyword to select the implicit integration method.

nimpli — the optional integer value following IMPLICIT which gives the number of cells to be solved implicitly. The first "nimpli" cells as numbered by the user are solved implicitly. The remaining ("ncells"-"nimpli") cells, if any, are solved explicitly. In practice, only environment cells are tractable when solved explicitly for timesteps typical of containment analysis. Use volumes of at least 10^{10} m^3 for these cells. The value of "nimpli" cannot be zero. Default = "ncells".

DROPOUT — keyword to remove all suspended liquid coolant from the atmosphere and deposit it in the appropriate pool. To be used only in the absence of aerosol modeling.

PERROR — keyword to define the degree to which the inventory of a cell, as measured by the pressure, is iterated to self-consistency. The error in the pressure difference between cells gives rise to an error in the flow rate. The cumulative error in the flow over the timestep leads to an inventory error. This is what is limited by "perror". (For very large flow areas, the driving pressure differences between cells have errors much less than "perror".)

perror — value of the self-consistency error. Default = 1. (Pa)

PIVOTMIN — keyword to define the minimum acceptable size of a divisor in the implicit solver analogous to the pivot element in Gaussian elimination. A smaller divisor is assumed to generate an effectively singular inverse matrix and is not used.

pvtmin — the minimum size of the pivot element. Increasing the value somewhat should increase robustness, at the expense of efficiency. The decrease in efficiency should be acceptable for a factor of two to four increase in value. Default = 0.01. (dimensionless).

ELEVCL,i = elevcl — the center of mass elevation of cell i. See Figure 2-2. Default = 0. (m)

ELEVFP,i,j = elevfp — the elevation of one end of the regular flow flowpath connecting i and j. ELEVFP,i,j defines the end of the path between cells i and j that is attached to cell j. In general, both ELEVFP,i,j and ELEVFP,j,i need to be specified. See Figure 2-2. The gravitational head developed across the flow path can be deduced from Equation (2-8). The default value for ELEVFP,i,j is that given by ELEVCL,j. The reader interested in using ELEVFP should read the cautionary note at the end of Section 2.2.3.2.1. (m)

CONTRACT,i,j = contr — area ratio for the vena contracta that may develop downstream of the flow path. The value between zero and one specified for "contr" is the ratio of the cross sectional area of the vena contracta to the geometric cross sectional area of the flow path. "Contr" is used only for choked flow. Default = 1. (dimensionless)

FPCOSN,i,j = fpcosn — the cosine of the angle of the flow path axis with respect to the vertical direction. The angle is measured between the upward direction and the flow path axis in the direction from i to j. The value is used to calculate aerosol settling through the flow path. The value for "fpcosn" should be 1 if the end of the flow path at cell j is directly above that at cell i, and -1 if the reverse is true. Only the component of aerosol settling velocities parallel to the flow path axis is considered. Default = 0. (dimensionless)

The following keywords are available only when the QUASI option is invoked. Because the QUASI option is typically much less efficient than the IMPLICIT option, the latter should be used in most cases.

QUASI — keyword to select the Runge-Kutta integration method and the quasi-steady flow model in all flow paths.

DPREF = dpref — the crossover pressure to the artificial linear viscosity regime. Default = 1000. (Pa)

REDUCE — keyword to instruct the code to reduce stiffness in the QUASI flow option by artificially reducing flow path areas when the pressure difference across the flow path is less than "dpref".

nred — an integer that determines the maximum degree of restriction, which is 2^{nred}.

The above parameters are discussed in Section 2.2.3.2.2 and in Appendix C.

The keyword FLOWS can be used by itself in nonflow problems (e.g., single cell systems) to activate the atmosphere thermodynamics and mass and energy accounting subroutines. Alternatively, the keyword THERMO can be used for this purpose.

THERMO alternative keyword to FLOWS to activate atmosphere thermodynamics and mass and energy accounting in problems without flow paths.

3.2.3.2 Engineered Vents. The engineered vent is an intercell gas flow path with a number of additional features and improved architecture when compared with the regular flow paths specified in the FLOWS block. For example, the number of vents which can be specified between any two cells is not restricted as it is with the regular flow paths. The modeling options for the flow are also more extensive. For example, the flow area as a function of pressure is calculated implicitly in the RVAREA-P option. This option allows the modeling of one way doors and liquid heads in the flow path without chatter. As another example, the user may specify either the mass or volumetric flow rate as a function of time. Only constant user-specified flow rates are available with the regular flow paths.

The ENGVENT engineered vent input block is separate from the FLOWS input block. One must, however, select the IMPLICIT solver option in the FLOWS input block whenever engineered vents are to be specified. The keyword NENGV in the global CONTROL block must also be used to specify the total number of engineered vents in the system.

```
**************************************************************************

ENGVENT
        (FROM=cellfr TO=cellto [VAREA=varea] [VAVL=vavl] [VCFC=vcfc]
        [VMFLOW=vmflow] [VVFLOW=vvflow] [VIFLOW=viflow] [VCOSN=vcosn]
        [VCONTRA=vcontra] [VDPB=vdpb] [VDPF=vdpf] [VELEVB=velevb]
        [VELEVF=velevf] [VTCLOS=vtclos] [VTCONS=vtcons] [VTOPEN=vtopen]
        [(AREA-T or IRAREA-P or MFLOW-T or RVAREA-P or VFLOW-T)
            [FLAG=iflag]
            X=n (x)
            Y=n (y)
        EOI]
    EOI)

**************************************************************************
```

If the engineered vent modeling is to be used, the following keywords are always required:

ENGVENT keyword to begin the specification of engineered vents.

FROM keyword to specify the nominal donor cell.

cellfr the number of the cell from which flow is occurring when the flow is considered positive. (This arbitrary sign convention is also used in the code output.)

TO keyword to specify the nominal acceptor cell.

cellto the number of the cell to which flow is directed when the flow is considered positive.

EOI — keyword to terminate the reading of the parameters of a given vent.

The keywords from the next group should be selected as necessary to define the flow for a given vent. Note that they may be used in conjunction with a number of table options (AREA-T, IRAREA-P, MFLOW-T, RVAREA-P, and VFLOW-T) defined below. The inertial flow model is used unless otherwise specified. For this model, VAVL, VCFC, and an option to define the flow area (VAREA, AREA-T, or IRAREA-P) are required. The quasi-steady flow model is invoked when the reversible-area-versus-pressure option RVAREA-P is specified. For this model only VCFC is required in addition to the RVAREA-P option. When any of the user-specified flow rate options are specified (VVFLOW, VMFLOW, VFLOW-T, or MFLOW-T), no other keywords from the following set are required, although VAREA should be specified to determine the settling rate of aerosols through the vent if VCOSN is specified.

VAREA = varea — the (constant) cross-sectional area of the vent when open. This should be specified unless a table option for the area is used (see below). In the user-specified flow rate options, VAREA may still be specified. Although it is not required for the gas flow calculation with those options, it may be used for calculating aerosol settling through the vent. (m^2)

VAVL = vavl — the vent area versus length (analogous to AVL in the FLOWS input) used to calculate the inertial mass in the flow path. This is required except in the case of the reversible pressure-dependent-area table option (RVAREA-P), which assumes quasi-steady flow, or a user-specified flow rate option. (m)

VCFC = vcfc — the vent turbulent flow coefficient (analogous to CFC in the FLOWS block). This is required unless a user-specified flow rate option is used. (dimensionless)

VMFLOW = vmflow — the constant mass flow rate for the vent when open. A time-dependent rate can be specified through the MFLOW-T table option discussed below. (kg/sec)

VVFLOW = vvflow — the constant volumetric flow rate for the vent when open. A time-dependent rate can be specified through the VFLOW-T table option discussed below. (m^3/sec)

VIFLOW = viflow — the flow rate at problem start. This should be specified only if the vent is initially open and the flow model is inertial. Default = 0. (kg/sec)

The following keywords are optional and may be specified independently of any other keyword.

VCOSN = vcosn — the cosine of the angle between the vent axis and the vertical direction. The value is used to calculate aerosol settling through the vent. The angle is measured between the upward direction and the vent axis in the direction from "cellfm" to "cellto." The value should be 1 if the

vent goes straight up in the direction from "cellfm" to "cellto" and -1 if it goes straight down. Only the component of the aerosol settling velocities parallel to the vent axis is considered. Default = 0.

VCONTRA = vcontra — the reduction factor for the flow area due to the vena contracta. Used only when the flow is choked (analogous to CONTRACT in the FLOWS block). Default = 1. (dimensionless)

VDPB = vdpb — the positive-definite pressure difference to open the vent in the backward (negative flow) direction. This option sets the vent initially closed. If VDPB is specified, then VDPF, discussed below, must also be specified. VDPF and VDPB may be used with VTOPEN and VTCLOS as long as the times specified imply the vent is initially closed. (Pa)

VDPF = vdpf — the positive-definite pressure difference to open the vent in the forward (positive flow) direction. See the comments regarding usage in the discussion of VDPB above. (Pa)

VELEVB = velevb — the elevation of the vent at cell "cellfr". Default = cell center elevation given by the ELEVCL keyword in the FLOWS block for cell "cellfr". The reader interested in using VELEVB or VELEVF should read the cautionary note at the end of Section 2.2.3.2.1. (m)

VELEVF = velevf — the elevation of the vent at cell "cellto". Default = cell center elevation given by the ELEVCL keyword in the FLOWS block for cell "cellto". The reader interested in using VELEVB or VELEVF should read the cautionary note at the end of Section 2.2.3.2.1. (m)

VTCLOS = vtclos — the time at which the vent should close or begin to close. Default = 10^{30}. (sec)

VTCONS = vtcons — the time period over which the vent should open or close after a VTOPEN, VTCLOS, VDPF, or VDPB is satisfied. The area variation on opening or closing is linear in time. Because of conflicts with the table values, this option should not be used with a table option. Default = 0. (sec)

VTOPEN = vtopen — the time at which the vent should open or begin to open. The vent by default is initially open. Specification of this option will result in the vent being initially closed unless "vtclos" is also specified and "vtclos" < "vtopen." Default = -10^{30}. (sec)

The user may introduce a number of different global table options in which the area or user-specified flow rate is specified as a function of time or pressure difference. The type of table is specified through a keyword picked from the list below and then followed by standard table keywords FLAG, X, and Y as indicated in the ENGVENT input template. (These keywords are also discussed in Section 3.5.) If any tables described below are used in the input, the user should take them into account in setting the number of global tables "numtbg" and maximum global table size "maxtbg" in the global CONTROL block.

AREA-T — keyword to initiate the specification of a table for area versus time.

IRAREA-P — keyword to initiate the specification of a table for area versus pressure difference. The area is treated as irreversible in this option. The table value will be used only if it is larger than the existing area.

MFLOW-T — keyword to initiate the specification of a table for mass flow versus time.

RVAREA-P — keyword to initiate the specification of a table for area versus pressure difference. The area is considered reversible in this option. Unlike the reversible area option for regular flow paths, the vent area is implicitly calculated as a function of pressure. The flow is calculated according to the quasi-steady flow expression, Equation (2-9), with $C_{LFC} = 0$ and the (i,j) indices interpreted as referring to the engineered vent in question.

VFLOW-T — keyword to initiate the specification of a table for volumetric flow versus time.

FLAG — keyword to introduce the interpolation flag for the table.

iflag — the interpolation flag for the table. A value of 1 denotes a step-function table, whereas a value of 2 denotes a linearly interpolated table. Note that in the RVAREA-P option, a linearly interpolated table must be used.

X — keyword to introduce the independent variable of the table.

n — the number of points in the table.

x — the independent variable in the table. In the AREA-T, MFLOW-T, and VFLOW-T tables, the independent variable represents time (s). In the IRAREA-P and RVAREA-P tables, the independent variable represents the pressure difference ΔP_{ij} given in Equation (2-8), where i="cellfr" and j="cellto" (Pa). Specify "n" monotonically increasing values. Note that outside of the range of the independent variable of the table, the table is extrapolated. A constant value equal to the closest endpoint value is used in the extrapolation.

Y — keyword to introduce the dependent variable of the table.

y — the dependent variable of the table. In the AREA-T, IRAREA-P, and RVAREA-T tables, the dependent variable represents the flow area (m^2). In the MFLOW-T table, the dependent variable represents a mass flow rate (kg/s). In the VFLOW-T table, the dependent variable represents a volumetric flow rate (m^3/s). Specify "n" values.

A table should not be specified if VTCONS, VMFLOW, or VVFLOW keywords are specified since these represent modeling options that conflict with those of the tables. For example, VTCONS gives a time constant for the opening of the vent to the value given by VAREA. This method of specifying the vent characteristics obviously could conflict with the vent characteristics given by the tables, and thus the combination is not allowed. Similarly, only one table may be specified for a given vent, since each represents an independent modeling option. A table may be used in conjunction with any of the keywords which change the vent state, such as VTOPEN, VTCLOS, and VDPF. VAREA may also be used with any table which does not represent the area, but it is used in that case only to define the aerosol settling rate through the vent. Note that the table values are accessed only when the vent is open. When the vent is closed, the flow and the flow area (if specified) are zeroed out.

3.2.3.3 Suppression Pool Vent Flow Path Model Options. The BWR suppression pool vent flow path model is activated through the SPVENT keyword. Only one SPVENT block is allowed, and only two cells may be connected by the suppression pool vents.

```
**************************************************************************

SPVENT
    NDRY=ndry NWET=nwet
    [NSVNTS=nsvnts] [AVNT=avnt] [VNTLEN=vntlen] [ELEVNT=elevnt]
    [DPDRY=dpdry] [DPWET=dpwet] [FDW=fdw] [FWD=fwd] [GINLEN=ginlen]
    [(SCRUB
        [BSIZI=bsiz] [VROVR=vrovr]
    EOI     or
    SPARC
         [BSIZI=bsiz] [RATIO=ratio] [NRISE=nrise]
    EOI)]
EOI

**************************************************************************
```

The following keywords specify geometrical and physical parameters of the suppression pool vent flow path system. Note that in addition to the input described here, a lower cell pool must be defined in the wetwell cell (see Section 3.3.2.5). Figures 2-4 and 2-5 illustrate the significance of the geometric parameters.

The following keywords are required:

SPVENT	keyword to begin the specification of the suppression pool vent path.
NDRY = ndry	the number of the cell on the drywell side of the suppression pool vents.
NWET = nwet	the number of the cell containing the wetwell pool.

The following keywords are optional. (The default values except for that for "elevnt" correspond to a Mark I configuration.)

NSVNTS = nsvnts — the number of vent pipes of cross-sectional flow area "avnt"; used for computing the total flow area. Default = 8.

AVNT = avnt — horizontal cross-sectional characteristic flow area for a single vent. For a Mark III, this should be the annulus flow area. Default = 6.71. (m^2)

VNTLEN = vntlen — for a Mark I or II, this is the vertical extent of the vent pipe. For a Mark III, this is the characteristic distance from the vent to the top of the weir wall. Default = 5. (m)

ELEVNT = elevnt — height of the vent opening above the bottom of the pool. Default = 0. (m)

DPDRY = dpdry — the range for the pressure difference between the drywell and wetwell over which the effective vent gas flow area goes from zero to its maximum value. This range applies when the flow is from the drywell to the wetwell. The gas flow area is taken to be zero at the pressure difference required to support the liquid head present when the vents just begin to clear. The total gas flow area changes linearly from zero to "nsvnts"*"avnt" over the range "dpdry". The flow solver may have difficulty converging if this range is too small. In most cases, if this range is much less than the cell pressures, the calculated results will not be sensitive to the value used. In such cases it may be adjusted to give better computational efficiency. Default = 10^4. (Pa)

DPWET = dpwet — the range for the pressure difference analogous to "dpdry", but referring to flow from the wetwell to the drywell. The total gas flow area changes from zero to "nsvnts"*"avnt" over "dpwet". Default = 10^4. (Pa)

FDW = fdw — overall liquid flow loss coefficient for flow from the drywell to the wetwell, including contraction, turning, and orifice losses but not expansion losses. (See Equation (2-11).) Default = 1. (dimensionless)

FWD = fwd — overall liquid flow loss coefficient for flow from the wetwell to the drywell. Default = 1. (dimensionless)

GINLEN = ginlen — the gas inertial length to be used when the vent flow bypasses the pool (as when the level is too low to cover the vent). The bypass gas flow is calculated considering the effects of inertia in the flow. Default = 5. (m)

For a THERMAL reactor, the user may choose either of two aerosol scrubbing models. The keyword SCRUB specifies the aerosol scrubbing model from the VANESA code.[Pow86] The keyword SPARC specifies the SPARC scrubbing model.[Owc85b] For a FAST reactor only SCRUB is available. The SCRUB model is the model by default provided aerosols are present.

The following keywords and values may be used in conjunction with the SCRUB model from the VANESA code (see Reference Pow86):

SCRUB — keyword to specify the VANESA aerosol scrubbing model.

BSIZI = bsiz — initial bubble diameter. Default = 0.01. (m)

VROVR = vrovr — ratio of bubble gas circulation velocity to computed rise velocity. Default = 1.

The following keywords and values may be used in conjunction with the SPARC scrubbing model (see Reference Owc85b):

SPARC — keyword to specify the SPARC aerosol scrubbing model.

BSIZI = bsiz — initial bubble diameter. This keyword replaces DIAM of the stand-alone version of SPARC. Default = 0.01. (m)

RATIO = ratio — ratio of major axis to minor axis for a symmetric oblate spheroid bubble. The ratio is taken to be greater than or equal to 1. If a value less than 1 is input, its inverse is automatically taken. Default = 1.

NRISE = nrise — number of integration zones used for bubble rise in the scrubbing region. Values ranging from 10 to 1000 are suggested for accuracy. Default = 10.

3.2.4 Aerosol Options.

The global aerosol characteristics are specified in the following input block. Note that aerosol initial conditions and sources are given on a cell-by-cell basis and are discussed in Section 3.3.1.9.

```
**************************************************************************

AEROSOL
        [NEWCOF=newcof] [DIAM1=diam1] [DIAM2=diam2] [TGAS1=tgas1]
        [TGAS2=tgas2] [PGAS1=pgas1] [PGAS2=pgas2] [TURBDS=turbds]
        [COLEFF=coleff] [DENSTY=rho] [CHI=chi] [GAMMA=gamma]
        [DELDIF=deldif] [TKGOP=tkgop] [NOCOND] [NOEVAP]
        [RELTOL=reltol] [ABSTOL=abstol]
        [AERTIM=ntb
                (NAME=aname
                [FLAG=iflag]
                X=n (x)
                VAR-Y=yname
                Y=n (y)
            EOI)]
    (mapaer amean avar)

**************************************************************************
```

The AEROSOL keyword is required to initiate this input block. The keywords following AEROSOL are optional. The block must be terminated by "nac" groups of values for "mapaer", "amean", and "avar".

AEROSOL — keyword to begin specification of the global aerosol characteristics.

NEWCOF = newcof — flag for calculating aerosol coefficient sets. The possible values of "newcof" are discussed at the end of this section. Default = 1.

DIAM1 = diam1 — smallest diameter allowed for aerosols. Default = 1.0×10^{-6}. (m)

DIAM2 = diam2 — largest diameter allowed for aerosols. Default = 1.0×10^{-4}. (m)

TGAS1 = tgas1 — lower temperature in the coefficient interpolation. Default = 273. (K)

TGAS2 = tgas2 — upper temperature in the coefficient interpolation. Default = 673. (K)

PGAS1 = pgas1 — lower pressure in the coefficient interpolation. Default = 10^5. (Pa)

PGAS2 = pgas2 — upper pressure in the coefficient interpolation. Default = 7.5×10^5. (Pa)

TURBDS = turbds — turbulent dissipation rate. Default = 0.001. (m^2/s^3)

COLEFF = coleff — constant collision efficiency. If a positive value is specified, it will be used. A zero value will set a flag to use an internal analytic expression. Default = 0.

DENSTY = rho — material density to use for all aerosol component materials. Default = 1000. (kg/m^3)

CHI = chi — dynamic shape factor. Default = 1.

GAMMA = gamma — agglomeration shape factor. Default = 1.

DELDIF = deldif — diffusion boundary layer thickness. Default = 1.0×10^{-5}. (m)

TKGOP = tkgop — ratio of thermal conductivity of atmosphere to that of the particle. Default = 0.05.

NOCOND — keyword to suppress condensation on aerosols.

NOEVAP — keyword to suppress evaporation from aerosols.

RELTOL = reltol — relative error tolerance per Runge-Kutta timestep. Default = 0.001.

ABSTOL = abstol — scaling factor for the absolute error tolerance per Runge-Kutta timestep. The actual absolute error tolerance is "abstol" times the maximum total mass concentration in a size class. A "reltol" of 0.001 and an "abstol" of 0.0001 have been used successfully for problems with a large dynamic range. As an example of such a problem, one component is present initially at a relative mass concentration of one part in ten thousand compared to the total mass concentration, and the relative and total mass concentrations then decay by a factor of one million). Default = 0.0001.

More complete definitions of the physical parameters introduced above are given in Reference Gel82.

Through the AERTIM global table option, the user may specify the aerosol size distribution parameters "amean" and "avar" (discussed more fully along with the "mapaer" variable below) as a function of time. The AERTIM option uses a number of global tables to specify this time dependence, with one table specifying "amean" or "avar" for one aerosol component. The FLAG, X, and Y keywords are standard table keywords defined in Section 3.5. Other keywords and values associated with the AERTIM option are discussed below. The user should consider the AERTIM tables in setting the "numtbg" and "maxtbg" parameters in the global CONTROL block.

When the time is within the range of the table, the table values of "amean" and "avar" will override the corresponding values specified after the "mapaer" variable, as discussed below. Note that the "amean" and "avar" parameters in use at a given time are global values that apply to the aerosol initial conditions and sources in any cell, with the possible exception of SRV aerosol sources. The size distribution of SRV aerosols may be specified completely independently of the global values through the SRV source tables themselves.

AERTIM — keyword to initiate the specification of global tables for "amean" and/or "avar" as a function of time.

ntb — the number of tables to follow.

NAME = aname — the name of the aerosol component to which the table applies. It should be among the names specified for "mapaer" below.

VAR-Y = yname — the name of the dependent variable in the table. "Yname" should be specified as either AMEAN or AVAR, depending on whether the dependent variable corresponds to "amean" or "avar", as defined below.

n — the number of points in the table.

x — the independent variable of the table, corresponding to time. Specify "n" values in ascending order. Note that for times prior to the first time in the table, the initial

values of "amean" or "avar", specified after "mapaer" as discussed below, will be used. Within the range of the table, the table value determined according to the interpolation flag "iflag" will be used. For times greater than the last time in the table, the value of "amean" or "avar" will remain fixed at the last value determined from the table.

y — the dependent variable of the table, corresponding to "amean" if the AMEAN keyword has been specified after VAR-Y or to "avar" if the AVAR keyword has been specified. Specify "n" values.

The last group of variables in this block specifies the aerosol components to be used in the problem and the initial values of the aerosol size distribution parameters "amean" and "avar". This group terminates the global aerosol block and thus should follow any of the keywords described above. The following group of three variables is repeated "nac" times, once for each aerosol component.

mapaer — aerosol component name. This name must be one of the materials specified in the COMPOUND or AERNAMES input blocks. (See Section 3.2.1).

amean — volume-equivalent mass median particle diameter to be used for initial distributions and sources of new particles. See Section 2.2.4 for a definition of "amean". Default = 1.0×10^{-6}. (m)

avar — natural logarithm of geometric standard deviation of the particle size distribution to be used for initial distributions and sources of new particles. See Section 2.2.4 for a definition of "avar". Default = 0.693.

These "amean" and "avar" values govern the particle size distribution for initial conditions and sources unless overridden by the AERTIM table option discussed above or by local size distribution parameters used in conjunction with SRV aerosol sources.

For aerosol condensation to be active, the last aerosol component specified for "mapaer" must be H2OL or H2OV. In addition, the reactor type must be THERMAL. If THERMAL and either H2OL or H2OV are specified, the amount of liquid condensed on aerosols from the vapor phase will be added to the mass of the last component. However, note that the use of H2OV is obsolete and is not recommended. Note also that there is currently no provision for condensation of sodium vapor on aerosols.

Another format for the AEROSOL block is available. This format, discussed in Appendix D, might be present in input files developed for earlier code versions. While upward compatible, it is considered obsolete.

The aerosol model uses a set of coefficients that must either be calculated or read in from an aerosol database file created in a previous calculation. The user has some control over the coefficient calculation through the "newcof" parameter, as discussed below.

The coefficients depend on the number of size classes or sections, "nsectn", specified in the global CONTROL block, and all the parameters that can be set by the keywords listed above, with the exception of "newcof", "abstol", and "reltol". The aerosol database file, if present, is first scanned for a match in all these parameters if $1 \leq$ "newcof" ≤ 4. If an appropriate set of coefficients is found, it is read in. If a set of coefficients is found that is appropriate except for a mismatch in deposition or condensation parameters (e.g., "tkgop"), only the deposition and condensation coefficients will be calculated. The other coefficients will be read in. Coefficients not otherwise available are calculated during input processing and then used throughout the rest of the calculation. If a complete set of coefficients is calculated, the set can be appended to the end of the aerosol database file.

The aerosol routine by default is set up to interpolate between the coefficients calculated at each of the four points ("tgas1", "pgas1"; "tgas1", "pgas2"; "tgas2", "pgas1"; "tgas2", "pgas2") to account for the temperature and pressure dependence of the coefficients. For problems with no temperature or pressure variation, the user may specify that coefficients be defined at one or two points by setting "newcof" = 2, 3, or 4 as discussed below. If the user specifies such a partial set, the database file will be scanned for a match in only the "pgas1", "pgas2", "tgas1", and "tgas2" parameters relevant to the partial set. However, the complete set of parameters will be read in. If no match with partial sets on the database file is found, the partial set will be calculated, and the coefficients not required will be set to zero.

The options selected by various values of "newcof" are as follows:

- newcof = 1 coefficients are requested at four combinations of temperature and pressure given by "tgas1", "tgas2", "pgas1", and "pgas2". If coefficients are not available on the database file, they will be calculated and appended to the end of that file.

- newcof = 2 coefficients are requested only at "tgas1" and "pgas1". This option is appropriate only for constant temperature and pressure problems.

- newcof = 3 coefficients are requested for "pgas1" at "tgas1" and "tgas2". This option is appropriate only for constant pressure problems.

- newcof = 4 coefficients are requested for "tgas1" at "pgas1" and "pgas2". This option is appropriate only for constant temperature problems.

- newcof = 99 coefficients are to be recalculated regardless of availability of coefficients in the database file but are not to be appended to the end of that file.

A more detailed discussion of the aerosol physics modeling is found in Section 2.2.4.

3.2.5 Fission Product Decay and Heating Input

Global fission product characteristics are specified in the following input block. These characteristics include the structure of the linear decay chains, the fission product half-lives, and the decay power coefficients. Initial fission product masses and the targeted release and acceptance parameters are defined at the cell level in the FPM-CELL input block (see Section 3.3.1.10).

```
**************************************************************************

FISSION
    (NFPCHN=nfpchn
        FPNAME=(fpname)
        HFLIFE=(hflife)
        [{FGPPWR=ndpcon
            POWER=(fpq)     or
        POWER=(fpq)}])
EOI

**************************************************************************
```

FISSION — keyword to initiate input of the global fission product parameters. There should be only one global FISSION block in any one input file.

NFPCHN — keyword to specify the number of fission product elements in a chain. It also marks the beginning of the input sub-block for that chain. All other keywords and values for that chain must be given before NFPCHN is specified again for the next chain. A total of "nchain" NFPCHN subblocks should be defined in the FISSION block, where "nchain" is specified in the global CONTROL block.

nfpchn — the number of fission chain elements in a chain. The sum of "nfpchn" over all chains must add up to the value of "nfce" given in the global CONTROL block.

FPNAME — keyword to initiate the specification of the names of each element of a chain.

fpname — the fission product name for the chain element. Specify "nfpchn" names, each taken from the ones declared after FP-NAMES in the MATERIAL input block.

HFLIFE — keyword to initiate the input of fission product half-lives for all elements in a chain.

hflife — the half-life of a chain element (s). Exactly "nfpchn" values must be entered. The last element in a chain may be specified as stable with a zero value of "hflife". (Since there is no such thing as a zero half-life, zero is assumed to represent an infinite half-life or a zero decay constant). If a negative value is given then its absolute value will be interpreted as the decay constant, λ, where "hflife" = $\ln(2)/\lambda$.

FGPPWR = ndpcon — the number of coefficients in the decay power expression for each element in a chain. These coefficients are specified after the POWER keyword discussed below and are used to define a general time-dependent specific decay power according to Equation (2-23). Note that each chain may have its own number "ndpcon" of such coefficients. The minimum value of "ndpcon" is 1 and the maximum is 4. If FGPPWR is omitted, the value of "ndpcon" is taken to be 1, and the decay power reduces to a constant. If specified, FGPPWR should be specified before POWER. Note that a time-dependent decay power is useful when fission product groups are modeled (see Section 2.2.5.4).

POWER — keyword to initiate input of the power coefficients.

fpq — the value of a power coefficient. Exactly "nfpchn"*"ndpcon" values should be specified. "Ndpcon" values for the first element in a chain should be given, then "ndpcon" values for the second, and so on. For each element, the first value is a_1, the second, a_2, and so forth, where these coefficients are defined in Equation (2-23). If FGPPWR is not specified, only a_1 should be specified. Default = 0. (W/kg for odd coefficients and 1/s for even coefficients)

An alternate format is also available for the FISSION input block as described in Appendix D. This alternate input format includes the specification of initial fission product masses and release/acceptance functions at the global level with the FPM-CELL keyword. The FPM-CELL input block can also be given at the global level when using the input format described above; however, this is not the recommended procedure. The recommended procedure is to define the FPM-CELL input block at the cell level as described in Section 3.3.1.10.

3.2.5.1 Fission Product Transport Efficiency in Liquid Pathways. The FPLIQUID block is used to define the efficiency factors for fission product transport in liquid pathways. These factors determine the rate of fission product transport with structure condensate runoff and pool-to-pool transfers of coolant via engineered systems components, as discussed in Section 2.2.5.5.

```
**************************************************************************

FPLIQUID
    (fpname=fpliq)
EOI

**************************************************************************
```

FPLIQUID — keyword to initiate the specification of transport efficiency factors for fission products in liquid pathways. This keyword should be followed by pairs of the following two variables.

fpname — fission product name that is among the list of fission product names given in the global FISSION input block.

fpliq — the transport efficiency factor for "fpname" in liquid pathways. This should be a real value between zero and one. It specifies the ratio of the relative amount of the fission product transferred to the relative amount of water transferred when condensate drains from structure surfaces to a recipient pool and when direct pool-to-pool coolant transfers occur through engineered systems components, such as a PIPE . In the first case, the fission product is transferred from the structure surface to the recipient pool. That pool can be designated through the cell OVERFLOW keyword discussed in Section 3.3.1.11. (This keyword should not be confused with the engineered systems OVERFLOW component discussed in Section 3.3.3.11.) In the second the fission product is transferred from one pool to another. Default = 0.

EOI — required keyword terminating the FPLIQUID input block.

3.2.6 Timestep and Time Zone Input

The TIMES block establishes the maximum system timestep size, the maximum edit timestep, and the total allowable CPU calculation time. The edit timestep by definition is the interval at which information is written to the plot file(s). It is smaller than or equal to the interval at which long edits are written to the main output file. The TIMES block also defines the times at which restart data are written to the restart file.

```
**************************************************************************

TIMES cput tstart (timinc edtdto tstop) [{(ctmfr)   or
    CTFRAC=(ctmfr)}]
    [TRESTART=n (tres)]
    [TSFRAC=tsfrac]
    [EDMULT=edmult]
[EOI]

**************************************************************************
```

TIMES — keyword initiating timestep and time zone input.

cput — maximum CPU time limit. (s)

tstart — problem start time. (s)

The following set of three variables is repeated "ntzone" times, one set for each time zone:

timinc — maximum system timestep size in the time zone. (s)

edtdto — maximum edit timestep, or interval at which plot information is written to the plot file(s). For the long and short edit frequency, see Section 3.2.7.1. (s)

tstop — end time of the time zone. (s)

CTFRAC — optional keyword for defining the maximum cell timestep. It does not have to be specified if "ctmfr" values follow immediately after the time zone information.

ctmfr — the ratio of the maximum allowed cell timestep to the system timestep. Specify a value less than or equal to one for each cell. Note that neither CTFRAC nor "ctmfr" has to be specified if the default value is acceptable. Default = 1.

TRESTART — optional keyword to specify the times at which restart blocks are to be saved on the restart file.

n — number of restart times to be defined. Maximum = 100.

tres — times at which restart blocks are to be saved. Specify "n" values. If no values are specified, the restart times by default are taken to be the end times of the time zones.

TSFRAC = tsfrac — a timestep scaling factor for internal system timesteps. Such timesteps are calculated during certain physical processes, such as hydrogen burns, as some fraction of the characteristic time for those processes. When calculated, the internal timesteps override the maximum user-specified system timesteps, if the latter are larger. The fraction of the characteristic time used for the internal timesteps is obtained by multiplying the default fraction by the "tsfrac" factor. The default value of "tsfrac" is 1 for an initial run and the previous value in a restart. In support of older input decks, the keyword MULTIPLE may also be given instead of TSFRAC.

EDMULT = edmult — a frequency factor for edits during processes for which an internal system timestep is calculated, such as hydrogen burns. The edit timestep will be the system timestep multiplied by "edmult" if the resulting timestep is less than "edtdto" (even if the internal timestep itself is not used). The default value of "edmult" is the ratio "edtdto"/"timinc" for an initial run and the previous "edmult" value in a restart.

EOI — optional terminator.

A maximum of 101 restart blocks can be present on the restart tape. The last is always the temporary restart block from the last edit time. (This block is overwritten each edit time.) Up to 100 restart blocks may also be permanently saved. These are specified through TRESTART, or if this is not used, by the "tstop" times marking the ends of the time zones. Note that on a restart, new restart blocks are added to those already present on the restart tape, and the original blocks count toward the maximum of 101 blocks allowed.

The TSFRAC option gives the user control over internal system timesteps. For example, hydrogen burns are accompanied by calculation of internal system timesteps which are equal to 0.1*"tsfrac" times the burn time. Within a time zone with relatively long "timinc" timesteps, the internal

timesteps will be used. The hydrogen and carbon monoxide combustion model is the only model that makes use of the TSFRAC and EDMULT options in CONTAIN 1.1.

The EDMULT keyword is useful for resolving hydrogen burns without producing massive quantities of output at other times in the run. For example, "edtdto" may be considerably larger than "timinc"; however, if "edmult" is, say, equal to 1.2, the edit interval during a burn will be 2 (1.2 rounded up) times the actual timestep used.

3.2.7 Output Control

Several options to control the formatted output written to the main output file are discussed in this section. However, there are other types of output, as discussed in Section 4.1. The most extensive of these is the unformatted output written to the plot file(s). Note that the latter can be post-processed using the POSTCON code.[Was87]

3.2.7.1 Frequency of Print Output. Output is written to the main output file in printer carriage control format. This output consists of short summary edits and long detailed edits. The frequency at which the short edits and long edits are produced in the main output file can be controlled with the SHORTEDT and LONGEDT options.

****

SHORTEDT=kshort

****

SHORTEDT = kshort — the number of system timesteps between short edits. Cannot be 0; default = 1.

For example, if the system timestep is 5 s and "kshort" is 4, then the short edit interval will be 20 s. The short edit interval is completely independent of other output intervals.

****

LONGEDT=klong

****

LONGEDT = klong — the number of edit timesteps between long edits. Cannot be 0; default = 1.

The LONGEDT option controls the frequency of the long edits in the same way that the SHORTEDT option controls the short edit frequency. Note that LONGEDT and SHORTEDT have no effect on the frequency with which information is written to the plot file(s). (That frequency is governed by the basic edit timestep, which is defined by parameters such as "edtdto" discussed in Section 3.2.6.) Thus the user can limit the quantity of long or short edits but still obtain detailed plot information on the plot file(s). A long edit will always occur at a "tstop" time, a restart time, an opening or closing time for a regular flow path,

and a CORCON edit time regardless of the number of edit timesteps that have elapsed since the last long edit.

3.2.7.2 Print Output Options. The following single-keyword options can be used in any order to obtain the indicated block of output in the long edits.

****

[PRFLOW]
[PRAER]
[PRAER2]
[PRLOW-CL]
[PRHEAT]
[PRFISS]
[PRFISS2]
[PRENGSYS]
[PRBURN]
[PR-USERO]

****

PRFLOW	intercell flow model.
PRAER	detailed suspended aerosol inventories and short aerosol deposition summaries.
PRAER2	detailed suspended aerosol and aerosol deposition inventories.
PRLOW-CL	lower cell model.
PRHEAT	heat transfer structure model.
PRFISS	fission product mass and decay power summaries.
PRFISS2	detailed fission product mass inventories and decay power distribution.
PRENGSYS	engineered system model.
PRBURN	hydrogen and carbon monoxide burn model.
PR-USERO	user-implemented output from the USERO subroutine.

The user may specify as many of these keywords as desired. The associated output occurs only in the long edits. (See the section above for a discussion of the LONGEDT option.) A discussion of the output obtained with each of the above keywords is presented in Section 4.

The PR-USERO option gives the user additional flexibility in obtaining output. It controls output from the USERO subroutine, from which essentially any variable in the code can be accessed. The user must add coding to the USERO subroutine specifying the output and the format to be used. (See Section 4.1.3.10.)

3.2.7.3 Title. This block specifies a descriptive title for the problem, which forms the heading for every long edit and is also written to the plot file(s) for use in post-processing.

```
**************************************************************************

TITLE
    lines

**************************************************************************
```

TITLE	keyword used to mark the start of title information
lines	a number of entire lines containing title information. Such lines consist of a maximum of 80 characters, and all characters on the lines, including comments (&&) are incorporated into the title. Specify "ntitl" such lines.

3.3 Cell Input and Cell Control

The input needed to activate and control models that operate at the cell level in CONTAIN is addressed in the following sections. The structure of the cell input for one cell is illustrated in Figure 3-3. The entire cell level input set is repeated "ncells" times, one set for each cell defined for the problem.

The present section discusses the CELL keyword and the cell level CONTROL block, which are given first and second, respectively, in the cell level input for each cell. In addition, the optional TITLE option for the cell is discussed.

```
**************************************************************************

CELL ncell

**************************************************************************
```

CELL = ncell	the number of the cell to which the following input data blocks apply.

The cell number is followed by the CONTROL keyword and the cell CONTROL information block. The cell CONTROL block is used to allocate storage space based on the models invoked in the cell. The storage allocation parameters should be set to reflect the models that will be used at any time in the calculation, not just what might be used at the initiation of the problem. For example, if a lower cell is specified for the cell, and it does not initially have a pool layer, but it is anticipated that a pool layer will form in the course of the calculation, then the "jpool" parameter should be given a value of 1. This allocates the necessary storage space for the pool.

```
**************************************************************************

CONTROL
    [NHTM=nhtm] [MXSLAB=mxslab] [NSOPL=nsopl] [NSPPL=nsppl]
    [NSOATM=nsoatm]
    [NSPATM=nspatm] [NSOSPR=nsospr] [NSPSPR=nspspr] [NSOAER=nsoaer]
    [NSPAER=nspaer] [NSOFP=nsofp] [NSPFP=nspfp] [NAENSY=naensy]
    [NSOENG=nsoeng] [NSPENG=nspeng] [JCONC=jconc] [JINT=jint]
    [JPOOL=jpool]
    [NUMTBC=numtbc] [MAXTBC=maxtbc] [NRAYCC=nray] [NVFPSM=nvfpsm]
    [NSOSAT=nsosat] [NSPSAT=nspsat] [NSOSAE=nsosae] [NSPSAE=nspsae]
    [NSOSFP=nsosfp] [NSPSFP=nspsfp]
EOI

**************************************************************************
```

CONTROL — keyword to begin the specification of the cell level storage allocation.

NHTM = nhtm — number of heat transfer structures in the cell.

MXSLAB = mxslab — maximum number of nodes in any heat transfer structure.

NSOPL = nsopl — number of external sources to the lower cell layers.

NSPPL = nsppl — maximum number of entries in the lower cell source tables.

NSOATM = nsoatm — number of external sources to the upper cell atmosphere.

NSPATM = nspatm — maximum number of entries in the atmosphere source tables.

NSOSPR = nsospr — number of external spray fire sources.

NSPSPR = nspspr — maximum number of entries in the spray fire source tables.

NSOAER = nsoaer — number of external aerosol sources.

NSPAER = nspaer — maximum number of entries in the aerosol source tables.

NSOFP = nsofp — number of external fission product sources.

NSPFP = nspfp — maximum number of entries in the fission product source tables.

NAENSY = naensy — number of separate engineering systems to be defined in the cell.

NSOENG = nsoeng — number of engineered system sources.

NSPENG = nspeng — maximum number of entries in the engineered system source tables.

JCONC = jconc — designator indicating use of a concrete layer in the lower cell. Specify a positive integer if the concrete layer is used. If "jconc" is greater than 5, then "jconc" is taken to be the number of nodes in the single concrete layer; if "jconc" is positive but less than 5, the concrete layer will have 5 nodes.

JINT = jint — number of intermediate layers in the lower cell.

JPOOL = jpool — designator indicating use of the pool layer in the lower cell. Specify 1 if the pool layer is used.

NUMTBC = numtbc — number of cell level tables used for the cell. This number should take into account all of the tables used in the Q-VOL, HT-COEF, and FORCED options. (Such tables are considered to be at the cell level since these options are processed at that level.) Each such table defines one dependent variable in terms of an independent variable. These tables should not be confused with source tables, which have a different format and different control parameters.

MAXTBC = maxtbc — maximum number of entries in any cell level table used in the cell.

NRAYCC = nray — number of CORCON rays used to model the cavity.

NVFPSM = nvfpsm — the total number of coefficients, representing mass fractions, used to describe the composition of the VANESA constituent materials in terms of CONTAIN fission products. See the discussion of the FPTRACK keyword in Section 3.3.2.3.2.

NSOSAT = nsosat — number of SRV gas and vapor source tables.

NSPSAT = nspsat — maximum number of entries in the SRV gas and vapor source tables.

NSOSAE = nsosae — number of SRV aerosol source tables.

NSPSAE = nspsae — maximum number of entries in the SRV aerosol source tables.

NSOSFP = nsosfp — number of SRV fission product source tables.

NSPSFP = nspsfp — maximum number of entries in the SRV fission product source tables.

EOI — required keyword terminating the cell CONTROL block.

Unless otherwise specified, any positive integer can be assigned to each of the control variables. However, computational storage requirements can increase rapidly as the values assigned to the control variables increase.

The keyword and value pairs in the above template may be entered in any order but must be terminated by the keyword EOI. The default for each value is 0. (Only the nonzero values need be specified.)

Another format for the CONTROL block is available. This format is discussed in Appendix D.

The CONTROL block should be followed by either the GEOMETRY block, or else the cell TITLE block and then the GEOMETRY block. The cell TITLE block is discussed below, and the GEOMETRY block in the next section.

The cell title forms the heading for the output for the cell in the long edit:

```
*******************************************************************************

TITLE
    line

*******************************************************************************
```

TITLE — keyword identifying the next line as a cell title.

line — one line of title information, with up to 80 characters, describing the cell. Only one line of information is allowed for each cell.

The cell title is optional.

3.3.1 Upper Cell Input

3.3.1.1 Upper Cell Geometry. The following input block gives the geometry information for the upper cell.

```
*******************************************************************************

GEOMETRY volume height

*******************************************************************************
```

GEOMETRY — keyword to specify the upper cell geometry.

volume upper cell atmosphere volume. (m^3)

height characteristic height of the upper cell. (m)

The keyword GEOMETRY and the geometry variables must immediately follow the cell CONTROL block or else the TITLE block if TITLE follows CONTROL.

3.3.1.2 Upper Cell Atmosphere Initial Conditions and Sources. This block specifies the initial atmosphere conditions and atmosphere sources in the upper cell.

```
**************************************************************************

ATMOS nma pgas tgas (gas frac)
    [SOURCE=nso
        (oname=n
            [IFLAG=ival] T=(times) MASS=(masses)
            {TEMP=(temps) or ENTH=(enths)}
        EOI)]

**************************************************************************
```

ATMOS keyword to initiate input of atmosphere initial conditions and sources.

nma number of materials initially in the atmosphere. Specify at least one gas or the coolant vapor.

pgas gas pressure (Pa) or an input option flag. See the discussion below of the options available for the initial conditions.

tgas gas temperature. (K)

The following group of two variables is repeated "nma" times, once for each material initially present in the atmosphere:

gas material name; must be among those specified after either the COMPOUND keyword or the USERDEF keyword in the MATERIAL block.

frac molar fraction (dimensionless) or material mass (kg). (See the discussion below of the options available for the initial conditions.)

The keyword SOURCE may be used here to introduce any nonaerosol material declared after the COMPOUND keyword or USERDEF keyword in the MATERIAL block to the upper cell atmosphere. Sources of condensed phases of materials that are not aerosol components will be carried along in the atmosphere gas as homogeneously dispersed material. For a discussion of the keywords following SOURCE, see Section 3.4.

SOURCE keyword to initiate input of source information.

nso number of source tables to follow.

Three different types of input options for the initial conditions are available to give the user considerable flexibility. The option type depends on the sign of the "pgas" parameter. Only completely dry and/or saturated initial conditions are allowed in the first two options; arbitrary conditions are allowed in the third.

If "pgas" is specified to be positive, then "pgas" is taken to be the initial atmosphere pressure, "gas" should be the name of a gas or the coolant vapor, and "frac" should be the gas or vapor molar fraction. Furthermore, if the coolant vapor, H2OV or NAV, is specified as one of the gases, the atmosphere will be assumed to be at the dew point (saturation), and the input value of the coolant vapor molar fraction will be ignored. The coolant vapor fraction will be redefined internally as the value that will bring the atmosphere to the dew point. The other values of "frac" will be rescaled so as to bring the total to 1. If the coolant vapor is not specified as one of the gases, the sum of all values of "frac" will be renormalized to 1.0 if necessary, and the atmosphere will have the composition given by the renormalized molar fractions. The atmosphere will be completely dry.

If "pgas" is specified to be negative, "gas" should be the name of a gas or the coolant vapor, and "frac" should be the corresponding molar fraction. One of the gases specified must be the coolant vapor, and the corresponding value of "frac" must be positive and less than 1. If the sum of all the molar fractions is not 1, the fractions of the gases other than the coolant vapor are rescaled so that the sum of all molar fractions becomes 1. The pressure is calculated as the value that places the atmosphere at the dew point and gives a composition corresponding to the adjusted molar fractions. If no other gases are present, the coolant vapor fraction must be unity. Note that the CONDENSE option models the diffusion of the condensable through the noncondensable gas boundary layer at a structure surface. This process is not defined if noncondensables are not present.

In the two options above, acceptable names for "gas" are N2, O2, H2, CO2, HE, CO, AR, H2OV, NAV or the name of a gas defined through the user-defined material option.

If "pgas" is specified to be zero, "gas" may be the name of any nonaerosol or non-fission-product material, and "frac" is taken to be a material mass. The pressure is calculated from equations of state at the temperature "tgas".

3.3.1.3 Structure Characteristics. This block provides the characteristics of the heat structures modeled in the cell.

```
**************************************************************************

STRUC
        ([NAME=name]  TYPE=type   SHAPE=shape
        NSLAB=nslab   CHRLEN=chrlen
        [SLAREA=slarea]    [CYLHT=cylht]
        [IOUTER=iouter]    [TOUTER=touter]
        [VUFAC=vufac]
        {TUNIF=tunif or TNODE=(tnode)}
        COMPOUND=(cname)
        X=(xvalue)
    EOI)

**************************************************************************
```

The keywords in the structure input are defined as follows:

STRUC	keyword to begin the definition of structures.
NAME = name	optional user-selected name for the structure. The name may have up to eight characters. Note that although the name is optional within CONTAIN, it is used in the POSTCON post-processing code discussed in Section 4.1.
TYPE = type	name of the type of structure, which may be either ROOF, WALL, or FLOOR. These names refer to the orientation of the structure inner surface.
SHAPE = shape	name of the shape of the structure, which may be either SLAB, CYLINDER or SPHERE. See the discussion below for the actual shapes invoked by these names.
NSLAB = nslab	number of nodes in the structure. The number must be less than or equal to "mxslab", defined in the cell CONTROL block.
CHRLEN = chrlen	characteristic length of the structure to be used in the Grashof number for heat transfer. (m)
SLAREA = slarea	area of the structure if it is a slab. (m^2)
CYLHT = cylht	height of the structure if it is a cylinder. (m)
IOUTER = iouter	number of the cell adjacent to the outer surface of the structure. The number must be that of a cell in the problem.
TOUTER = touter	temperature of the gas adjacent to the outer face. Specify only if a cell in the problem is not specified to be adjacent to outer face and if nonadiabatic, fixed temperature boundary conditions on the outer face are desired. Note that a heat transfer coefficient will control the heat transfer between the outermost node and the gas, which will be at the temperature specified. An

adiabatic outer surface is assumed if neither IOUTER or TOUTER is specified. (K)

VUFAC = vufac — the parameter defined in Equation (2-60) for modeling radiation from the lower cell to the inner structure surface. Default = 0.

TUNIF = tunif — initial uniform temperature of the structure. (K)

TNODE — keyword to begin the specification of the initial temperature for each of the nodes of the structure. Use either TUNIF or TNODE, but not both.

tnode — the value of the initial temperature of a node. Specify "nslab" values, going from the inner to the outer node. (K)

COMPOUND — keyword to begin the specification of the material constituting each node. Each material must be among the materials specified after either the COMPOUND keyword or the USERDEF keyword in the MATERIAL block.

cname — the name of the material in a node. Specify "nslab" names,going from the inner to the outer node.

X — keyword to begin the specification of the position of each of the node interfaces.

xvalue — the position of a node interface. Specify "nslab"+1 values, going from the inner surface to the outer surface. For hemispherical or half-cylindrical structures, the position should be given in terms of the radial coordinate for the interface. The numerical values may be given in either ascending or descending order depending on which surface is to be considered the inner surface. (m)

EOI — end of input for the present structure.

The above keywords should be repeated for each of the "nhtm" structures declared in the cell CONTROL block.

The three allowed shapes for structures are SLAB, CYLINDER, and SPHERE. Cylinders and spheres are actually half-cylinders and hemispheres whose inner surfaces are defined as a ROOF, WALL, or FLOOR by the TYPE keyword. Thus, to model a whole cylinder or a complete sphere, two structures are required. Note that the outer face of a ROOF is a floor, and the outer face of a FLOOR is a roof. Radiative heat transfer from a lower cell to the outer face is not currently modeled. Neither condensation nor aerosol deposition is modeled on the outer face if the face is in another cell. The distinction between "inner" and "outer" is arbitrary. The "inner" face is the one whose node position is given first following the X keyword.

An alternative input format is given in Appendix D. The format above may be used in conjunction with the alternative one, provided the alternative format is placed first in the STRUC block.

3.3.1.4 Convection and Condensation. This block activates the surface condensation model for all structures in the cell. It also allows the user to specify forced-convection/condensation heat transfer for selected structures in the cell using the FORCED table option.

```
**************************************************************************

CONDENSE
    [FLMAX=flmax]
    [FORCED nmtb
            ([FLAG=iflag]
            X=n (x)
            VAR-Y=option
            Y=n (y)
        EOI)
    STR-COND nprs (istruc itabl)]

**************************************************************************
```

CONDENSE — keyword indicating that convective and condensation heat transfer to surfaces is to be modeled in the cell. If natural convection correlations and the default surface film depth are desired, this is the only entry required. In the absence of this keyword, heat transfer between the atmosphere and heat transfer structures is modeled with a constant (dry) heat transfer coefficient of 6.08 W/m^2-K.

FLMAX = flmax — the maximum condensate film depth. Default = 5.0×10^{-4}. (m)

The FORCED keyword activates the forced convection option for selected structures in the cell. The forced convection option utilizes a number of cell level tables to specify either the velocity, the Reynolds number, or the Nusselt number as a function of time. A given table is associated with a given structure through the STR-COND input discussed below. The definitions of the standard table keywords FLAG, X, and Y are given in Section 3.5. The other keywords and values associated with FORCED are defined below.

FORCED — keyword to specify that a number of forced convection tables follow.

nmtb — number of tables to be used with the FORCED option. The tables are numbered in the order that they are entered, the first being 1, the second 2, and so forth.

n — the number of points in the table.

x — the independent variable of the table, corresponding to time. Specify "n" values in ascending order. Note that outside of the range of times given in the table, natural

convection and not forced convection will be assumed to occur.

VAR-Y — keyword to specify the type of dependent variable represented by the table.

- option — character flag determining the dependent variable in the table. Specify either VELOCITY, REY-NUM, or NUS-NUM depending on whether velocity, Reynolds number, or Nusselt number is given by the table.
- y — the dependent variable of the table. Specify "n" values of velocity (m/s), Reynolds number, or Nusselt number depending on the choice made for "option".

EOI — keyword used to terminate each table.

STR-COND — keyword to specify the correspondence between the forced convection tables and the structures. Natural convection correlations are used for any structure for which a correspondence has not been established.

- nprs — the number of pairs of values of "istruc" and "itabl" to follow.
- istruc — the number of the structure associated with table "itabl". The structure number is determined by the order of input of structures in the STRUC input block.
- itabl — the number of the table containing the forced convection information for structure "istruc".

The keyword CONDENSE by itself enables condensation of coolant vapor on structures and the lower cell pool, if any. The growth of a condensate film on initially dry structure surfaces increases the thermal resistance to heat transfer. The optional keyword FLMAX allows the user to set the maximum film depth assumed for all structures in the cell; any excess condensate will either drain to a lower cell or be lost from the problem. That lower cell can be specified through the cell OVERFLOW option discussed in Section 3.3.1.11

The following is an example of the STR-COND input:

```
STR-COND 3  (1,1) (2,1) (3,2)
```

This input implies at least two tables and at least three structures. In this example, the first table defines the forced convection associated with the first and second structures, while the second table defines the forced convection associated with the third structure.

3.3.1.5 Radiation Input. The radiation model is activated at the cell level by the keyword RAD-HEAT. In the following descriptions, "nhtm" is the number of heat transfer structures in the cell as specified in the cell CONTROL block.

```
**************************************************************************

RAD-HEAT
    [EMSVT (emsvt)]
    [CESS]
    [{ABSORB absorb  or  KMX kmx}]
    {ENCLOS
        VUFAC (vufac)  [BEAML (beaml)]
    EOI
        or
    GASWAL gaswal
        or
    GEOBL (geobl)}
EOI

**************************************************************************
```

The following keywords control the gas and surface emissivities:

RAD-HEAT — keyword to begin the specification of the radiation model in the cell.

EMSVT — keyword to begin the specification of the dry surface emissivities.

emsvt — the dry surface emissivity. Specify "nhtm" values if no lower cell is present. Specify "nhtm"+1 values if a lower cell model is logically present in the cell, with the last value equated to emissivity, ϵ', of the uppermost lower cell layer. (The atmosphere or null layers are not taken into account in determining this layer.) A lower cell is logically present if space has been reserved for the lower cell model; i. e., if "jint" + "jpool" + "jconc" is greater than 0. Specify a corrected emissivity ϵ' if the GASWAL option is chosen (see the definition of ϵ' in Section 2.3.1.5.4); otherwise, specify a proper dry surface emissivity. If water is present on a surface, a value of 0.94 is used for the emissivity. If "emsvt" is not specified, all dry surface emissivities default to a value of 0.8.

CESS — keyword specifying use of the Cess-Lian correlation for the steam emittance (see Sec. 2.3.1.5.3). If this option is activated, carbon dioxide and carbon monoxide are treated as transparent gases and therefore do not participate in the radiative heat transfer. If CESS is not specified, the default Modak model is used for the gas emittance.

Two options are available for characterizing the contribution of the aerosols to the gas mixture radiative properties, as discussed in Section 2.3.1.5.2. The first option uses a constant user-specified absorption coefficient, "absorb", which is applied under all conditions. An alternative treatment of aerosol absorption uses a multiplier, "kmx", in an expression for the absorption coefficient which is proportional to the aerosol mass concentrations calculated by CONTAIN. In the model used in the latter option, small soot-like aerosols with a material density of

2000 kg/m^3 have been found to give a "kmx" of approximately one, as discussed in Section 2.3.1.5.2. If both options are specified, the ABSORB option will override the "kmx" option. If neither option is chosen, CONTAIN will use a value of zero for the aerosol absorption coefficient. (It should be noted that the scattering effects of aerosols are presently not treated.)

ABSORB = absorb — aerosol absorption coefficient. Default = 0. (m^{-1})

KMX = kmx — aerosol mass concentration multiplier. Default = 0.

The user can activate either a net enclosure model through the keyword ENCLOS or a simpler model through the keyword GEOBL or GASWAL. The net enclosure model treats multiple reflections correctly but does not consider the outer surfaces of structures within the cell. The simpler method treats reflections approximately but allows radiative heat transfer between the atmosphere and the inner and outer surfaces in the cell. Only one of these three keywords may be chosen.

ENCLOS — keyword to activate the net enclosure model.

BEAML — optional keyword to initiate the input of the upper triangle of the array of beam lengths.

beaml — beam length between two structure inner surfaces. Specify "beaml" between structure 1 and structures 2 through "nhtm" and then between 1 and the lower cell, if logically present. Then specify "beaml" between structure 2 and structures 3 through "nhtm" and so forth. The input corresponds to rows in the upper right triangle of an "nhtm" + 1 square matrix if the lower cell is present, and to the upper right triangle of an "nhtm" square matrix, otherwise. If the "beaml" input is omitted, a single value for each surface pair is calculated, using

"beaml" =

3.6*(cell volume)/(total inner surface area in cell).

VUFAC — keyword to initiate the input of the upper triangle of the array of view factors.

vufac — view factor from one surface to another surface. Specify the view factor from structure 1 to structure 2, and so forth, in the order used for "beaml". (The view factor from 1 to 2 corresponds to the fraction of radiation leaving 1 within the solid angle subtended by 2.) The lower triangle "vufac" is calculated automatically using the reciprocity relation for view factors:

area(1)*vufac(1 to 2) = area(2)*vufac(2 to 1)

The input corresponds to the upper triangle of an "nhtm" + 1 square matrix if the lower cell is logically present, and

to the upper triangle of an "nhtm" square matrix, otherwise. The sum of the elements in each column of the view factor matrix (including both user-specified elements and those calculated by CONTAIN from reciprocity) must equal 1. Thus, the user will generally need to perform side calculations with the above reciprocity relation to ensure that the constraint of the columns adding to 1 is satisfied.

EOI — terminates the net enclosure input.

GASWAL = gaswal — geometric mean beam length for the enclosure. If specified this single value has the effect of activating the simple atmosphere-to-structure radiation model. It is used for all structures and the uppermost lower cell layer.

GEOBL — keyword to activate the simple atmosphere-to-structure radiation model. Unlike the GASWAL keyword, the GEOBL keyword allows for a separate geometric beam length for each structure.

geobl — geometric beam length for a structure or the uppermost lower cell layer. As described above for the EMSVT input, "nhtm" values for "geobl" should be specified in absence of a lower cell and "nhtm" + 1 values if a lower cell is logically present.

EOI — keyword which terminates the RAD-HEAT radiation input block.

An obsolete radiation input format which uses the keyword RADIAT is also available. It should be noted, however, that only the simple radiation model and NOT the net enclosure model is available when this obsolete input format is exercised. Also, the Cess-Lian correlation is used as the default, as opposed to Modak, when using the RADIAT input option. The format of the RADIAT input block is given in Appendix D.

3.3.1.6 Heat Transfer Control Options. This block allows the user to activate or deactivate certain heat transfer mechanisms.

```
**************************************************************************

HT-TRAN htflag1 htflag2 htflag3 htflag4 htflag5

**************************************************************************
```

An ON or OFF value must be specified for each of the five flags following HT-TRAN. These flags control the heat transfer between the entities described below.

HT-TRAN — keyword to begin specification of the heat transfer control flags

htflag1 — atmosphere to structures for all heat transfer processes.

htflag2 — first non-null layer in the lower cell to the basemat, which is assumed to be at constant temperature "txl" (See Section 3.3.2.1).

htflag3 — between two adjacent layers in the lower cell. The heat transfer to the basemat or the atmosphere layer is not controlled by this flag.

htflag4 — uppermost lower cell layer to the upper cell for all heat transfer processes. The uppermost layer by definition is not the atmosphere layer or a null layer.

htflag5 — radiative transfer from the lower cell to the upper cell and from the atmosphere to structures. In case of conflict between "htflag5" and "htflag1" or "htflag4", the latter flags take precedence.

The processes controlled by each of the flags are discussed more fully in Section 2.3.1.6. If this optional block is not selected, then all flags are set to ON. If one or more of the heat transfer mechanisms are to be turned off, then all five flags must be included in the input.

Example: HT-TRAN OFF ON OFF OFF ON

3.3.1.7 Hydrogen and Carbon Monoxide Burn Input. This optional block activates the hydrogen and carbon monoxide combustion model in CONTAIN.

```
**************************************************************************

H-BURN
    [BURNT=burnt]   [CHRL=chrl]     [FLAM=flam]
    [CFRMNG=cfrmng] [MORMNG=mormng]
    [ELEV=elev]     [KPROP=kprop]   [MFCIG=mfcig]   [MFOIG=mfoig]
    [MFSIG=mfsig]   [MFCDN=mfcdn]   [MFODN=mfodn]   [MFSDN=mfsdn]
    [MFCHZ=mfchz]   [MFOHZ=mfohz]   [MFSHZ=mfshz]   [MFCUP=mfcup]
    [MFOUP=mfoup]   [MFSUP=mfsup]   [TACTIV=tactiv] [TDEACT=tdeact]
[EOI]

**************************************************************************
```

H-BURN — keyword to activate the combustion model.

BURNT = burnt — compartment burn time. Default = internally calculated value. (s)

CHRL = chrl — compartment characteristic length. Default = cube root of cell volume. (m)

FLAM = flam — flame speed. Default = internally calculated value. (m/s)

CFRMNG = cfrmng — fraction of the initial amount of combustible remaining after the burn. Default = internally calculated value.

MORMNG = mormng — mole fraction of oxygen remaining after the burn. Default = 0.005.

ELEV = elev — compartment elevation used only in the burn model to determine the relative positions of the cells for burn propagation. Default = 0. (m)

KPROP = kprop — propagation delay factor. A burn will be allowed to propagate to another cell after a time "kprop"*"burnt" has elapsed after the start of the burn, if the conditions in that cell are suitable. A burn will not propagate after the time "burnt" has elapsed. Default = 0.5.

MFCIG = mfcig — mole fraction of combustible for ignition. Default = 0.07.

MFOIG = mfoig — mole fraction of oxygen for ignition. Default = 0.05.

MFSIG = mfsig — mole fraction of steam plus carbon dioxide for inerting. Default = 0.55.

MFCDN = mfcdn — mole fraction of combustible in adjacent cells for propagation down. Default = 0.09.

MFODN = mfodn — mole fraction of oxygen in adjacent cells for propagation down. Default = 0.05.

MFSDN = mfsdn — mole fraction of steam plus carbon dioxide in adjacent cells for inerting against propagation down. Default = 0.55.

MFCHZ = mfchz — mole fraction of combustible in adjacent cells for propagation horizontally. Default = 0.06.

MFOHZ = mfohz — mole fraction of oxygen in adjacent cells for propagation horizontally. Default = 0.05.

MFSHZ = mfshz — mole fraction of steam plus carbon dioxide in adjacent cells for inerting against propagation horizontally. Default = 0.55.

MFCUP = mfcup — mole fraction of combustible in adjacent cells for propagation up. Default = 0.041.

MFOUP = mfoup — mole fraction of oxygen in adjacent cells for propagation up. Default = 0.05.

MFSUP = mfsup — mole fraction of steam plus carbon dioxide in adjacent cells for inerting against propagation up. Default = 0.55.

TACTIV = tactiv — time to activate burns. Default = -1×10^{30}. (s)

TDEACT = tdeact — time to deactivate burns. This time must be larger than "tactiv". Default = 1×10^{30}. (s)

EOI — terminates the H-BURN block. The EOI may be omitted if just the H-BURN keyword is specified.

The keyword H-BURN must be included if hydrogen or carbon monoxide burns are desired in a problem. The other keywords and associated variables need to be input only if the defaults are to be overridden.

The user should note that the default option to have the code calculate "cfrmng", the fraction of the initial combustible remaining, may be incompatible with a mole fraction of combustible for ignition which is too low. For a mole fraction for ignition of less than 0.0376, the correlation for burn completeness used in the code may return a fraction of initial combustible of unity, which may result in nothing being burned. The user must specify "cfrmng" through the keyword CFRMNG for a mole fraction for ignition of less than 0.0376.

The keyword CFRMNG serves the same function as the obsolete (but upward compatible) keyword HFNL. The keyword HFNL implies a final hydrogen concentration rather than final fraction of initial hydrogen and is therefore not recommended.

3.3.1.8 Aerosol Initial Conditions and Sources. This optional block specifies initial aerosol component masses and aerosol sources in the cell.

```
**************************************************************************

AEROSOL=[naero (omat mass)]
    [SOURCE=nso
        (oname=n
            IFLAG=ival
            T=(times)
            MASS=(masses)
        EOI)]

**************************************************************************
```

AEROSOL — keyword to begin the specification of initial masses and sources in the cell.

naero — number of aerosol components which have nonzero initial suspended mass. Default = 0.

The following group of two variables is repeated "naero" times:

omat — name of an aerosol component material specified in the global AEROSOL block.

mass — initial total mass of the aerosol component. The initial particle size distribution will be governed by the "amean", "avar" parameters specified in the global AEROSOL block, as discussed in Section 3.2.4. (kg)

Aerosol source tables are optional. If desired, they are initiated by the SOURCE keyword. Note that SOURCE and the keywords that follow use a standard notation for source tables discussed in Section 3.4. The particle size distribution of the aerosol mass introduced through the source tables is governed by the "amean" and "avar" parameters discussed in Section 3.2.4.

SOURCE optional keyword to initiate the input of aerosol sources.

nso the number of source tables to follow. (The input from "oname" to EOI should be repeated "nso" times.)

oname name of the aerosol component material to be introduced by the table.

n number of source table points.

The other keywords and values are described in Section 3.4. Note that TEMP or ENTH is not used for aerosols.

3.3.1.9 Fission Product Sources. This optional block is used to specify fission product source tables.

```
**************************************************************************

FISSION
    SOURCE=nso
        (oname=n
            [IFLAG=ival] [HOST=i]
            [CHAIN=j]
            T=(times)
            MASS=(masses)
        EOI)

**************************************************************************
```

Note that many of the keywords and values used above follow a standard notation for source tables discussed in Section 3.4.

FISSION keyword to initiate the specification of fission product source tables.

SOURCE keyword which must immediately follow FISSION.

nso number of fission product source tables. (The parameters from "oname" to EOI should be repeated "nso" times.)

oname name of the fission product that is to be introduced by the table. It should be a name specified in the global FISSION input block.

n number of table points.

HOST keyword to specify to which host the fission product should be attached.

i an integer indicating the host to which the mass introduced by the table will be attached. Hosts are arranged in the following order: the upper cell atmosphere gas host, "nac" aerosol hosts in the order specified in the global AEROSOL input block, the inner surface host and the outer surface host for each structure, and one host for every lower cell layer. An additional DUMMY host is also provided after the

lower cell hosts for miscellaneous targeted release and acceptance purposes. The structure hosts are arranged with the inner surface of structure 1 first, the outer surface of structure 1 second, and so forth. The structure number is determined by the order in which the structures are given in the STRUC input. The lower cell hosts are arranged with the bottommost layer first, the layer above it second, and so forth. The atmosphere layer is counted as a host if other lower cell layers are present. Since there may be many structures and/or lower cell layers in a given cell, care should be taken when specifying host numbers for nonairborne hosts. Furthermore, old input decks with sources for nonairborne fission product hosts should be examined for correctness since the fission product host numbering scheme has undergone a non-upward-compatible evolution.

CHAIN — keyword to specify the decay chain which is to receive the fission product mass. This keyword is required only when the same fission product name appears more than once in the linear chain decomposition (as a result of branching or merging decays). If CHAIN is not given then the first chain containing the fission product "oname" will receive the mass introduced by the table.

j — an integer between 1 and "nchain" that indicates which decay chain will be searched for the specified fission product "oname" (see Section 3.2.5).

The definitions of keywords and values not given above are discussed in Section 3.4. Note that the effects of decay on source material prior to the time of source will not be calculated by CONTAIN. For example, for a two-element decay chain representing F1 decaying into F2, one must generally specify a source of both F1 and F2 in the ratio appropriate to the time of the source, even if only F1 was present initially.

The decay and power characteristics are specified in the global input under the FISSION keyword. Initial fission product masses and release and acceptance parameters are specified in the cell input under the FPM-CELL keyword as described in the following section.

3.3.1.10 Fission Product Initial Conditions and Release Rates. The optional FPM-CELL block is used to specify initial fission product masses on the hosts within a cell. User-specified host-to-host transfer rates for fission products within the targeted release and acceptance model are also defined in this input block. An obsolete nontargeted release and acceptance model is also available, as described in Appendix D.

```
**************************************************************************

FPM-CELL
    [(HOST = hname (masses))]
    [TARGET
        (fpname aval  bval  tth
            (FROM=rname
                TO=aname))
    EOI]
EOI

**************************************************************************
```

FPM-CELL — keyword to initiate the specification of fission product initial masses and user-specified host-to-host transfers of fission products.

HOST — keyword to initiate the input of fission product initial masses for a given host.

hname — a simple name or a name and qualifier that identify the host to which the fission product mass will be assigned. Valid simple names are: GAS, "aername", "strname", and DUMMY, where "aername" is a valid aerosol component name and "strname" is the name of a structure in the cell (the inner surface is the indicated host in this case). The DUMMY host is used for miscellaneous release and acceptance purposes. Names with qualifiers may be used in the following combinations: INNER "strname", OUTER "strname", AEROSOL "aername", AEROSOL "n", LAYER "n", and LAYER POOL. The INNER and OUTER qualifiers are used to specify a particular side of a given structure since each structure is a double host. Either a name ("aername") or a number ("n") may follow the AEROSOL word to specify an aerosol component. Only the pool layer may be accessed by name as shown above; all other lower cell layers must be denoted by LAYER followed by a number, "n". Layers are numbered beginning with 1 at the bottom. Three more simple names, ROOF, WALL, and FLOOR, are also accepted. These generic names refer here to all inner surfaces of structures of type ROOF, WALL, and FLOOR, respectively, and certain outer surfaces of structures of type FLOOR, WALL, and ROOF. To be considered among one of the generic surface types, an outer surface must be defined to be within the cell in which the structure is defined.

masses — initial mass of each fission product associated with the host specified by "hname". Exactly "nfce" values must be specified (one for each chain element). (kg)

TARGET — keyword to initiate input of targeted release and acceptance parameters for the cell. Note that the parameter "ntgt" in the global CONTROL block must be set to use this option. (See Section 3.2 and the discussion below.)

fpname — name of the fission product to which the targeted release and acceptance parameters apply. The transfer rates specified in this block for "fpname" are applied to all fission chain elements corresponding to "fpname" in the linear chain decomposition. (Multiple occurrences of "fpname" may arise as the result of branching or merging decays.)

aval — the multiplicative coefficient "a" in the temperature-dependent release rate given by Equation (2-20). The value of a may be negative. In that case, it is interpreted as shown in that equation. (s^{-1})

bval — the exponential factor "b" in the release rate given by Equation (2-20). (K)

tth — the host threshold temperature below which the release rate will be set to zero (see Equation (2-20)). (K)

FROM = rname — "rname" is nominally the releasing host in a targeted transfer; "rname" must obey the same rules as outlined above for "hname." Note that if "rname" is one of the generic surface names ROOF, WALL, or FLOOR, multiple target equations will be generated and the number "ntgt" in the global CONTROL block must be set as discussed below.

TO = aname — "aname" is nominally the receiving host in a targeted transfer; "aname" must obey the same rules as outlined above for "hname" and "rname". In order to simplify input for large problems, FROM/TO pairs may be repeated for a given fission product without repeating "fpname", "aval", "bval", and "tth" as long as these parameters do not need to be changed. The TO keyword must follow the FROM keyword. Note that use of a generic surface name for "aname" will also generate multiple target equations, and in such a case, the number "ntgt" in the global CONTROL block must be set as discussed below.

EOI — terminating keyword used at the end of the TARGET block and also at the end of the entire FPM-CELL block.

Note that the keyword HOST should appear once for each host which has finite initial fission product masses. The keyword TARGET should appear only once in each FPM-CELL block, and only one FPM-CELL block should appear in the input for a given cell.

The following discussion applies only to TARGET input involving the generic fission product host names ROOF, WALL, and FLOOR. In situations where "rname" and/or "aname" are ROOF, WALL, or FLOOR, the following guidelines should be followed to determine the smallest allowable value of "ntgt" in the global control input block. Note that the generic meaning of these names will apply even if ROOF, WALL, or FLOOR is used in an attempt to reference a single structure that happens to be named either ROOF, WALL, or FLOOR. Consequently, structures named ROOF, WALL, or FLOOR cannot be explicitly referenced in the targeted release model to release or accept fission products. Thus, cell structures should not be

named ROOF, WALL, or FLOOR if explicit reference to them in the targeted release input is desired.

Two variables, nl and n2, are used to assist in the following description. If either ROOF, WALL, or FLOOR is specified as the FROM host, the value of "nl" is the number of structure surfaces of the corresponding orientation in the cell. The inner surface of a structure of type ROOF, WALL, or FLOOR has an orientation corresponding to the structure type. The outer surface has an orientation of the opposite type (i.e., FLOOR, WALL, and ROOF) and is included among surfaces of that orientation if the outer surface is in the cell in which the structure is defined. (Note that while ROOF, WALL, and FLOOR refer here only to certain surfaces within the cell, the outer surfaces of structures are always hosts regardless of the cell specified or boundary condition used.) If the FROM host is not ROOF, WALL, or FLOOR, the value of "nl" is one. Identical guidelines apply to the name of the TO host in determining the value of "n2". The number of equations associated with a given FROM/TO pair is given by the product of "nl" and "n2". If multiple FROM/TO pairs are specified without repeating "fpname", this product should be formed for each pair. The sum of all "nl"*"n2" products for one "fpname" is then multiplied by the number of chain elements that are named "fpname". The sum of such values for each "fpname" in the targeted release input for all cells is the smallest allowed value for "ntgt".

Fortunately, "ntgt" does not have to be exactly equal to the number of targeted release equations; instead, it is only required that "ntgt" not be smaller than this number. For this reason, it is highly recommended that "ntgt" not be computed when complex targeted release and acceptance input is used. Instead, it is recommended that a large value (e.g., 1000) be specified. The fission product input routine will report an error message if "ntgt" is too small to run the problem.

3.3.1.11 Cell Overflow. This input block is used to specify the cell to which condensate runoff from structures and aerosols lost from the aerosol size mesh are diverted. The condensate runoff and the fission products associated with the runoff are transferred to the pool of the overflow cell, if it is present, or lost from the problem. As discussed in Section 2.2.5.5, the amounts of fission products transferred with the runoff are determined through the "fpliq" transport efficiency factors. The "fpliq" values are assigned in the FPLIQUID input block described in Section 3.2.5.1. The treatment of aerosol mesh losses and the fission products associated with those losses is discussed in Section 2.2.4.2.

****

OVERFLOW=novcel

****

OVERFLOW= novcel — an integer giving the destination cell for overflow masses consisting of aerosol mesh losses, condensate runoff from structures, and fission products transported with the condensate runoff. The absolute value of this integer should be either zero or the cell to which the overflow masses are to be transferred. A value of zero will cause all transfers of the overflow masses to be lost from the problem,

although the cumulative amounts of overflow will still be reported. A negative number indicates that aerosols which become undersized are to be returned to the smallest size class. Caution: when aerosols are returned to the smallest size class, the cumulative amount of aerosols reported in the underflow bin may count the same mass more than once and thus should not be used for mass conservation checks.

NOTE: The cell OVERFLOW option should not be confused with the ESF OVERFLOW component which models liquid transfers between lower cell pools.

3.3.2 Lower Cell Input

The cell level keyword LOW-CELL activates the input for the lower cell models. The lower cell consists of a series of layers in the bottom of a cell. The following layer types are considered: a concrete layer, multiple intermediate layers, a pool layer, and an atmosphere layer. For all but the atmosphere layer, a set of physics modeling options can be activated through input in the LOW-CELL block. The initial configuration of the layers and initial material masses are also specified in this input block. The atmosphere layer is used as an interface between the lower cell and the upper cell; therefore, it is automatically created and requires no user input.

Due to the complexity of the lower cell models, the lower cell input can often be quite extensive. This is particularly true when the CORCON and VANESA models are specified. The lower cell input descriptions are therefore given at two levels of detail. The first level of detail shows the overall structure of the lower cell input. This level of detail is most useful for determining the order of the major subblocks in the lower cell input (see Section 3.3.2.1 below). The second level of detail gives the minor subblocks within each major subblock. Complete descriptions of each keyword in the major and minor subblocks are given in the detailed descriptions. These descriptions are given in separate sections beginning with Section 3.3.2.2. The descriptions of the CONCRETE and INTERM input blocks are further subdivided into problems without CORCON modeling of core-concrete interactions and those with CORCON.

3.3.2.1 Overall Lower Cell Input Structure. There are two general classes of problems that can be modeled with the lower cell capabilities. The first such class consists of problems in which there are no explicitly modeled core-concrete interactions and the CORCON model is not active. Lower cell modeling is confined to heat transfer effects in such problems. The second class consists of problems in which core-concrete interactions are modeled with CORCON. In these cases the VANESA model may also be activated. The overall lower cell input structure given below applies to both general classes of lower cell modeling.

Only the major lower cell subblocks are shown in this section. These major subblocks include the subblocks that define the three possible types of layers (concrete, intermediate, and pool) in the lower cell. Layers in the lower cell are defined from the bottom to the top of the cavity, with the bottom layer given first in the input, the next layer up given second, and so forth. In the following, the order of layers from bottom to top is assumed to be the concrete layer, if present, then the

intermediate layer(s), if present, and then the pool. This order applies to both general classes of problems.

```
**************************************************************************

LOW-CELL
    GEOMETRY carea
        BC txl
        [DECAY-HT
             (data)
        EOI]
        [CONCRETE
             (data)
        EOI]
        ([INTERM
             (data)
        EOI])
        [POOL
             (data)
        EOI]
EOI

**************************************************************************
```

The major subblock keywords are GEOMETRY, BC, DECAY-HT, CONCRETE, INTERM, and POOL. A brief description of these blocks and their usage in the two general classes of problems is provided below. The required GEOMETRY and BC input blocks are described in detail at the end of this section. More complete input descriptions of the optional DECAY-HT, CONCRETE, INTERM, and POOL input blocks are given in Section 3.3.2.2 through Section 3.3.2.5, respectively.

The CONCRETE layer input block is described in detail in Section 3.3.2.3. If the CORCON model is used, a concrete layer is required to specify the concrete type and other CORCON model parameters, including the starting time for the interactions. If CORCON is not specified, the concrete layer is optional but may be specified with respect to initial material masses and other parameters for the modeling of conduction heat transfer. Input for problems not involving CORCON is described in Section 3.3.2.3.1, and input for those involving CORCON is described in Section 3.3.2.3.2.

The INTERM intermediate layer input block is described in detail in Section 3.3.2.4. If the CORCON model is specified, only one intermediate layer may be defined. This single CONTAIN intermediate layer is used to initialize the CORCON melt layers. If CORCON is not specified, multiple intermediate layers may be specified. Each such layer will be included in the heat transfer modeling. Input for problems not involving CORCON is described in Section 3.3.2.4.1, and input for those involving CORCON is described in Section 3.3.2.4.2.

The POOL layer input block is described in detail in Section 3.3.2.5. A pool layer may be specified in any problem with a lower cell. The pool layer is used as a repository for coolant in the lower cell. Even if coolant is not initially present in a problem, the pool layer should be specified if coolant is expected to accumulate in the lower cell. A pool layer is also required if coolant boiling is to be modeled.

The layers specified will depend on the problem being analyzed. Only those expected to play a role in the analysis need be specified in the input. If a layer is initially empty, but could be created in the course of the calculations (or through user-specified material sources), then it should be specified in the lower cell input. With the exception of the intermediate layer used with CORCON, any layer may have zero initial mass. With CORCON, the user should specify the CORCON layer compositions at the CORCON start time through the intermediate layer input. Materials may thereafter be introduced into the CORCON layers to reflect time-dependent additions to the debris.

Detailed descriptions of the GEOMETRY and BC subblocks are given below.

GEOMETRY = carea — the area of the layers in the lower cell. This area should be given immediately after the LOW-CELL keyword. If CORCON is not specified, "carea" is used for heat transfer between all layers in the lower cell. If core-concrete interactions are modeled with CORCON, "carea" is only used in modeling the transfer of heat to the coolant pool, and other aspects of the geometry of the cavity are specified with the GEOMETRY keyword in the CORCON subblock of the CONCRETE layer input (see Section 3.3.2.3.2). (m^2)

BC = txl — the basemat boundary condition temperature. The basemat is defined as the region below the bottommost layer in the lower cell and is assumed to be at a constant temperature "txl". This constant temperature boundary condition is used only if CORCON is not active. (For upward compatibility, an obsolete pressure boundary condition value, "pbot", may be given immediately after "txl". The "pbot" value is no longer used by the code, and any value entered will be ignored.) (K)

3.3.2.2 Makeup Decay Power. This optional block activates the ANSI-standard decay power model used by CONTAIN. It may be utilized in any number of cells. If DECAY-HT input has been defined in more than one cell, the total reactor power is the sum of the "rpwr" values in each cell. The general structure of the DECAY-HT input block and detailed descriptions of the DECAY-HT input options are given below.

```
**************************************************************************

DECAY-HT rpwr
    DIST-PWR (dpwr)
    [Q235U=q235u] [Q238U=q238u]   [Q239PU=q239pu] [P235U=p235u]
    [P238U=p238u] [P239PU=p239pu] [R239U=r239u]   [ROPT=ropt]
    [TTOSD=ttosd] [PSCALE=pscale]
EOI

**************************************************************************
```

DECAY-HT — keyword to begin the specification of parameters for the decay power model.

rpwr — the reactor thermal power associated with the current cell. This is part or all of the nominal power at which the

reactor operated in the time period prior to shutdown. Values of this quantity for all cells will be summed to obtain the total reactor power. (W)

DIST-PWR — keyword to initiate input of the power distribution fraction for each layer in the lower cell.

dpwr — fraction of the makeup decay power to be allocated to each layer in lower cell. Exactly one fraction must be specified for each layer, including the atmosphere layer, which is always considered present. The specified fractions apply to the concrete layer, each intermediate layer, the pool layer, and the atmosphere layer, in that order. If a layer has no mass, the power distribution fractions are renormalized by the code to those layers with mass. Default = 0.

Q235U = q235u — total recoverable energy per fission for U-235. Default = 199.27. (MeV/fission)

Q238U = q238u — total recoverable energy per fission for U-238. Default = 199.59. (MeV/fission)

Q239PU = q239pu — total recoverable energy per fission for Pu-239. Default = 210.48. (MeV/fission)

P235U = p235u — fraction of reactor power generated from U-235. Default = 0.6716.

P238U = p238u — fraction of reactor power generated from U-238. Default = 0.0421.

P239PU = p239pu — fraction of reactor power generated from Pu-239. Default = 0.2863.

R239U = r239u — ratio of U-239 atoms produced per fission at time of shutdown. Default = 0.53.

ROPT = ropt — reactor operating time prior to problem start time. The reactor is assumed to have been at full power during operation. Default = 5.05×10^7. (s)

TTOSD = ttosd — time of reactor shutdown (should be prior to problem start time.) Default = 0. (s)

PSCALE = pscale — reactor power scale factor. Default = 0.947.

EOI — terminates the DECAY-HT input.

If the required DIST-PWR input is not specified, the default power distribution fractions of zero will be used. The makeup power would thus be lost from the problem. Note that a portion (or all) of the makeup power may be directed to the upper cell atmosphere by setting the atmosphere layer fraction to a nonzero value.

The DECAY-HT option may be used in conjunction with the CORCON model only if time-dependent core debris sources are not used. The internally computed CORCON decay heat (see CORESTAT and DKPOWER in Section 3.3.2.4.2) will be normalized to the value computed by the makeup decay power model.

3.3.2.3 Concrete Layer. The configuration of the lower cell concrete layer is specified in the CONCRETE block. If core-concrete interactions are being modeled with CORCON, the CONCRETE input block is also used to specify the concrete type and various other input parameters for the CORCON and VANESA models. If CORCON is not used, the CONCRETE input block is used to define the initial layer masses, temperatures, user-specified sources, and heat transfer coefficients. The following two sections give the overall input structure for the CONCRETE block for both general classes of lower cell modeling.

3.3.2.3.1 Concrete Layer Input Without CORCON. The structure shown below applies to problems in which core-concrete interactions are not explicitly modeled with CORCON. Such problems involve the modeling of heat transfer in the lower cell.

```
*************************************************************************

CONCRETE
    [COMPOS=nma (omat cmass)]
    TEMP=ctemp
    [DELTA-Z=cdzin]
    [PHYSICS
        [SOURCE=nso
            (oname=n IFLAG=ival
                T=(times) MASS=(masses)
                {TEMP=(temps) or ENTH=(enths)}
            EOI)]
        [Q-VOL
            [FLAG=iflag]
            X=nq (timeq)
            Y=nq (qvol)
        EOI]
        [HT-COEF
            [FLAG=iflag]
            NAME=olay
            VAR-X=oxopt
            X=nh (xhtval)
            Y=nh (htcoef)
        EOI]
    EOI]
EOI

*************************************************************************
```

CONCRETE — keyword to initiate the definition of the concrete layer.

COMPOS — keyword to initiate the specification of initial material masses in the concrete layer. If this keyword and its associated input are omitted, the concrete layer will be initially empty.

nma — number of materials (including CONC) initially present in the concrete layer.

omat — name of a CONTAIN material being specified as initially present in the concrete layer. This name must be among the materials specified either after the COMPOUND or USERDEF keyword in the MATERIAL input block. In most instances, at least one "omat" name will be CONC for concrete; other materials may also be included in the concrete layer to simulate steel rebar or other constituents. Note that the specific concrete types discussed in the next section under the CONCRETE keyword are only used in the CORCON and VANESA models. For upward compatibility, input for a specific concrete type may still be given here. However, the code will substitute the CONC material for that specific concrete if this is done.

cmass — initial mass of material "omat" in the layer. If DELTA-Z is not specified, this mass will be equally divided among the nodes in the concrete layer. By default the thicknesses of the nodes and the entire concrete layer are determined by the code from the volume occupied by the materials and the area "carea" of the layer. (kg)

TEMP = ctemp — required initial temperature of the concrete layer. (K)

DELTA-Z = cdzin — optional initial concrete node thickness. If this option is used, initial material masses in the layer will be uniformly loaded into each node from the bottom to the top until either each node has been filled, or all initial mass has been exhausted. In the latter case, some of the top nodes will be empty and will therefore be excluded from the heat transfer modeling. The number of nodes corresponds to the larger of 5 or "jconc". This option is useful for fixing the initial thickness of the concrete layer as opposed to the mass. (m)

PHYSICS — keyword to initiate input of the layer physics options. This keyword is required if any of the options described below are selected.

The SOURCE subblock for specifying materials to be introduced into the CONCRETE layer uses a standard notation. The SOURCE keywords and values not discussed below are defined in Section 3.4.

SOURCE — keyword to initiate input of material source tables for the layer.

oname — name of the material to be introduced. It should be the name of a material specified after the COMPOUND keyword or USERDEF keyword in the MATERIAL input block. The material does not have to be present initially in the layer.

The Q-VOL and HT-COEF blocks use cell level tables that require the user to set appropriate values for "numtbc" and "maxtbc" in the cell CONTROL block.

The standard table keywords X, Y, NAME, VAR-X, and FLAG are defined in Section 3.5. The variables associated with Q-VOL and HT-COEF are defined below.

Q-VOL — keyword to begin the specification of a volumetric heating table. (This option should not be confused with the DECAY-HT option.) Only one Q-VOL table may be specified in a given layer.

- nq — number of points in the Q-VOL table.
- timeq — the independent variable of the Q-VOL table, which corresponds to time. Specify "nq" values in ascending order. Note that the heating is set to zero if the time is outside of the range of the table. (s)
- qvol — the volumetric heating rate of the layer. Specify "nq" values. (W)

HT-COEF — keyword to begin the specification of a heat transfer coefficient table. Within the range of the table, the table values will override an internally calculated heat transfer coefficient. Outside of the range, the internally calculated coefficient will be used. The applicable heat transfer coefficient may be that between the present layer and one above it or between the present layer and the basemat. The independent variable name "oxopt" and the name "olay", which specifies the boundary to which the heat transfer coefficient applies, must be specified. Only one HT-COEF table may be specified for a given layer.

NAME — keyword to specify the boundary to which the heat transfer coefficient table applies.

- olay — either the name of a layer above the present layer or the word BAS-MAT. The table values will be applied (1) when the present layer is not a null layer and (2) when the layer specified is not a null layer and is physically adjacent to the present layer or, in the case of the basemat, when the basemat is physically adjacent to the present layer. (Null layers between the present layer and the layer considered physically adjacent.) Intermediate layer names are given after the LAY-NAM keyword (see Section 3.3.2.4). Other layer names match the type of the layer (i.e., CONCRETE, POOL, and ATMOS).
- oxopt — a character flag that indicates the type of independent variable represented by "xhtval". Replace with either TIME, TEMP, or DELTA-T. These choices represent time, temperature, or temperature difference across the boundary.
- nh — the number of points in the heat transfer coefficient table.
- xhtval — the independent variable of the table. It represents either time (s), temperature (K), or temperature difference (K).

The temperature difference is defined as the temperature above the boundary at which the heat transfer coefficient applies minus the temperature below the boundary. Note that if the time, temperature, or temperature difference at a given point in time lies outside of the range of the table, the internally calculated heat transfer coefficient will be used. Specify "nh" values in ascending order.

htcoef — the dependent variable of the table, which represents the heat transfer coefficient across the boundary specified by "olay". (W/m^2-K)

EOI — input block terminator.

3.3.2.3.2 Concrete Layer Input With CORCON. The overall input structure for the CONCRETE input block when core-concrete interactions are modeled with CORCON is given below. The SOURCE, Q-VOL, and HT-COEF physics options are not given in this summary, since they have no effect on the calculation when CORCON is active. These options may however be specified, since they will affect the heat conduction model that is active before CORCON begins and after CORCON completes. Input descriptions for these options are given in the previous section. Time-dependent sources of core debris to CORCON may be specified by the user in the required CORCON intermediate layer (see Section 3.3.2.4.2).

```
**************************************************************************

CONCRETE
    COMPOS=1
        (CONCRETE=otyp
                    [[TSOLID=tsolct] [TLIQID=tliqct] [RHOCON=rhoc]
                    [REBAR=rbr] [TABLAT=tabl] [EMCONC=ew]
                EOI]
            cmass     or
        CONCRETE
            OTHER fsio2 ftio2 fmno fmgo fcao fna2o fk2o ffe2o3
            fal2o3 fcr2o3 fco2 fh2oe fh2ob tabl efusn
                        TSOLID=tsolct TLIQID=tliqct RHOCON=rhoc
                        [REBAR=rbr] [EMCONC=ew]
                    EOI
                cmass)
    TEMP=ctemp
    [PHYSICS
        [CORCON
            TIMES tstart ndelt (dtmin dtmax dedit timdt)
            GEOMETRY ro zo
                (HEMICYL rs hc rw hbc  or
                FLATCYL zt rad hit radc rw hbb nbot ncorn  or
                ARBISHP nbot rtang rw htotl (ri zi))
            EMISIV
                OXIDE oflag neo  (tort1 eo)
                METAL oflag nem  (tort2 emm)
                [SURRND oflag ns (tort6 es)]
            EOI
            [MOVIES]
```

```
            [MMCHEM]
        EOI]
        [VANESA
            EDITDELT=vdtedt
            {CONCCOMP=otypv          or
            CONCCOMP=
                OTHER fcao fal2o3 fna2o fk2o fsio2 ffeo}
            [REBAR=ffe] [FDELT=fdelt] [DIFCO=difco]
            [BUBD=bubd] [PTBB=ptbb] [PTDIA=ptdia]
            [AERCONST=numaer (aername ncnams (ovnam))
                [FPTRACK
                    {SIMPLE=nvanfp (ovnam) or
                    DETAIL=nvcons (ovnam nfp (ofpnam wfrac ohost))}]]
            {[MELTCOMP (cmelt)]  or
            [CES=ces] [KRY=kry] [SN=sn] [ZR=zr] [FEO=feo] [RB=rb] [RH=rh]
            [CE=ce] [SM=sm] [MN=mn] [SB=sb] [IOD=iod] [TE=te] [RU=ru]
            [ZRO2=zro2] [MO=mo] [Y=y] [PD=pd] [PR=pr] [PU=pu] [NI=ni]
            [NB=nb] [XEN=xen] [BA=ba] [UO2=uo2] [FE=fe] [SR=sr] [TC=tc]
            [LA=la] [ND=nd] [CR=cr] [AG=ag]}
            [SCRUB
                [BSIZI=bsizi]
                [VROVR=vrovr]
            EOI]
            [OXPOT=vnoxpt]
            [MOLEC]
            [STABLE]
        EOI]
    EOI]
EOI
```

****

CONCRETE — keyword to initiate the definition of the concrete layer.

COMPOS=1 — required composition keyword and value. The properties of the concrete layer in CORCON problems are controlled by the CONCRETE type specification. Note that when CORCON is inactive, the material CONC will be assumed to be present in the concrete layer with a mass "cmass" for the purpose of doing heat conduction calculations. The concrete type specified here through "otyp" has no effect on the properties of the CONC material.

CONCRETE — required keyword to initiate the concrete type specification when the CORCON model is used.

otyp — the concrete type designator. Allowed values are BASALT, LIME, and GENERIC. The type LIME refers to limestone/common sand concrete while GENERIC refers to limestone concrete. See Table 2-5 for the composition and properties of each type.

OTHER — keyword to allow the user to specify the composition and properties of the concrete, as defined by the next 15 variables.

fsio2	mass fraction of SiO_2 in solid concrete.
ftio2	mass fraction of TiO_2 in solid concrete.
fmno	mass fraction of MnO in solid concrete.
fmgo	mass fraction of MgO in solid concrete.
fcao	mass fraction of CaO in solid concrete.
fna2o	mass fraction of Na_2O in solid concrete.
fk2o	mass fraction of K_2O in solid concrete.
ffe2o3	mass fraction of Fe_2O_3 in solid concrete.
fal2o3	mass fraction of Al_2O_3 in solid concrete.
fcr2o3	mass fraction of Cr_2O_3 in solid concrete.
fco2	mass fraction of CO_2 in solid concrete.
fh2oe	mass fraction of evaporable water.
fh2ob	mass fraction of chemically bound water.
tabl	ablation temperature of concrete. (K)
efusn	heat of fusion associated with concrete decomposition. (J/kg)
TSOLID = tsolct	concrete solidus temperature. Defaults are given in Table 2-5 for "otyp" = BASALT, LIME, and GENERIC. (K)
TLIQID = tliqct	concrete liquidus temperature. Defaults are given in Table 2-5 for "otyp" = BASALT, LIME, and GENERIC. (K)
RHOCON = rhoc	concrete density. Defaults are given in Table 2-5 for "otyp" = BASALT, LIME, and GENERIC. (kg/m^3)
REBAR = rbr	mass ratio of reinforcing steel to concrete in the layer. Default = 0.
TABLAT = tabl	ablation temperature of the concrete surface. Defaults are given in Table 2-5 for "otyp" = BASALT, LIME, and GENERIC. (K)
EMCONC = ew	emissivity of the concrete surface. Used in radiation modeling between the concrete surface and the ablating material. Default = 0.8.
EOI	terminating keyword to be used if one or more of the concrete keywords TSOLID, TLIQID, RHOCON, REBAR, TABLAT, or EMCONC described above is given.

cmass	initial mass of concrete in the layer. This required value represents the end of the COMPOS input block. (kg)
TEMP = ctemp	required initial temperature of the concrete layer. (K)
PHYSICS	keyword to initiate input for the layer physics options. If CORCON or VANESA are to be activated, the PHYSICS keyword is required.
CORCON	keyword to begin the specification of the CORCON core-concrete interaction model.
TIMES	keyword to begin the specification of time zones within the period that CORCON will be active.
tstart	time to begin the CORCON calculation. This value may be greater than the CONTAIN starting time, in which case CONTAIN will run for a period without invoking CORCON. Note that this time should be the same as the time from scram, "time0", input under the INTERM keyword. (s)
ndelt	number of contiguous time zones during which CORCON is active. The limits on the CORCON internally computed timestep and the edit frequency may be specified in each zone. This number must be followed by "ndelt" sets of ("dtmin", "dtmax", "dedit", "timdt"). The maximum value of ndelt is 10.
dtmin	minimum allowed CORCON timestep. (s)
dtmax	maximum allowed CORCON timestep. (s)
dedit	time interval between CORCON edits. (s)
timdt	end time of the time zone. (s)
GEOMETRY	keyword to begin the selection of the geometrical model used by CORCON for the cavity shape. Schematics of the allowed cavity shapes are shown in Reference Col84.
ro	radial coordinate of the center of the ray system. The value of this parameter must be 0. (m)
zo	axial coordinate of the center of the ray system. (m)
HEMICYL	keyword to select a cylindrical cavity with a hemispherical floor. The following four parameters must be specified.
rs	radius of the hemispherical floor as measured from the point (ro, zo). (m)
hc	height of the cylindrical top section. (m)
rw	outside radius of the cylindrical top section. (m)

hbc	height from the external base of the cavity to the base of the cylindrical top section. (m)
FLATCYL	keyword to select a cylindrical cavity with a flat floor. The following eight parameters must be specified.
zt	cylindrical z coordinate of cylinder top edge. (m)
rad	inside radius of cylinder. (m)
hit	height of cylinder from the floor. (m)
radc	radius of inner corner. (m)
rw	outside radius of the cylinder. (m)
hbb	height from the external base of the cavity to the floor of the cavity; i.e., the thickness of the concrete at the bottom. (m)
nbot	number of ray points equally spaced along the flat floor of the cavity.
ncorn	number of ray points equally spaced around corner (not including tangent points).
ARBISHP	keyword to select the arbitrarily shaped cavity option. The number of parameters which must be specified depends on the value "nrays" given in the cell CONTROL block, and the "nbot" value below. A total of "nrays" - "nbot" pairs of cylindrical coordinates ("ri", "zi") must be specified to define the cavity shape.
nbot	number of ray points equally spaced along a flat bottom.
rtang	cylindrical radial coordinate at the point where the floor is no longer flat. (m)
rw	external radius of the cylindrical cavity. (m)
htotl	height from the external base to the top of the cavity. (m)
ri, zi	cylindrical radial and vertical coordinates of body points. Specify "nrays" - "nbot" pairs of values. (m)
EMISIV	required keyword to begin the specification of the emissivities that will be used by CORCON. The surface emissivity will either be that of the oxide or metal depending on the material at the surface.
OXIDE	keyword to begin the specification of the emissivities of the oxide layers.

oflag	a character flag indicating the type of specification being used. The use of TIME for "oflag" indicates that the emissivities are being specified as functions of time, while TEMP implies that they are being specified as functions of surface temperature.
neo	the number of oxide emissivities in the table.
tort1	time (s) or temperature (K) values for the emissivity table.
eo	values of oxide emissivities.
METAL	keyword to begin the specification of the emissivities of the metal layers.
oflag	same as above.
nem	the number of metal emissivities in the table.
tort2	time (s) or temperature (K) values for the emissivity table.
emm	values of metal emissivities.
SURRND	keyword that begins specification of emissivities of the surrounding environment for the cavity. These values will be used only if a radiation model has <u>not</u> been specified in the CONTAIN problem definition.
oflag	same as above.
ns	the number of surrounding's emissivities in the table.
tort6	time (s) or temperature (K) values for the emissivity table.
es	values of surrounding's emissivities.
MOVIES	optional keyword to add CORCON cavity shape information to a separate plot file.
MMCHEM	optional keyword to invoke the older CORCON mechanical mixture chemistry model. By default, the ideal solution chemistry model is used in CORCON.
VANESA	keyword to begin the input of parameters for the VANESA aerosol/fission product model.
EDITDELT = vdtedt	time interval for producing VANESA edits in the output. (s)
CONCCOMP	keyword to initiate the specification of a concrete type for melted concrete.

otypm — the melted concrete type designator. The three predefined types are BASALT, LIME, and GENERIC. As with the concrete specification, LIME refers to limestone/common sand concrete and GENERIC refers to limestone concrete. The melted concrete type specified here may differ from the solid concrete type specified in the CORCON input block. Default compositions for the three predefined types are given in Table 2-6.

OTHER — keyword to allow the user to specify the mass fractions present in melted concrete. Note that this input refers to the composition of melted concrete and is distinct from the mass fractions for solid concrete.

fcao — mass fraction of CaO in melted concrete.

fal2o3 — mass fraction of Al_2O_3 in melted concrete.

fna2o — mass fraction of Na_2O in melted concrete.

fk2o — mass fraction of K_2O in melted concrete.

fsio2 — mass fraction of SiO_2 in melted concrete.

ffeo — mass fraction of FeO in melted concrete.

REBAR = ffe — mass ratio of iron to concrete. Iron will be added to the VANESA metallic phase according to the "ffe" value as concrete is ablated. Note: in order to reproduce standard VANESA results, this value must be set to 0.25. Also, the solid concrete rebar fraction in the CORCON input block (REBAR = rbr) should be nonzero. Default = 0.

FDELT = fdelt — the fraction of the CORCON timestep used as the VANESA calculational timestep. Default = 0.05.

DIFCO = difco — the condensed phase diffusion coefficient. Default = 1.0×10^{-8}. (m^2/sec)

BUBD = bubd — diameter of bubbles rising through the melt. Default = 1.0×10^{-2}. (m)

PTBB = ptbb — the number of particles created per bubble burst. Default = 2000.

PTDIA = ptdia — the diameter of the particles created by bursting. Default = 1.0×10^{-6}. (m)

AERCONST — keyword to initiate the specification of the mapping of VANESA constituent materials onto the CONTAIN aerosol components. At least one aerosol component must be defined in the global AEROSOL block. If AERCONST is not specified, the VANESA constituent materials will all be assigned to the first aerosol component. The AERCONST input is required in order to obtain other than the default setup.

numaer — the number of CONTAIN aerosol components used to represent the VANESA constituent materials. This value must not exceed the value of "nac" given in the global CONTROL block. The following group of three values must be repeated "numaer" times.

aername — the name of an aerosol component, as declared in the global AEROSOL input block, or alternatively a number between 1 and "nac" corresponding to the aerosol component.

ncnams — the number of VANESA constituents assigned to the above aerosol component.

ovnam — a list of VANESA constituent names, "ncnams" in length. The 24 legal constituent names are: FE, CRCO3, NI, MO, RU, SN, SB, TE, AG, MN, CAO, AL2O3, NA2O, K2O, SIO2, UO2, ZRO2, CS2O, BAO, SRO, LA2O3, CEO2, NB2O5, CSI.

FPTRACK — keyword to initiate the specification of the mapping of the VANESA constituent materials onto the CONTAIN fission product inventory system. This mapping allows CONTAIN to track VANESA materials that are calculated to be volatilized and/or aerosolized as a result of the core-concrete interactions. If specified, this keyword and its associated input must follow the AERCONST specification. By default, VANESA constituents are not introduced into the CONTAIN fission product system. The user must specify which VANESA constituents are to be tracked and supply either the SIMPLE or DETAIL tracking parameters.

SIMPLE — keyword to indicate that the simplified fission product tracking option will be used. With this option individual VANESA constituents may be tracked as fission products on aerosols; however, any VANESA constituent that is tracked must match the name of a fission product declared in the FISSION global input. The fission products representing VANESA constituents are assigned to aerosol component hosts in the same proportion that VANESA constituents are assigned to aerosol components in the AERCONST input.

nvanfp — the number of VANESA constituents to be tracked individually as CONTAIN fission products. When the SIMPLE option is used, the value of "nvanfp" must be the same as that of "nvfpsm" in the cell CONTROL block.

ovnam — a list of VANESA constituent names, "nvanfp" in length. The legal names are as given above for the aerosol assignment. In the SIMPLE tracking option, these names also must have been defined previously as fission products in the global FISSION input block.

DETAIL — keyword to select the detailed fission product tracking option. With this option, the VANESA constituents may be assigned in a general manner to the airborne (gas or aerosol) hosts of the CONTAIN fission product system. (VANESA constituents may not enter the CONTAIN fission

product system directly on nonairborne hosts.) With this form of fission product tracking, the parameter "nvfpsm" on the cell CONTROL line must equal the value obtained by summing the "nvcons" values of "nfp", two parameters discussed below.

nvcons — the number of VANESA constituents that will be tracked as CONTAIN fission products. The following groups of input must be repeated "nvcons" times.

ovnam — VANESA constituent name. In the DETAIL tracking option, this name need not match the name of any CONTAIN fission product; however, it must be one of the 24 allowed VANESA constituents.

nfp — number of CONTAIN fission products associated with the VANESA constituent "ovnam". The following three keywords must be repeated "nfp" times. (This is done for each "ovnam" given.)

ofpnam — the name of a CONTAIN fission product specified in the global FISSION input block.

wfrac — mass fraction of VANESA constituent "ovnam" which will be assigned to the fission product "ofpnam" on host "ohost". There is no restriction on this value; therefore, the mass tracked as CONTAIN fission products will differ from the mass produced by VANESA, if the "wfrac" values do not sum to 1.

ohost — simple or composite name indicating the airborne host to which the fission product mass should be assigned. "Ohost" may be either the word GAS to indicate the atmosphere gas as a host or the words AEROSOL_"aername", where "aername" is the name of an aerosol component, to indicate that aerosol component as a host. An alternative form to indicate an aerosol component host is AEROSOL_"n", where "n" the number of the aerosol component. (The component number lies between 1 and "nac" and corresponds to the order in which "mapaer" is specified in the global AEROSOL input block.)

MELTCOMP — keyword to specify the composition of the melt layer. This is one of the two possible methods for specifying the composition. The MELTCOMP format is used in the stand-alone VANESA code and has been included to accommodate the users who wish to use that format.

cmelt — the masses of melt components following the MELTCOMP keyword. The user must provide a list of 32 numbers specifying in the following order the mass of each of the materials: Cs, I, Xe, Kr, Te, Ba, Sn, Ru, UO_2, Zr, ZrO_2, Fe, FeO, Mo, Sr, Rb, Y, Tc, Rh, Pd, La, Ce, Pr, Nd, Sm, Pu, Cr, Mn, Ni, Ag, Sb, and Nb. (kg)

CES = ces, etc. — this value and the ones that follow in the template are used in the second method for specifying melt composition. As an alternative to MELTCOMP method, the user may specify one of the indicated material keywords (such as CES) and then the material mass for that material. The masses may be given in any order, and only the masses that are nonzero need be included. The material keywords and the associated materials are given in Table 3-1. Default = 0. (kg)

SCRUB — keyword to activate the VANESA aerosol scrubbing model for overlying pools. The depth of the coolant pool used by the scrubbing model is determined from the conditions of the pool layer.

BSIZI = bsizi — initial bubble diameter for pool scrubbing. Default = 0.01. (m)

VROVR = vrovr — ratio of internal gas velocity to rise velocity. This is an adjustable parameter for simulating nonspherical bubble effects and the effects of impurities on the bubble-liquid interface. Default = 1.

OXPOT = vnoxpt — real value between 0 and 1 governing calculation of the oxygen potential value in VANESA. A value of 0 corresponds to a standard VANESA calculation (see Section 2.3.2.3.3). Default = 0.

MOLEC — keyword to activate the nonstandard VANESA molecularity assumption (see Section 2.3.2.3.3).

STABLE — keyword to activate the nonstandard VANESA condensed phase stability assumption (see Section 2.3.2.3.3).

Table 3-1

Melt Component Keywords and Chemical Symbols

Keyword (Symbol)	Keyword (Symbol)	Keyword (Symbol)
CES (Cs)	IOD (I)	XEN (Xe)
KRY (Kr)	TE (Te)	BA (Ba)
SN (Sn)	RU (Ru)	UO2 (UO_2)
ZR (Zr)	ZRO2 (ZrO_2)	FE (Fe)
FEO (FeO)	MO (Mo)	SR (Sr)
RB (Rb)	Y (Y)	TC (Tc)
RH (Rh)	PD (Pd)	LA (La)
CE (Ce)	PR (Pr)	ND (Nd)
SM (Sm)	PU (Pu)	CR (Cr)
MN (Mn)	NI (Ni)	AG (Ag)
SB (Sb)	NB (Nb)	

EOI — input block terminator. The CONCRETE, PHYSICS, CORCON, EMISIV, VANESA, and SCRUB blocks all must be terminated with the EOI keyword.

3.3.2.4 Intermediate Layers. This input block is used to define the characteristics of an intermediate layer in the lower cell. Like the concrete layer input, the intermediate layer input differs for problems with and without core-concrete interaction modeling with CORCON. The two sections that follow describe the intermediate layer input for problems without CORCON and problems with CORCON, respectively.

3.3.2.4.1 Intermediate Layer Input Without CORCON. Multiple intermediate layers may be defined in problems that do not include core-concrete interaction modeling with CORCON. The number of intermediate layers, "jint", is specified in the cell CONTROL block. The intermediate layer definition block should be repeated "jint" times. The first INTERM layer input block corresponds to the lowest intermediate layer in the lower cell system. The layers proceed upward in the order that they are defined, with the last intermediate layer corresponding to the uppermost of the intermediate layers.

Descriptions of the SOURCE, Q-VOL, and HT-COEF keywords and associated input are the same as described for the CONCRETE layer without CORCON (see Section 3.3.2.3.1). Detailed descriptions of these keywords and their associated input are therefore not repeated in this section.

```
**************************************************************************

INTERM
    LAY-NAM=olay
    [COMPOS=nma (omat mass)]
    TEMP=temp
    [PHYSICS
        [SOURCE=nso
            (data)]
        [Q-VOL
            (data)
        EOI]
        [HT-COEF
            (data)
        EOI]
    EOI]
EOI

**************************************************************************
```

INTERM — keyword to initiate the definition of an intermediate layer.

LAY-NAM = olay — the name of the intermediate layer. Intermediate layer names may be anything the user desires; however, each intermediate layer name should be unique. In the HT-COEF input for specifying a heat transfer coefficient between layers, "olay" is used to identify the intermediate layer.

COMPOS	keyword to initiate the specification of materials initially in the intermediate layer. If this keyword and its associated input are omitted, this layer will be initially empty.
nma	number of materials initially present in the layer. The following two inputs must be repeated "nma" times.
omat	name of a material which is initially present in the intermediate layer. This material must be among the materials specified after either the COMPOUND or the USERDEF keywords in the MATERIAL input block.
mass	initial mass of material "omat" in the layer. (kg)
TEMP = temp	required initial temperature of layer. (K)
PHYSICS	keyword to initiate input for the layer physics options. This keyword is required if any of the options described below are to be selected.
SOURCE	keyword to initiate the specification of material sources to the layer. The source input template for the intermediate layer is identical to that for the concrete layer shown in Section 3.3.2.3.1. Additional details are also given in Section 3.4.
nso	the number of source tables specified for the layer. A description of the "nso" data groups that must follow this number is given in Sections 3.3.2.3.1 and 3.4.
Q-VOL	keyword to initiate the specification of a volumetric heat source table in the layer. The input description of this option for intermediate layers is identical to that given in Section 3.3.2.3.1 for concrete layers. Only one Q-VOL table may be specified in a given layer. Additional details on such tables are also given in Section 3.5.
HT-COEF	keyword to initiate the specification of a heat transfer coefficient table to override the internal heat transfer coefficient either between the present layer and one above it or between it and the basemat. The input description of this option for intermediate layers is identical to that given in Section 3.3.2.3.1 for concrete layers. Only one HT-COEF table may be specified in a given layer. Additional details on such tables are also given in Section 3.5.
EOI	input block terminator.

3.3.2.4.2 Intermediate Layer Input With CORCON. When the CORCON model is used, only one intermediate layer may be defined. This single CONTAIN intermediate layer is used to initialize the CORCON melt layers. This layer must be defined after the CONCRETE layer and before the POOL layer. The name for this single layer is always CORCON. The user does not have the option to change this name through the LAY-NAM keyword.

```
**************************************************************************

INTERM
    COMPOS
        CORCON
            [OXIDES=nosi (namosp smo)]
            [METALS=nmsi (nammsp smm)]
            [TOXIDE=toi] [TMETAL=tmi] [LAYERS=ilyr]
        EOI
    [PHYSICS
        [SOURCE=nso
            (oname=n  IFLAG=ival
                T=(times) MASS=(masses) TEMP=(temps)
            EOI)]
        {[CORESTAT time0 xmtu xmwth num (fpl reti)]  or
        [DKPOWER
            [OXIDEPWR=ndeco (tio pio)]
            [METALPWR=ndecm (tim pim)]
        EOI]}
    EOI]
EOI

**************************************************************************
```

INTERM — keyword to begin the specification of an intermediate layer.

COMPOS — keyword to begin the specification of CORCON layer initial conditions. It must be followed immediately by the keyword CORCON.

CORCON — second keyword used for specifying the CORCON layer initial conditions. Note that prior to the CORCON start time, the CORCON intermediate layer is assumed to be absent in the heat conduction calculations. However, after CORCON finishes, an intermediate layer will be constructed for use in the heat conduction calculations as described in Section 2.3.2.4.

OXIDES — keyword to begin the specification of the initial CORCON oxidic layer composition.

- nosi — number of oxidic species used in the CORCON oxide layer.
- namosp — name of an oxidic species, taken from the list of CORCON species given in Table 3-2.
- smo — mass of the oxidic species. (kg)

METALS — keyword to begin the specification of the initial CORCON metallic layer composition.

- nmsi — number of metallic species used in the CORCON metal layer.
- nammsp — name of a metallic species, taken from the list of CORCON species given in Table 3-2.

Table 3-2

Names of CORCON Species

Oxides		Metals
SIO2	FE2O3	FE
TIO2	AL2O3	CR
FEO	UO2	NI
MNO	ZRO2	ZR
MGO	CR2O3	MN
CAO	NIO	C
SRO	FE3O4	NA
BAO	MN3O4	
LI2O	PUO2	
NA2O	K2O	

smm — mass of the metallic species. (kg)

TOXIDE = toi — initial CORCON oxidic layer temperature. (K)

TMETAL = tmi — initial CORCON metallic layer temperature. (K)

LAYERS = ilyr — index that specifies the type(s) of melt layers initially present in CORCON. The CORCON melt layers are treated as separate nodes in the single CONTAIN intermediate layer. A value of 0 implies an oxidic and a metallic layer; a value of 1 implies a metallic layer; and a value of 2 implies an oxidic layer.

PHYSICS — keyword to begin the specification of models for the CORCON intermediate layer.

SOURCE — keyword to begin the specification of sources of material to the CORCON intermediate layer. With the exception of the allowed material names and the required temperature specification, the input description for these sources is the same as that discussed in Section 3.3.2.3.1 for the concrete layer. Time-dependent sources of the materials listed in Table 3-2 may be introduced into the CORCON layers by means of these source tables. Note: only temperature specification and not enthalpy specification of the incoming CORCON material is allowed.

CORESTAT — keyword to begin the specification of one of two models for decay heating of the CORCON layers. In this option, the gross fuel mass and operating power are specified so that the code may calculate the decay power. The user may

modify the CORCON calculation by specifying new fission product retention fractions to replace those used in the code.

time0	time after scram. Because of assumptions about the time of scram in CORCON, this time must be equal to the CORCON start time "tstart". (s)
xmtu	core mass in metric tons of uranium. (MTU)
xmwth	core operating power. (MWt)
num	number of radioactive species in the intact core inventory for which the retention factor will be modified. This value must be less than or equal to 27. A nonzero value of "num" implies that this value is followed by "num" pairs of "fpl" and "reti".
fpl	name of radioactive species whose retention factor is to be modified. The allowed names are given in Table 3-3. This table also shows the assumed mass concentrations at scram and the default retention factors for each species.
reti	user-specified retention factor for the "fpl" species.
DKPOWER	keyword to begin the specification of the second of two models for decay heating of the CORCON layers. In this method the user can specify the power to be delivered to the oxide and/or metal layers as a function of time.
OXIDEPWR	keyword to begin specification of an oxidic-phase power table.
ndeco	number of points in the table representing oxidic-phase power versus time. The value must be less than or equal to 30 and followed by "ndeco" pairs of values of "tio" and "pio".
tio	time value in oxidic-phase power table. (s)
pio	oxidic-phase power. (W)
METALPWR	keyword to begin specification of a metallic-phase power table.
ndecm	number of points in the table of metallic-phase power versus time. The value must be less than or equal to 30 and followed by "ndecm" pairs of values of "tim" and "pim".
tim	time value in the metallic-phase power table. (s)
pim	metallic-phase power. (W)
EOI	input block terminator.

Table 3-3

CORCON Decay Heat Elements

Element	Mass Concentration [g-atom/MW(thermal)]	Retention Factor
MO	.6053	.97
TC	.1545	.97
RU	.3885	.97
RH	.0690	.97
SB	.00244	.85
TE	.0627	.85
SR	.2155	.90
BA	.1915	.90
ZR	.7352	.99
CE	.3870	.99
NP	.0422	.99
CM	.00204	.99
NB	.01139	.99
PU	.7921	.99
AM	.00593	.99
Y	.1099	.99
LA	.1662	.99
PR	.1446	.99
ND	.4638	.99
SM	.0539	.99
EU	.01705	.99
RB	.0819	.19
CS	.3776	.19
BR	.0053	.10
I	.0320	.10

3.3.2.5 Pool Layer. The POOL input block is used to specify the configuration of a coolant pool layer. The overall input format for the pool layer is the same for all problems, regardless of whether CORCON is used to model core-concrete interactions.

```
**********************************************************************

POOL
    [COMPOS=nma (omat pmass)]
    TEMP=ptemp
    [PHYSICS
        [BOIL]
        [SOURCE=nso
            (data)]
        [Q-VOL
            (data)
        EOI]
```

```
        [HT-COEF
            (data)
        EOI]
    EOI]
EOI
```

****

POOL	keyword to initiate the definition of the pool layer.
COMPOS	keyword to initiate the specification of the initial material in the pool layer. If this keyword and its associated input are omitted, the pool layer will be initially empty.
nma	number of materials initially present in the pool layer. The following two variables must be repeated "nma" times.
omat	name of a material initially present in the pool layer. This material must be among the materials specified after either the COMPOUND or USERDEF keywords in the MATERIAL input block. If the BOIL physics option is invoked, only coolant material (H2OL or NAL) may be present.
pmass	initial mass of material "omat" in the pool layer. (kg)
TEMP = ptemp	required initial temperature of layer. (K)
PHYSICS	keyword to initiate input of the layer physics options. This keyword is required if any of the options described below are to be selected.
BOIL	keyword to activate the pool boiling model. If the implicit intercell flow option has been selected, pool boiling is modeled implicitly under the direction of the implicit flow solver. Otherwise, a semi-implicit boiling algorithm is used.
SOURCE	keyword to initiate the specification of material sources to this layer. With the exception of possible restrictions on the materials present when boiling is allowed, the source input description for the pool layer is identical to that given in Section 3.3.2.3.1 for the concrete layer. Additional details are also given in Section 3.4.
Q-VOL	keyword to initiate the specification of a volumetric heat source table for the pool layer. The input description of this option for a pool layer is identical to that described in Section 3.3.2.3.1 for a concrete layer. (While that section describes the concrete layer without CORCON, volumetric heating of the pool layer can also be specified with CORCON.) Only one Q-VOL table is allowed in a given layer. Additional details on such tables are also given in Section 3.5.

HT-COEF — keyword to initiate the specification of heat transfer coefficient tables to override the internally calculated heat transfer coefficient either between the pool and the layer above it (for the pool layer this is the atmosphere, i.e., ATMOS) or between the pool and the basemat. If the CONDENSE option has been selected, convective heat transfer from the surface of the pool will be modeled independently through that option and any heat transfer coefficient table given for the interface between the pool and the atmosphere will have no effect. The input description of these tables for the pool is identical to that described in Section 3.3.2.3.1 for concrete layers. Only one HT-COEF table is allowed in a given layer. Additional details on such tables are also given in Section 3.5.

EOI — an input block terminator.

3.3.2.6 Atmosphere Layer. The atmosphere layer input which was available in earlier versions of CONTAIN is now disabled. An atmosphere layer is still present within the code, but user input to this layer is not allowed. The main purpose of this layer is to provide a collection point for mass and energy which will be passed to the upper cell atmosphere. Lower cell atmosphere layer sources which were formerly allowed can be replaced by either upper cell atmospheric sources or SRV sources. The name of the atmosphere layer (for use in HT-COEF input in other layers) is ATMOS.

3.3.3 Engineered Safety Systems

The cell level keyword ENGINEER is used to specify engineered safety features and/or engineered system components that form the coolant redistribution system connecting lower cell pools. The three available ESFs are the containment spray, the fan cooler, and the ice condenser, activated by the keywords SPRAY, FANCOOL, and ICECOND, respectively. Only one ESF or one redistribution system component may be defined after each ENGINEER keyword, but any number of ENGINEER keywords can be specified in a cell. Each ENGINEER keyword is considered to define an "engineered system." (The number of such systems "naensy" should be specified in the cell level CONTROL block.) For example, a given cell may include one fan cooler, two pumps, and five valves as engineered systems for that cell. Each of the pumps and each of the valves should be specified as a separate system.

In the specification of an engineered safety feature, the keyword SOURCE indicates that the inlet coolant flow to either a containment spray or the cooling coils of a fan cooler is to be specified as an external source with mass flow rate and temperature given as a function of time. A tank, activated by the keyword TANK, may also provide the source for a containment spray. If the source of the spray is recirculated water from a pool, a heat exchanger model activated by the keyword HEX must be used. Water to be recirculated may come from a pool in another cell, specified by the input variable "iclin". The residual liquids from an ESF may be diverted to the cell specified by the input variable "iclout".

The redistribution of coolant liquid from the pool of one cell to that of another may also be modeled through an engineered system component. If any one of the PIPE, ORIFICE, or VALVE components is specified, the flow rate is determined by the pressure difference between the two cells and the hydraulic head of the respective pools. Specification of a valve between the two cells allows opening and closing of the flow path. If PUMP is specified as the component, a constant flow rate is maintained from "iclin" to "iclout" as long as liquid is available in "iclin". Overflow modeling activated by the keyword OVERFLOW will allow coolant to overflow from the pool of one cell to that of another.

The complete input template for the ENGINEER input block is given below. Detailed descriptions of the three ESF models and the liquid redistribution components are given in the following sections. It should be noted that only one ESF model and certain logical combinations of components are allowed in any one engineered system as discussed in the following subsections.

```
**************************************************************************

ENGINEER onmsys numcom iclin iclout delev
    [SOURCE=nso
        (H2OL=n IFLAG=ival
            T=(times)
            MASS=(masses)
            {TEMP=(temps) or ENTH=(enths)}
        EOI)]
    [SPRAY
        [SPDIAM=spdiam] [SPHITE=sphite] [SPPCI2=sppci2]
        [SPPCMI=sppcmi] [SPSTPR=spstpr] [SPSTTM=spsttm]
    EOI]
    [FANCOOL
        {CONDENSE
            [FCQR=fcqr] [FCWIN=fcwin] [FCTCLI=fctcli] [FCCLMD=fcclmd]
            [FCCLOD=fcclod] [NRWSFC=nrwsfc] [FCEFAR=fcefar]
            [FCFLAR=fcflar] [FCHNTR=fchntr]     or
        MARCH
            [FCQR=fcqr] [FCTCLI=fctcli] [FCCLMD=fcclmd]
            [FCTPIR=fctpir]}
    EOI]
    [ICECOND
        [HITICI=hitici] [TMSICI=tmsici] [CITICE=citice] [CITLEX=citlex]
        [CIARFL=ciarfl] [ARHTIN=arhtin] [ICLLP=icllp] [AREASED=areased]
        [FRACSED=fracsed] [AREAIMP=areaimp] [DIAMIMP=diamimp]
        [DIAMDIF=diamdif] [AREADIF=areadif]
    EOI]
    [TANK tnkmas tnktem tnkflo]
    [PUMP pmpmdt]
    [ORIFICE orifid orifdr]
    [PIPE pipeid pipel pipekf]
    [VALVE
        {PRESSURE valvar valvkf valopp   or
        TIMES valvar valkf (valtim)}]
```

```
    [HEX {otype hxticl hxclmd hxarea hxcoef or
        USER hxdelt}]
    [OVERFLOW iclfrm iclto flovht]
EOI

*************************************************************************
```

ENGINEER — keyword to initiate the specification of an engineered system. This system can consist of up to 10 components of which only one may be an ESF model (SPRAY, FANCOOL, or ICECOND). Multiple systems may however be specified by repeating the ENGINEER input block.

onmsys — name of the engineered system.

numcom — number of components in the engineered system. This number includes the ESF component (SPRAY, ICECOND, or FANCOOL) and the engineered system components. The SOURCE table input, if used, is also considered a component of the system. In CONTAIN versions prior to 1.1, an accurate value for this parameter is required; however, the number of components is now automatically determined by the code. Any nonzero value specified is acceptable since it will be overridden at execution time.

iclin — cell number from which the liquid to the system originates. Default = current cell.

iclout — cell number to which the system diverts residual liquid. This residual liquid may include spray droplets, condensate, melted ice, or diverted flow.

delev — drop in elevation from the bottom of pool in "iclin" to that of "iclout". It is used in redistribution of coolant from cell to cell. (m)

3.3.3.1 External Engineered System Source. An external source table is the simplest way to specify a time-dependent mass flow rate and temperature to a spray or fan cooler engineered system. Engineered system source tables may only be used to specify liquid water for a containment spray or a fan cooler. The input format for such a source is similar to that for other sources in CONTAIN (see Section 3.4); however, the material name is restricted to H2OL.

```
*************************************************************************

[SOURCE=nso
    (H2OL=n
        [IFLAG=ival]
        T=(times)
        MASS=(masses)
        {TEMP=(temps) or ENTH=(enths)}
    EOI)]

*************************************************************************
```

SOURCE — keyword to initiate the specification of source tables which determine the rate at which water is supplied to the engineered system.

nso — the number of water source tables to be defined. If "nso" is greater than one, the multiple tables are additive.

H2OL — material name required to indicate that the source consists of liquid water. Engineered system external source tables are restricted to water.

The remaining keywords and input parameters shown in the above input template are described in Section 3.4.

3.3.3.2 Containment Spray. This input block is used to specify the containment spray model. Note that all of the spray parameters have defaults.

```
**************************************************************************

SPRAY
    [SPDIAM=spdiam] [SPHITE=sphite] [SPPCI2=sppci2] [SPPCMI=sppcmi]
    [SPSTPR=spstpr] [SPSTTM=spsttm]
EOI

**************************************************************************
```

SPRAY — keyword to initiate the input for the containment spray model.

SPDIAM = spdiam — representative droplet diameter. Default = 0.001. (m)

SPHITE = sphite — spray fall height. Default = cell height specified in the cell GEOMETRY block. (m)

SPPCI2 = sppci2 — partition coefficient used to model removal of elemental iodine. Fission products having names that begin with the letters "MOLI" are assumed to be elemental iodine. Default = 5000.

SPPCMI = sppcmi — partition coefficient used to model removal of organic iodides. Fission products having names that begin with the letters "ORGI" are assumed to be organic iodides. Default = 0.

SPSTPR = spstpr — containment pressure at which the spray is initiated. If this value is 0., the spray is initiated by a finite flow rate or "spsttm". Default = 0. (Pa)

SPSTTM = spsttm — containment temperature at which the spray is initiated. If this value is 0, the spray is initiated by a finite coolant flow rate or "spstpr". Default = 0. (K)

EOI — an input block terminator.

If the spray model is selected as the ESF in an engineered system, certain combinations of components must be specified. One combination consists of SOURCE and SPRAY, with OVERFLOW optional. The other combination consists of TANK, PUMP, HEX, and SPRAY, with OVERFLOW optional. An example of the input for the latter combination is given below.

```
ENGINEER SAMPLE1 4 2 2 0.0
                          && engineered system has four components
                          && outlet to and recirculation from cell 2
                          && elevation difference = 0
    SPRAY
        SPPCI2=6000.0     && elemental iodine partition coeficient
        SPSTPR=2.0e5      && pressure initiation at 2.0 x 10^5 Pa
    EOI
    TANK
        5000.0            && mass of water available in the tank
        280.0             && source water temperature
        200.0             && water flow rate from the tank
    PUMP
        200.0             && flow rate for recirculation
    HEX
        USER=50.          && user-specified temperature drop of 50 K
EOI
```

3.3.3.3 Fan Cooler. Two fan cooler models are available--a mechanistic condensation heat transfer model activated by the keyword CONDENSE and a simple heat transfer model, similar to that used in the MARCH code and activated by the keyword MARCH.

****

```
FANCOOL
    {CONDENSE
        [FCQR=fcqr] [FCWIN=fcwin] [FCTCLI=fctcli]
        [FCCLMD=fcclmd] [FCCLOD=fcclod] [NRWSFC=nrwsfc]
        [FCEFAR=fcefar] [FCFLAR=fcflar] [FCHNTR=fchntr]
            or
    MARCH
        [FCQR=fcqr] [FCTCLI=fctcli]
        [FCCLMD=fcclmd] [FCTPIR=fctpir]}
EOI
```

****

FANCOOL — keyword to begin specification of the fan cooler model.

CONDENSE — keyword to specify the mechanistic condensation heat transfer model.

FCQR = fcqr — estimated fan cooler heat removal rate. Because the CONDENSE model is iterative, this value is only used to initiate the iteration. The rated capacity should normally be used for this value. Default = 2.17×10^7. (W)

FCWIN = fcwin — volumetric flow rate of the air/steam mixture through the fan cooler. Default = 25.01. (m^3/s)

FCTCLI = fctcli — cooling water inlet temperature. If an external source is specified this value is ignored. Default = 300. (K)

FCCLMD = fcclmd — cooling water mass flow rate through cooler. If an external source is specified, this value is ignored. Default = 123.1. (kg/s)

FCCLMOD = fcclod — outside diameter of the cooling tubes. Default = 0.0159. (m)

NRWSFC = nrwsfc — number of rows from front to back of cooler. Default = 12.

FCEFAR = fcefar — effective area for heat transfer across one row of tubes. Because tubes have closely spaced fins, this value is several times the tube area. Default = 26.5. (m^2)

FCFLAR = fcflar — frontal area of the fan cooler. Default = 3.0. (m^2)

FCHNTR = fchntr — heat transfer coefficient between the tube external surface and the cooling water, based on "fcefar". Default = 1000. (W/m^2-K)

MARCH — keyword to specify the simple heat transfer model.

FCQR = fcqr — cooler rated capacity. Default = 2.17×10^7. (W)

FCTCLI = fctcli — rated coolant inlet temperature. Default = 300. (K)

FCCLMD = fcclmd — rated coolant mass flow rate. Default = 123.1. (kg/s)

FCTPIR= fctpir — rated inlet air/steam temperature. Default = 405.9. (K)

EOI — input block terminator

If the SOURCE option is used with FANCOOL, the data provided in the SOURCE tables overrides the default or user-specified values of the cooling water flow rate and temperature.

3.3.3.4 Ice Condenser. The input for the ice condenser model is described in this section. Use of the ice condenser model requires a problem with at least two cells. For realistic analysis, three or more cells are preferable. The cell in which the the model is invoked is the ice chest itself. Note that the default upstream cell "icllp" is somewhat arbitrary; the user should specify the proper cell if the default is not appropriate.

```
**************************************************************************

ICECOND
    [HITICI=hitici] [TMSICI=tmsici] [CITICE=citice]
    [CITLEX=citlex] [CIARFL=ciarfl] [ARHTIN=arhtin] [ICLLP=icllp]
    [AREASED=areased] [FRACSED=fracsed] [AREAIMP=areaimp]
    [DIAMIMP=diamimp] [DIAMDIF=diamdif] [AREADIF=areadif]
EOI

**************************************************************************
```

ICECOND — keyword to initiate the specification of the ice condenser model.

HITICI = hitici — initial height of ice in bed. Default = 14.6. (m)

TMSICI = tmsici — initial mass of ice. Default = 1.1×10^6. (kg)

CITICE = citice — initial ice temperature. Default = 264. (K)

CITLEX = citlex — temperature at which melted ice and condensate are assumed to leave the ice chest. Tests have produced values between 335 and 373 K, depending on blowdown rate, with lower rates yielding higher temperatures. Default = 350. (K)

CIARFL = ciarfl — cross-sectional flow area through the ice chest. Default = 100. (m^2)

ARHTIN = arhtin — initial area of ice available for heat transfer. Default = 1×10^4. (m^2)

ICLLP = icllp — cell number of the upstream cell. This cell number is used only to determine the flow rate through the ice chest. The default value is normally the "iclin" value specified after the ENGINEER keyword. However, if "iclin" is the same as the current cell and if the current cell number is not 1, "icllp" will be set to the current cell number minus one.

AREASED = areased — effective floor areas for sedimentation, including tops of baskets and support structures but not including the ice surfaces. Default = 1535. (m^2)

FRACSED = fracsed — fraction of total ice area on which sedimentation may occur. Default = 0.5.

AREAIMP = areaimp — total area for impaction of aerosols on the basket wires. Default = 1240. (m^2)

DIAMIMP = diamimp — effective wire cylindrical diameter for modeling impaction and interception of aerosols on the basket wires. Default = 0.00191. (m)

DIAMDIF = diamdif — effective wire cylindrical diameter for modeling diffusion of aerosols to the basket wire surfaces. Default = 0.00526. (m)

AREADIF = areadif — total area for diffusion of aerosols to the basket wires. Default = 3430. (m^2)

The ice condenser aerosol scrubbing model includes only effects attributable to the ice and basket structure. The walls, floors, and ceiling of the ice chest compartment should be modeled as structures (see Section 3.3.1.3).

3.3.3.5 Tank. A tank provides water for a containment spray. The water in the tank is used until it is exhausted, and then the spray water is drawn from the pool in cell "iclin" in a recirculation mode.

****

TANK tnkmas tnktem tnkflo

****

TANK — keyword to specify a tank component.

tnkmas — initial mass of liquid in the tank. (kg)

tnktem — temperature of liquid in the tank. (K)

tnkflo — flow rate from the tank. (kg/s)

3.3.3.6 Pump. A pump provides a constant mass rate of flow from a pool to a containment spray or to a pool in another cell.

****

PUMP pmpmdt

****

PUMP — keyword to specify a pump component.

pmpmdt — constant mass flow rate. (kg/s)

When used as part of a SPRAY system that includes a TANK water supply, the pump is activated only after the TANK supply is exhausted.

3.3.3.7 Orifice. An orifice provides a model for pressure-driven flow between one pool and another through an orifice.

****

ORIFICE orifid orifdr

****

ORIFICE — keyword to specify an orifice component.

orifid diameter of the orifice. (m)

orifdr ratio of orifice diameter to free stream diameter.

3.3.3.8 Pipe. A pipe provides a flow rate between one pool and another based on a user-specified flow loss coefficient.

```
**************************************************************************

PIPE pipeid pipel pipekf

**************************************************************************
```

PIPE keyword to specify a pipe component.

pipeid inside diameter of the pipe. (m)

pipel the pipe length. (m)

pipekf the flow loss coefficient, which may include the Moody friction factor, entrance and exit loss factors, and form loss factors.

3.3.3.9 Valve. The keyword VALVE may activate one of two options. Followed by the keyword PRESSURE, it simulates a pressure-activated rupture disk, i.e., once the activating pressure differential is reached, the valve opens and remains open, regardless of subsequent changes in the driving pressure. If VALVE is followed by the keyword TIMES, the user must specify five open and close times. The valve is assumed to be initially closed, and the first time specified is the open time; at the next time the valve closes; at the third time it opens again; etc. For a valve that is initially open, the first time specified would be the problem start time. If all five times are not needed, the extra times can be set to very large values which would not be encountered during the course of a run.

```
**************************************************************************

VALVE
    {PRESSURE valvar valvkf valopp
        or
    TIMES valvar valvkf (valtim)}

**************************************************************************
```

VALVE keyword to initiate the specification of a valve component.

PRESSURE keyword indicating that the valve is a pressure-activated rupture disk.

valvar flow area through the valve. This input has the same meaning in the PRESSURE and TIMES options. (m^2)

valvkf flow loss coefficient, which may include the Moody friction factor, entrance and exit loss factors, and form loss

factors. This input has the same meaning in the PRESSURE and TIMES options.

valopp — absolute value of the pressure difference at which the valve opens. (Pa)

TIMES — keyword indicating that the valve is opened and closed up to five times according to the input below. The first two parameters that must follow this keyword are the same as the ones that are required when the PRESSURE option is used.

valtim — array of five alternating open and close times, beginning with the first opening time. (s)

3.3.3.10 Heat Exchanger. Five liquid-liquid heat exchanger options are available. The keyword SHELL invokes the appropriate heat transfer correlations for a shell and tube, single-pass heat exchanger. CROSS denotes a cross-flow heat exchanger; COUNTER, a counterflow type; PARALLEL, a parallel flow type; and USER, a user-specified constant temperature drop across the hot leg. The heat exchanger component is used only with the spray ESF.

****

HEX (otype hxticl hxclmd hxarea hxcoef **or**
USER hxdelt)

****

HEX — keyword to initiate the specification of the heat exhanger component.

otype — heat exchanger type keyword. Either SHELL, CROSS, COUNTER, or PARALLEL must be specified.

hxticl — cold leg inlet temperature. (K)

hxclmd — cooling water flow rate through the cold leg. (kg/s)

hxarea — effective heat transfer area of the exchanger. (m^2)

hxcoef — overall heat transfer coefficient. (W/m^2-K)

USER — heat exchanger keyword used to specify a constant temperature drop, "hxdelt", across the hot leg.

hxdelt — temperature drop across the hot leg. (K)

3.3.3.11 Engineered Systems Overflow. This input block describes the engineered systems overflow component. Overflow of coolant from the pool in one cell to that of another can be simulated through this component. It can be placed by itself in an engineered system or in a system with any other ESF model or engineered system component. The overflow model is useful in applications in which the liquid level in the pool to which coolant is transferred cannot rise above the overflow height of donor

pool. Note that unphysical conditions may result if the amount of water that overflows during any given timestep is comparable to the amount in the pool.

```
**************************************************************************

OVERFLOW iclfrm iclto flovht

**************************************************************************
```

OVERFLOW keyword to specify the overflow engineered system component.

iclfrm cell number from which the overflow originates.

iclto cell number to which the overflow is directed.

flovht height above pool bottom in cell "iclfrm" which defines the level above which any additional coolant is diverted to cell "iclto". (m)

3.3.4 Safety Relief Valve Discharge Model

This block of input is used to activate the SRVSOR model for modeling the effects of a pool on the discharge of gases, aerosols, and fission products below the pool surface. The model may be activated in any cell with a pool specified in the LOW-CELL block. Space must be reserved for the SRV source tables in the cell level CONTROL block using the variables "nsosat", "nspsat", "nsosae", "nspsae", "nsosfp", and "nspsfp" described in Section 3.3.

The source table input in the ATMOS, AEROSOL, and FISSION blocks shown in the template below are similar to those described in Sections 3.3.1.2, 3.3.1.8, and 3.3.1.9, respectively. Thus, only those keywords unique to the SRVSOR block are discussed in this section.

Provided the discharge level is below the pool surface, the materials introduced through the SRVSOR sources are equilibrated in and/or scrubbed by the pool prior to being introduced into the atmosphere above the pool. The user may select either of two aerosol scrubbing models discussed in Section 3.2.3.3: the SCRUB model from VANESA or the SPARC model. Note that aerosol scrubbing depends strongly on the gas composition in the SRV ATMOS sources. For example, in the absence of a noncondensable gas, the aerosols will be trapped in the pool with the maximum decontamination factor (1.0×10^5).

The only SRV fission product sources allowed are those which have an aerosol component as a host. The HOST keyword must be used and the value associated with it must lie between 2 and 1+"nac", a number which corresponds to an aerosol component. If the host aerosol source rate is zero for any time period during which the fission product source rate is nonzero, the fission product mass introduced will be retained entirely in the pool if the discharge level is below the pool surface and assigned directly to the airborne aerosol component if the discharge level is above the surface.

```
**************************************************************************

SRVSOR
    [ELESRV=elesrv]
    {[SCRUB
        [BSIZI=bsiz] [VROVR=vrovr]
    EOI]  or
    [SPARC
        [BSIZI=bsiz] [RATIO=ratio] [NRISE=nrise]
    EOI]}
    [AEROSOL
        SOURCE=nsosae
            (oaer=na
                [IFLAG=ival]
                [AMEAN=(mmd)] [AVAR=(loggsd)]
                T=(times)
                MASS=(masses)
            EOI)]
    [FISSION
        SOURCE=nsosfp
            (ofp=nf
                [IFLAG=ival]
                HOST=nhost [CHAIN=jchain]
                T=(times)
                MASS=(masses)
            EOI)]
    [ATMOS
        SOURCE=nsosat
            (omat=nat
                [IFLAG=ival]
                T=(times)
                MASS=(masses)
                {TEMP=(temps)  or  ENTH=(enths)}
            EOI)]
EOI

**************************************************************************

ELESRV =        the elevation of the SRV discharge point above pool bottom.
  elesrv        Default = 0.  (m)

SCRUB           keyword to specify the VANESA scrubbing model.  By default
                this model is used if neither SCRUB nor SPARC is specified.

BSIZI =         initial bubble diameter for pool scrubbing purposes.
  bsizi         Default = 0.01.  (m)

VROVR =         ratio of internal gas velocity to rise velocity.  This is
  vrovr         an adjustable parameter for simulating nonspherical bubble
                effects and the effects of impurities on the bubble-liquid
                interface.  Default = 1.

SPARC           keyword to specify the SPARC scrubbing model.
```

BSIZI = bsizi — initial bubble diameter for pool scrubbing. This keyword replaces DIAM in the stand-alone version of SPARC. Default = 0.01. (m)

RATIO = ratio — ratio of major axis to minor axis in an axially symmetric oblate spheroid bubble. The ratio is taken to be greater than or equal to 1. If a value less than 1 is specified, its inverse is automatically taken. Default = 1.

NRISE = nrise — number of integration zones used for bubble rise in the scrubbing region. Values ranging from 10 to 1000 are suggested for accuracy. Default = 10.

AEROSOL — keyword to specify SRV aerosol sources. Note that the keywords and values associated with these sources but not discussed below are discussed in Sections 3.3.1.8 and 3.4.

SOURCE — keyword to specify that source table input follows.

nsosae — the number of aerosol source tables to be specified. This number should agree with the value specified in the cell CONTROL block.

oaer — name of an aerosol component declared in the global AEROSOL block.

na — number of time points in the aerosol table. The value of "nspsae" in the cell CONTROL block must be greater than or equal to "na".

One unique feature available for SRV aerosol sources, but not for other types of aerosol sources, is that aerosol size distribution parameters for the aerosol source may be specified as a function of time through the source table using the AMEAN and AVAR keywords described below.

AMEAN = (mmd) — keyword to specify the values of the mass median diameter "mmd". Specify "na" values of "mmd". The definition of "mmd" is identical to that of "amean", defined in the global AEROSOL input block discussed in Section 3.2.4. A nonzero value of "mmd" will override the global "amean" value. A zero value for "mmd" will result in the global "amean" value being used instead. Default = global value of "amean". (m)

AVAR = (loggsd) — keyword to specify the logarithm of the geometric standard deviation "loggsd". Specify "na" values of "loggsd". The definition of "loggsd" is identical to that of "avar", defined in the global AEROSOL input block discussed in Section 3.2.4. A nonzero value of "loggsd" will override the global "avar" value. A zero value of "loggsd" will result in the global value "avar" being used instead. Default = global value of "avar".

FISSION — keyword to specify SRV fission product sources. The keywords and values associated with these sources but not specified below are discussed in Sections 3.3.1.9 and 3.4.

SOURCE	keyword to specify that source table input follows.
nsosfp	the number of fission product source tables to be specified. This number should agree with the value specified in the cell CONTROL block.
ofp	name of a fission product declared in the global FISSION block.
nf	the number of points in the fission product source table. The value of "nspsfp" in the cell CONTROL block must be greater than or equal to "nf".
HOST = nhost	required keyword to specify the host number associated with the fission product in the table. Specify a number between 2 and 1+"nac" which corresponds to the aerosol host.
CHAIN = jchain	the number of the fission product chain which is to receive the "ofp" mass. This should be given if "ofp" appears more than once in the linear chain decomposition.
ATMOS	keyword to specify SRV gas and condensable vapor sources. The keywords and values associated with these sources but not discussed below are discussed in Sections 3.3.1.2 and 3.4. (The former section describes atmosphere sources that enter the atmosphere directly without equilibrating with the pool.)
SOURCE	keyword to specify that source table input follows.
nsosat	the number of gas source tables to be specified. This number should agree with the value specified in the cell CONTROL block.
omat	the name of a gas or the condensable vapor. This material must be among the materials specified after either the COMPOUND or USERDEF keywords in the global MATERIAL input block.
nat	the number of points in the gas source table. The value of "nspsat" defined in the cell CONTROL block must be greater than or equal to "nat".

An example of the SRVSOR input is given below. The elevation of the discharge point is 1 meter above pool bottom. The aerosol sources, in addition to the usual time and mass rate specifications, use the optional keywords for specifying size distribution parameters, AMEAN and AVAR. The SCRUB aerosol scrubbing option, by default, is in effect, with default parameters. The UO2 aerosol is intended to be the first aerosol component in this example, and the fission product LA2O3 is associated with this component through the HOST=2 specification. The control parameters which need to be specified in the cell level CONTROL block to accommodate the tables are "nsosat"=2, "nspsat"=4, "nsosae"=1, "nspsae"=4, "nsosfp"=1, and "nspsfp"=4.

SRVSOR input example:

```
SRVSOR                                  && safety relief valve input
    ELESRV=1.0                          && elevation of discharge

    ATMOS SOURCE=2                      && gas sources
        H2OV=4 IFLAG=1                  && steam; step interpolation
        T=28200. 30000. 31800. 33600.   && time points
        MASS= 14.96 10.16 6.63 7.43     && mass rates
        ENTH=2.85e6 2.92e6 3.07e6 3.24e6 && specific enthalpies
        EOI                             && end of first source table
        H2=4 IFLAG=1                    && hydrogen; step interpolation
        T=28200. 30000. 31800. 33600.   && time points
        MASS=0. 0. 0.002 0.033          && mass rates
        TEMP=569.3 594.1 645.0 705.9    && temperatures
        EOI                             && end of second table

    AEROSOL SOURCE=1                    && aerosol source
        UO2=4 IFLAG=1                   && uo2 aerosol
        T=  0. 37300. 40506. 42648.     && time points
        MASS= 0. 9.576e-5 2.971e-3 0.   && mass rates
        AVAR= 0.7 0.72 0.72 0.7         && log of standard deviation
        AMEAN= 1.e-6 1.1e-6 1.2e-6 1.e-6 && mass median diameter
        EOI                             && end of table

    FISSION SOURCE=1                    && fission product source
        LA2O3=4 IFLAG=1                 && la2o3 fission product
        HOST=2                          && host is first aerosol
                                        && component
        T=0. 37300. 40506. 42648.       && time points
        MASS=0. 4.683e-5 1.453e-3 0.    && mass rates
        EOI                             && end of table

EOI                                     && end of SRVSOR input
```

3.4 Source Table Input

Provisions are made in CONTAIN to specify external sources of mass and energy. The input description for these external sources uses a standard format to the extent possible not only for regular materials but for fission products and aerosols. This section lists the definitions of the standard keywords and values used in source tables. The reader should note that although the basic definitions of most of the keywords and values used in source tables are the same, the source tables for a particular model may require special keywords and values or impose special requirements on the values associated with standard keywords. Thus the present section cannot replace entirely the discussion of source tables in conjunction with the particular models that use them. If a definition of a common keyword or value appears in conjunction with the discussion of a particular model, that definition supersedes the definition given below.

Upper cell atmosphere material sources are discussed in Section 3.3.1.2; upper cell aerosol sources are discussed in Section 3.3.1.8; fission product sources are discussed in Section 3.3.1.9; lower cell material sources are discussed in Sections 3.3.2.3 to 3.3.2.5; engineered system

sources are discussed in Section 3.3.3.1; and SRV sources are discussed in Section 3.3.4.

Source tables should not be confused with the global and cell level tables discussed in Section 3.5 and elsewhere. Unlike source tables, the latter types of tables establish a functional relationship between one independent and one dependent variable.

The common keywords and values used in source tables appear in the following template:

```
**************************************************************************

SOURCE=nso
    (oname=n
        [IFLAG=ival]
        T=(times)
        MASS=(masses)
        [{TEMP=(temps)  or  ENTH=(enths)}]
    EOI)

**************************************************************************
```

SOURCE — keyword to indicate that source table input follows.

nso — the number of source tables to follow. In the template above, the items between "oname" and EOI should be repeated "nso" times.

oname — name of the source material. Depending on the particular type of source table, this name should be the name of a compound, aerosol, or fission product. The names used should be defined in the global input or be available as a default.

n — number of source table points used for material "oname". Each entry ("times", "masses", "temps", and "enths") in the source table for this material must consist of this number of points. The minimum is two points. Space for the source table must generally be provided in the cell CONTROL block for the cell in which the source table is used. The name of the control parameter depends on the model invoking the source table.

IFLAG — keyword to introduce the interpolation flag for the table.

ival — if "ival" = 1, tabular values are treated as step functions. If "ival" = 2, linear interpolation is used between tabular values. With the step function option ("ival" = 1), the value returned from the table remains constant in the interval between adjacent specified times. When the code calculational time reaches the next source time, the value changes to the corresponding tabular value. With the "ival" = 2 option, the value is assumed to vary linearly between the specified tabular values. The source rates are taken to be zero outside of the time range of the table.

T	keyword to introduce time values.
times	source times. Specify "n" monotonically increasing values. (s)
MASS	keyword to introduce mass values.
masses	source mass rates. Specify "n" values. Note that the source rate is taken to be zero outside of the time range of the table. (kg/s)
TEMP	keyword to introduce source temperature values. The temperature is converted internally to an equivalent source specific enthalpy. For compounds that are not CORCON materials, either TEMP or ENTH should be specified, but not both. For CORCON materials only TEMP should be specified. For aerosol or fission product source tables, neither TEMP nor ENTH should be specified since only the mass source rate is pertinent.
temps	source temperatures. Specify "n" values. (K)
ENTH	keyword to introduce specific enthalpy values. See the discussion above for TEMP on when to use TEMP or ENTH.
enths	source specific enthalpies. Specify "n" values. (J/kg)
EOI	input block terminator. Note that <u>each</u> source table is terminated by an EOI; however, <u>the SOURCE block itself is not terminated by an EOI</u>.

For all but engineered system source tables, both positive and negative mass rate values are allowed. Positive values signify mass additions, negative values signify mass removal from the cell. However, note that net negative masses are not allowed in any cell. If negative mass sources are specified, care should be taken to avoid conditions wherein the net mass of the material in question could go negative in any cell. For most models, the code checks for negative masses and sets the mass to zero if this condition is detected. In some cases, however, intermediate calculations are performed prior to the negative mass check, and thus some error could be introduced into the calculation. In some models, a diagnostic is given in the error file if a negative mass condition is encountered. Aerosol suspended masses are checked for negative masses and reset but a diagnostic is not given. Fission product masses are not checked by the code to detect a possible negative mass condition.

The following example indicates how the injection of steam into a cell atmosphere could be modeled. That steam may be due, for example, to a blowdown of the primary system. Only one source is needed, and thus "nso" = 1. The source material is injected into the cell as steam, so the "oname" is H2OV. Linear interpolation is desired, so "ival" = 2. There are fourteen times, mass flow rates, and enthalpies defined in the tables, and "n" = 14. Initially, the flow rate is small but rapidly builds and then slowly decreases as the pressure driving the steam flow drops, and the steam remaining in the tank decreases. At 23.2 s, the blowdown is complete, with the mass flow rate dropping to 0.

```
SOURCE=1
  H2OV=14
  IFLAG=2
  T=     0.0       0.2       0.7       1.2       2.2       3.2
         4.2       8.2       10.2      15.2      20.2      22.7    23.2   100.0
  MASS=  0.691E4   2.971E4   2.717E4   2.457E4   1.964E4   1.693E4
         1.516E4   0.965E4   0.827E4   0.381E4   0.216E4   0.011E4 0.0 0.0
  ENTH=  1.131E6   1.126E6   1.127E6   1.131E6   1.117E6   1.113E6
         1.108E6   1.142E6   1.138E6   1.102E6   0.629E6   0.454E6 0.0 0.0
  EOI
```

3.5 Global and Cell Level Table Input

This section gives the generic definitions of the standard keywords and values used in global and cell level tables. Such tables provide a standard format to specify the relationship between one dependent and one independent variable, such as a heat transfer coefficient versus time, and should not be confused with the source tables discussed in the preceding section.

The distinction between global and cell level tables is made on the basis of the level of the model using the table format. The tables used in global models, such as the flow model, are considered global, whereas tables used in cell level models, such as the lower cell model, are considered at the cell level. Global tables require that the user specify "numtbg" and "maxtbg" in the global CONTROL block; whereas cell level tables require specification of "numtbc" and "maxtbc" in the appropriate cell level CONTROL block.

The reader should note that although the keywords used in all global and cell level tables are the same, the definition and utilization of the values associated with the keywords depends on the application. Also a particular application may impose special requirements on the values that may be selected. Thus the present section cannot replace the discussion of such values in conjunction with the particular models that use them. If a definition of a table keyword or value appears in conjunction with the discussion of a particular model, that definition supersedes the generic definition given below.

In the input for global and cell level tables, a keyword initiating the input of one or more tables is given. That keyword may or may not be followed by application-specific parameters that are then followed by the body of the table. Since the application-specific parameters are nonstandard, the template below shows only the body of one table.

```
**************************************************************************

        [FLAG=iflag]
        NAME=oname
        VAR-X=xname X=n (x)
        VAR-Y=yname Y=n (y)
    EOI

**************************************************************************
```

FLAG = iflag	the table interpolation parameter. "Iflag" = 1 specifies step function interpolation between table points. "Iflag" = 2 specifies linear interpolation between table points. Default = 1.
NAME = oname	the name of the table. The table name in some cases is required to identify the table type. In tables where the name is optional, it may still be given for identification purposes.
VAR-X= xname	name of the independent variable. In some tables only one type of independent variable is considered, in which case this input is optional.
X	keyword to specify the values of the independent variable.
n	the number of independent variable entries in the table. It is also the number of dependent variable entries.
x	the independent variable values. Exactly "n" monotonically increasing values should be specified.
VAR-Y= yname	name of the dependent variable. In some tables only one type of dependent variable is considered, in which case this input is optional.
Y	keyword to specify the values of the dependent variable.
y	the dependent variable values. Exactly "n" values should be specified.
EOI	terminator for each table.

Note that the value of "y" returned from the table for values of "x" outside of the range of the table depends on the application. In some applications, the table is ignored in this case, and the value of "y" is calculated in some other fashion. In other applications the "y" value is determined by using the appropriate endpoint value. The method used is discussed with each specific application.

3.6 Restart Input

A CONTAIN calculation can be restarted at times for which restart blocks are present in the restart file from the preceding run. Such restart block times are controlled by the TIMES input block. (See Sections 3.2.6 and 3.6.1.1 below.) One may use a restart to continue a given problem or alter the course of the calculation. The calculation in a restart is controlled by an input file similar to that used to initiate the calculation. In the simplest case (e.g., when a CPU time limit was encountered in the prior run), the only input required is the machine type, a RESTART keyword, a TIMES block, and an EOF. If changes in some parameters are desired, additional input may be used to make these changes. In a restart run, plot information is added to the existing plot file so that

continuous plots can be generated. New restart blocks are also added to the restart file.

The basic and most important premise of the restart capability is that the user may not restart a calculation with the intention of invoking a new physical model or option or of changing an old model in a manner which would increase array dimensions. Thus, the user should invoke all of the required physical models or options in the original run. In general what can be changed in a restart are values of parameters or arrays related to models or options used in the original run. Such parameters or arrays should either have been explicitly specified in the original run or have default values (as indicated in the input description) that were used in that run. The basic premise does not rule out a reduction in size in such arrays. However, prudence dictates that array sizes whenever possible be kept exactly the same as in the original run. While one cannot invoke new models or options, it is possible in a restart in a number of instances to turn off models, since this does not increase the array space required. In some cases, one may also turn on models which were turned off in a previous restart. Note that the restriction on what can be changed in a restart does not apply to certain execution-time control flags that are directly controlled by the user, such as those specified after HT-TRAN or the output option flags.

The keyword RESTART indicates to CONTAIN that the restart file and plot file(s) generated in the previous run should be used. As discussed in Section 3.6.1.1 below, restart calculations begin at time "tstart" specified in the new TIMES block or at the closest time following "tstart" found in the restart file. If "tstart" is larger than any time found on the restart file, the calculation will abort. However, the restart block times found will be written to the error file for inspection. (The user should backup the restart and plot files before any attempt at restart.)

The template for the restart input has the same basic structure as that for an original run: the machine control input is given first, then the global input, and finally the cell input. For parameters and arrays that are not specified in a restart, a rule different from that in an original run governs default values: a parameters remain the same unless specifically changed. For the cell input, it follows that only those cells for which changes are made need to be specified. The input template for a restart has the following form:

****

```
omach
RESTART
TIMES cput tstart (timinc edtdto tstop) [{(ctfrac) or
    CTFRAC=(ctmfr)}]
    [TRESTART=n (tres)]
    [TSFRAC=tsfrac]
    [EDMULT=edmult]
[EOI]
[LONGEDT=klong]
[SHORTEDT=kshort]
[PRFLOW
    {ON or OFF}]
```

```
[PRAER
    {ON or OFF}]
[PRAER2
    {ON or OFF}]
[PRLOW-CL
    {ON or OFF}]
[PRHEAT
    {ON or OFF}]
[PRFISS
    {ON or OFF}]
[PRFISS2
    {ON or OFF}]
[PRBURN
    {ON or OFF}]
(CELL=ncell
    [ATMOS
        SOURCE
            {OFF or ON
                nso
                    ((data)
                    EOI)}]
    [FISSION
        SOURCE
            {OFF or ON
                nso
                    ((data)
                    EOI)}]
    [AEROSOL=naero (omat mass)
        [SOURCE=nso
            ((data)
             EOI)]]
    [H-BURN
        {ON or OFF}]
    [STRUC
        OFF]
    [HT-TRAN (htflags)]
    [LOW-CELL
        {OFF or ON}
            [CORCON
                {OFF or
                TIMES tstart ndelt (dtmin dtmax dedit timdt)}]
            [SOURCE
                {OFF or ON
                    nso
                        ((data)
                        EOI)}]
    EOI])
EOF
```

****

In the following sections, keywords or input parameters that are unique to a restart run or that have special meanings in a restart run are described. Other keywords and input parameters are described in earlier sections and are not discussed in great detail. The input template shown above includes all of the input that is allowed in a restart run;

therefore, portions of this template are not repeated in the following sections.

3.6.1 Global Level Input for a Restart

The global level restart input is described in detail in this and the following two sections. Restart input decks must begin with a single word indicating the machine type. That word is followed by the single word RESTART.

Plot file reassignment is not allowed on restart. The plot and restart files produced in the original run must be available to CONTAIN in a restart, and these files must have the same names that they had in the original run. (These files should always, of course, be backed up.)

omach — the machine identifier. Since the restart file is created with unformatted FORTRAN writes, it is a binary file and must be read with the same type of machine that it was written with.

RESTART — keyword used to denote a restart.

3.6.1.1 The TIMES Block in a Restart. The TIMES block for a restart has exactly the same format as the TIMES block for an original run. That format is discussed in Section 3.2.6. The number of time zones specified in a restart run must be the same as that originally specified; however, the problem restart time can be any time within the new time zones. Values specified in a restart will override values specified in the previous run.

Only one parameter in the TIMES block, "tstart", has a meaning somewhat different from that in an original run:

tstart — problem restart time. Use a time less than or equal to the time of the restart block from which the job should start. Such times, with one exception, are given in the error or event summary file from the previous run. The exception is the temporary restart block from the last edit time encountered in the previous run. The time for that block is not given in the error or event summary files. However, that block will be the one used if the restart time is set slightly greater than the times of the other restart blocks but less than the problem time attained in the previous run. If the user wishes to know the time of the temporary restart block or any other block in the restart file, a restart can be attempted with a restart time greater than the problem time attained in the previous run. In that case, the restart run will abort after the input processing stage. However, the times for all restart blocks found in the restart file will be given for inspection in the new error file.

As indicated in Section 3.2.6, the user can put as many as 101 restart blocks on the restart tape. One of these restart blocks will always be a temporary block corresponding to the last edit time encountered (a plot

file write and a restart dump are always made at an edit time). In general such blocks are saved permanently in the restart file only at times specified through the TRESTART option or supplied as a default to that option. The exception is a temporary restart block which is used to restart a run. That block becomes a permanent part of the restart file.

Note that if TRESTART is not specified in a restart, the times at which restart blocks will be permanently saved in the restart run will be the end times of the time zones present on restart, not the restart times defined in the previous run. This selection of default restart block times on a restart constitutes a change from the practice prior to CONTAIN 1.1. This change, strictly speaking, violates the convention that in a restart the default values are those present in the previous run. However, it appears that many users expect that changing the end times of the time zones in a restart will also change the times that new restart blocks are saved on the restart file.

New data will be added to the existing plot and restart files starting at the time of the restart block used to restart. If the restart is initiated at a point prior to the problem time previously attained, the old plot and restart information after the restart point will be overwritten in order to accommodate the new data from the restart run. Note that the main output file, the error file, and the event summary file will always be completely overwritten in a restart.

3.6.1.2 Print Output Options in a Restart. The output options for the long edits written to the main output file are the same for a restart as those for an original run (see Section 3.2.7). However, in order to have the flexibility to turn off an option used in the previous run, each output option keyword must be followed by either the word ON or OFF. The word ON will enable the option, and the word OFF will disable it. If an output option keyword is omitted entirely then the status of that option will be the same as in the previous run.

Example:

```
PRFLOW OFF
PRLOW-CL ON
```

In the above example, flow output is suppressed, and lower cell output is activated.

3.6.2 Cell Level Input for a Restart

Certain models within any cell may be deactivated and certain parameters within any cell may be changed in a restart run. Certain models may also be activated, if deactivated on a previous restart. If no changes are desired in a given cell, that cell can be omitted from the restart input.

3.6.2.1 Upper Cell Restart Block. The upper cell models and parameters that may be modified on restart are shown in the restart input template between the keywords CELL and LOW-CELL. Only those portions of the upper cell restart input that differ from the initial input are described. Unless otherwise noted, the keywords described below are followed by either ON or OFF to activate or deactivate a particular model.

ATMOS SOURCE OFF — keyword sequence to turn off all atmospheric sources in the cell.

ATMOS SOURCE ON — keyword sequence to initiate the respecification of all atmospheric sources in the cell. Note that the first number required after the word ON is "nso", the number of tables to be specified. The "(data... EOI)" sequence in the input template is explained in detail in Sections 3.3.1.2 and 3.4. The number of tables and number of data points in the tables must not be greater than those initially specified.

FISSION SOURCE OFF — keyword sequence to turn off all fission product sources in the cell.

FISSION SOURCE ON — keyword sequence to initiate the respecification of all fission product sources in the cell. Note that the first number required after the word ON is "nso", the number of tables to be specified. The "(data... EOI)" sequence in the input template is explained in detail in Sections 3.3.1.9 and 3.4. The number of tables and the number of data points in the tables must not be greater than those initially specified.

AEROSOL — keyword to specify a new set of aerosol component masses and/or sources. These replace the current inventories and sources in the cell. The number of tables and the number of data points in the tables must not be greater than those initially specified. The format for this restart block is the same as that described in Section 3.3.1.8 for the original run. The words ON and OFF are not used in this restart input block.

H-BURN ON or OFF — keyword sequence to activate or deactivate the hydrogen and carbon monoxide burn model.

STRUC OFF — keyword sequence to deactivate heat transfer structures in the cell. Note that heat transfer structures cannot be reactivated in a restart run.

HT-TRAN — keyword to specify a set of five heat transfer flags. All five flags must be specified as either ON or OFF if HT-TRAN is specified. The flags are discussed in Section 3.3.1.6.

3.6.2.2 Lower Cell Restart Block. All lower cell processes may be disabled on restart or certain lower cell parameters may be modified. The lower cell models and parameters that may be modified on restart are shown in the restart input template after the LOW-CELL keyword.

LOW-CELL OFF — keyword sequence to deactivate the entire lower cell calculation in the cell. If the word OFF is given after the LOW-CELL keyword, additional lower cell input for the cell will not be allowed.

LOW-CELL ON	keyword sequence to initiate changes to various parameters or to activate or deactivate certain models in the lower cell as described below.
CORCON OFF	keyword sequence to disable the core-concrete interaction modeling using the CORCON model. The word ON cannot be specified after the CORCON keyword.
CORCON TIMES	keyword sequence to initiate changes in the timestep and edit frequency values specified in the previous run for the CORCON calculation. The TIMES keyword initiates the specification of the range of times during which CORCON will be active.
tstart	time to begin the CORCON calculation. This value will be ignored if the CORCON model is already active at the time of the restart. (s)
ndelt	number of time zones to be used for the CORCON calculation. In each time zone the bounds on the CORCON timestep and the edit frequency may be specified. This value must be followed by "ndelt" sets of ("dtmin", "dtmax", "dedit", "timdt"). The maximum value of "ndelt" is 10 and is not limited by the initial value of "ndelt".
dtmin	minimum allowed CORCON timestep. (s)
dtmax	maximum allowed CORCON timestep. (s)
dedit	time interval between CORCON edits. (s)
timdt	end time of the time zone. (s)
SOURCE OFF	keyword sequence to deactivate all lower cell sources.
SOURCE ON	keyword sequence to initiate the respecification of all lower cell sources in the cell. Such sources normally are specified independently for each layer. Here they must all be specified together, in the order presented in the lower cell input in the original run. Also note that the first number required after the word ON is "nso", the total number of tables to be specified. Note that the total number of tables and the number of tables for each layer may not be changed from those specified in the original run. The input represented by the sequence "(data... EOI)" in the input template is shown, for example, in Section 3.3.2.3.1 and described in Section 3.4.

4. OUTPUT

In a CONTAIN run, formatted output is written to the main output file, the error file, and the event summary file. (The characteristics of these files are given in Appendix B.) Because of its extent and variability, the output available on the main output file is the principal subject of discussion in the following sections. However, the latter two files are also discussed.

Section 4.1 discusses most of the output available in the main CONTAIN output file. There are two major types of output in this file: information from the initial processing of the input dataset and results from the time-dependent calculations. The input processing information states the models chosen, the parameters to be used, and, in some cases, the initial conditions. (In other cases, the initial conditions are given only in the initial edit for the time-dependent calculations.) The input processing is split into global and cell level portions corresponding to the level of the model being processed. Global input processing is discussed in Section 4.1.1, whereas cell level input processing is discussed in Section 4.1.2. The output from the time-dependent calculations is discussed in Section 4.1.3. Extensive examples of both the input processing information and the time-dependent output are given in these sections.

A significant part of the output on the main file that is not discussed in Section 4.1 is the output from the CORCON/VANESA module within CONTAIN. Because of the documentation available for CORCON/VANESA [Col84,Pow86], the discussion of the CORCON/VANESA output is given separately in Section 4.2. Section 4.2 does not attempt to reproduce the discussion in the separate documentation. However, it does illustrate how CORCON/VANESA output has been merged into the CONTAIN output file.

Finally, Section 4.3 discusses how to find diagnostic messages that are written to the output files. Diagnostic messages are normally written to the error file, although in some cases they are also written to the main output file. As discussed in Section 4.3, the user should always check the error file for diagnostic messages about conditions that may adversely affect the calculation, even if the code does not abort.

In addition to the formatted output, the code writes data to plot files in binary form for use in producing tabular and graphic displays of code results (see Appendix E). The POSTCON postprocessor program reads the plot files and produces a wide variety of results in tabular and graphic form. The user is directed to Reference Was87 for a discussion of the latter program.

4.1 CONTAIN Output

The first part of the output in the main output file is an echo of the input file. It is provided to give the user an accurate record of the input used in a particular run. (The input file is also echoed to the error file, along with any diagnostic messages, to help the user locate input errors.)

The second part of the output is the input processing section. This part of the output is fairly extensive and complete. It presents both the user-specified input data and default values for data that are not specified. The input processing is divided into global and cell level parts. The global input processing is done first. The cell level input processing is then done for each cell in the problem. The output from global input processing is discussed in the next section, whereas the output from cell level input processing is discussed in Section 4.1.2.

The input processing information from a particular input block is in general bracketed by lines that have a special format. These lines may be used to help find the processing for that input block in output file. The input processing for a given input block begins with a line of the form "++++ input (xxxxxx) - process ... section" and is terminated by a line "++++ input (xxxxxx) ... section completed", where xxxxxx is the keyword for the input block.

The third and final part of the output in the main output file is that from the time-dependent calculations. This output is discussed in Section 4.1.3. The user should note that some of the time-dependent output is optional and must be requested through keywords. These keywords are discussed in Section 4.1.3 in conjunction with the output that they control. (The output that in general is not optional includes the input processing information, a minimal amount of information from the time-dependent calculations, messages about certain events occurring in the calculation, and diagnostic output. Diagnostic output may be written to either the main output file or the error file; event messages are normally written to either the main output file or error file and the event summary file.)

Most of the CONTAIN output is self-explanatory; however, some of the labeling of the output is quite concise to keep the output reasonably compact. That labeling may require more explanation, and where necessary that explanation is given below. Portions of the output that are self-explanatory are not discussed.

The figures in the following sections give examples of selected parts of the output. The numbers in boxes in the figures are used to indicate that that portion of the figure is discussed separately in the text. The discussion of that portion follows the corresponding number in parentheses in the text.

4.1.1 Global Input Processing

Figures 4-1 through 4-5 show examples of the output from the global input processing. That output always starts with the global control parameter information, followed by the material names information. After this output, the input processing information for specific input blocks are in general given in the order in which the input blocks appear in the input file. Exceptions include single keyword options, such as PRAERO, and the FPM-CELL input block. Separate input processing information blocks are in general not given for single keyword options that simply result in the setting of appropriate flags. The user, however, may determine the

```
****************************************
*                                      *
*         global input section         *
*                                      *
****************************************

global control parameters ...

    total number of cells ..................... ncells =   3
    number of title cards ..................... ntitl =   1
    number of time zones ...................... ntzone =   2
    number of fission product chain elements ... nfce =  11
    number of fission product chains ......... nchain =   4
    number of aerosol sections ............... nsectn =  10
    number of aerosol components ................ nac =   4
    total number of chain elements targeted .... ntgt =  30
    number of extra material hosts (unused) ... nhmo  =   0
    number of engineered vents ................ nengv =   0
    number of words reserved for u.d.m. .......nwdudm =   0
    number of global tables ................... numtbg =   0
    max. no. of table entries (per table) .... maxtbg =   0

adjusted global control parameters ...

    number of fission product chain elements ... nfce =  11
    number of fission product chains ......... nchain =   4
    total number of structures ................ nhtmt =   6
    total number of lower-cell layers ......... nlays =   6

derived global control parameters ...

    number of materials ........................... nm =  13
    number of fission product names ............. nnuc =  11
    total number fission product hosts .......... nhm =  39
    number of user defined materials ............nudm =   0
    extended storage option ................... iver = incore

   13 materials present
      gas       n2        o2        h2        co        co2       fe        fel       fev       ss
      conc      h2ol      h2ov
```

1

2

Figure 4-1 Global Control Parameters and Material List

```
++++ input (times    ) - process global times section.


    maximum cpu time limit ... cput =  1.8000e+03 (s)
    problem start time ..... tstart =  0.0000e+00 (s)

    time-zone       system time         long edit         time-zone
       no.            step size         increment             end

          1          1.0000e+01        1.0000e+01        2.0000e+02
          2          1.0000e+02        1.0000e+02        1.0000e+03

                      step size
     cell no.          fraction

          1          1.0000e+00
          2          1.0000e+00
          3          1.0000e+00

    internal timesteps will be reduced by a factor   1.00000e+00


    edits for internal timesteps will occur every default number of timesteps

    problem restart times (s) :

                2.00000e+02  1.00000e+03

++++ input (times    ) - global times section completed.
```

3

4

Figure 4-2 Timestep Control

```
++++ input (flows    ) - process global flow section.


    intercell flow - initial conditions


         intercell flow from cell number ..... i =  1
         intercell flow to cell number ..... j =  2
         x-sectional area of path (m**2) ..... area =  1.00000e-01
         initial state of flow path ..... ofstat =closed
         specified time to open (s) ..... topen =  1.00000e+01
         specified time to close ..... tclose =  1.00000e+30
         pressure req'd to open forward (pa) ..... dp =  0.00000e+00
         pressure req'd to open reverse (pa) ..... dp =  0.00000e+00

         flow calculation will be inertial, with
         initial flow rate (kg/s) ..... flow =  0.00000e+00
         area to length ratio (m) ..... avl =  1.00000e-02
         turbulent flow coefficient ..... cfc =  8.00000e-01

                                                                  5

         intercell flow from cell number ..... i =  1
         intercell flow to cell number ..... j =  3
         x-sectional area of path (m**2) ..... area =  1.00000e-05
         initial state of flow path ..... ofstat =closed
         specified time to open (s) ..... topen =  1.00000e+02
         specified time to close ..... tclose =  1.00000e+30
         pressure req'd to open forward (pa) ..... dp =  0.00000e+00
         pressure req'd to open reverse (pa) ..... dp =  0.00000e+00

         flow calculation will be inertial, with
         initial flow rate (kg/s) ..... flow =  0.00000e+00
         area to length ratio (m) ..... avl =  1.00000e-04
         turbulent flow coefficient ..... cfc =  2.00000e+00


    note> buoyancy, choked flow, and special flow path options are modeled only with the implicit flow solver option

         the implicit flow solver option will be used

         parameters relevant to the implicit solver

         for flow path from cell ..... j =  1
                        to cell ..... i =  2
         reference elevation for pressure in cell j . =  0.00000e+00
         reference elevation for pressure in cell i . =  0.00000e+00
         elevation of flow path end at cell j ..... =  0.00000e+00
         elevation of flow path end at cell i ..... =  0.00000e+00
         multiplier for choked flow vena contracta  . =  1.00000e+00

                                                                  6

         for flow path from cell ..... j =  1
                        to cell ..... i =  3
         reference elevation for pressure in cell j . =  0.00000e+00
         reference elevation for pressure in cell i . =  0.00000e+00
         elevation of flow path end at cell j ..... =  0.00000e+00
         elevation of flow path end at cell i ..... =  0.00000e+00
         multiplier for choked flow vena contracta  . =  1.00000e+00


++++ input (flows    ) - global flow section completed.
```

Figure 4-3 Intercell Flow Paths and Flow Options

```
++++ input (fission ) - process global fission product section.


    global fission product input : names, half lives, and power coefficients


    chain no.  1 is comprised of  3 linear chain elements
    no.  name       halflife   (units)       power coeficients
     1  moli133    7.44800e+04  seconds     1.23000e+04
     2  xe133      4.53600e+03  seconds     3.46000e+03
     3  cs133      0.00000e+00  seconds     0.00000e+00

    chain no.  2 is comprised of  2 linear chain elements
    no.  name       halflife   (units)       power coeficients
     1  cs137      1.81000e+03  seconds     1.17300e+03
     2  ba137      0.00000e+00  seconds     0.00000e+00

    chain no.  3 is comprised of  3 linear chain elements
    no.  name       halflife   (units)       power coeficients
     1  te132      7.80000e+01  hours       2.15000e+02
     2  orgi132    2.29000e+00  hours       1.61000e+03
     3  xe132      0.00000e+00  hours       0.00000e+00

    chain no.  4 is comprised of  3 linear chain elements
    no.  name       halflife   (units)       power coeficients
     1  sr90       2.46000e+05  seconds     5.46000e+03
     2  y90        2.30000e+05  seconds     2.28000e+04
     3  zr90       0.00000e+00  seconds     0.00000e+00


++++ input (fission ) - global fission product section completed.
```

7

Figure 4-4 Global Fission Product Parameters

```
++++ input (aerosol ) - process global aerosol section.

    the aerosol coefficients exist in the data base ... they were generated on 87/09/18

        number of aerosol sections ..... nsectn =       10
        lower diameter limit (m) ..... diam1 =  1.00000e-07
        upper diameter limit (m) ..... diam2 =  1.00000e-04
        lower temperature limit (k) ..... tgas1 =  2.73000e+02
        upper temperature limit (k) ..... tgas2 =  1.20000e+03
        lower pressure limit (pa) ..... pgas1 =  5.00000e+04
        upper pressure limit (pa) ..... pgas2 =  1.20000e+06
        turbulent diss rate (m**2/s**3) ..... turbds =  1.00000e-03
        collision efficiency ..... coleff = (calculated)

        aerosol material density (kg/m**3) .. densty =  1.00000e+03
        dynamic shape factor ..... chi =  1.00000e+00
        agglomeration shape factor ..... gamma =  1.00000e+00
        diffusion boundary thickness (m)..... deldif =  1.00000e-05
        thermal conductivity ratio ..... tkgop =  5.00000e-02
        relative error tolerance ..... reltol =  1.00000e-03
        absolute error tolerance ..... abstol =  1.00000e-04

    the aerosol materials are :

        cs137-a   te132-a   sr90-a    h2ol

    condensation on aerosols will occur for a <thermal> reactor

    evaporation from aerosols will occur for a <thermal> reactor

    the ranges (meters) of particle size diameters are :

          1.00000e-07  to   1.99526e-07
          1.99526e-07  to   3.98107e-07
          3.98107e-07  to   7.94328e-07
          7.94328e-07  to   1.58489e-06
          1.58489e-06  to   3.16228e-06
          3.16228e-06  to   6.30957e-06
          6.30957e-06  to   1.25893e-05
          1.25893e-05  to   2.51189e-05
          2.51189e-05  to   5.01187e-05
          5.01187e-05  to   1.00000e-04

++++ input (aerosol ) - global aerosol section completed.
```

8

9

Figure 4-5 Global Aerosol Parameters

status of the relevant flags by inspecting the flag table given later on in the output, as discussed in Section 4.1.2.12. Also, if the FPM-CELL input block is given as part of the FISSION input block at the global level, the input processing information about FPM-CELL will be given at the end of the input processing section. As discussed in Section 4.1.2, that may also happen under certain circumstances when the FPM-CELL block is given at the cell level.

4.1.1.1 Global Control Parameters and Material List. (1) The global control parameter information is shown in Figure 4-1. The values of global control parameters are displayed in three groups as shown in that figure. The values that are specified by the user in the global CONTROL block are included in the first group. The values in the second group are those that have been determined by the code by scanning and counting the relevant items in the input file. Thus, the values of "nfce" and "nchain" in the second group may differ from those specified by the user. (The user is allowed to specify such values for upward compatibility. However, in the event of a discrepancy, the values in the second group are used.) The "nhtmt" and "nlays" values represent a sum over all cells of the number of structures and lower cell layers, respectively. Other values that are obtained by scanning the input and counting the relevant items, but that may not also be specified by the user, are shown in the third group. The "nnuc" and "nudm" parameters are obtained by counting the number of fission product names and user-defined material names specified by the user. The "nm" and "nhm" values are described below.

"Nm" is the total number of materials that are used in the calculation, excluding those that are strictly associated with aerosols and fission products. This value is automatically determined from the number of materials specified in the COMPOUND and USERDEF input blocks and the number of default materials that are automatically included in every CONTAIN calculation. The default materials are N2, O2, H2, CO, CO2, H2OL, and H2OV. In addition, if CORCON is specified in one of the cells, the materials UO2, FE, LCCHOX, LCCMET, and LCCLOX are automatically included as default materials. For certain materials, if the solid phase of a material is specified, space for all three phases (gas, liquid, solid) is automatically allocated in the storage arrays. The materials for which this is automatically done are H2O, NA, FE, UO2, and PUO2.

"Nhm" is the total number of fission product hosts in all cells. This value is automatically determined from the number of aerosol components, the total number of structures, the total number of lower cell layers, and the number of cells in the problem. The actual formula used is "nhm" = (1+"nac")*"ncells" + 2*"nhtmt" + "nlays" + 2*"ncells".

(2) The names of the (nonaerosol and non-fission-product) materials used in the run are printed by the code as shown in Figure 4-1. Exactly "nm" names will be shown. These materials will be a combination of those specified by the user and the default materials as described above. This output always immediately follows the global control parameter output.

4.1.1.2 Timestep Control. (3) An example of the input processing information for the TIMES input block is shown in Figure 4-2. The labels "system timestep size" and "long edit increment" in this figure are not strictly correct. The first should refer to the maximum system timestep

and the second should refer to the edit timestep. Long edits may actually occur at some multiple (specified through the LONGEDT keyword) of the edit timestep. Both of these timesteps are discussed in Section 3.2.6. Cell modules use a maximum cell timestep equal to the product of the system time step and the cell step size fraction shown in Figure 4-2. The internal timesteps referred to in this output are system timesteps calculated by the code to be used instead of the user-specified timestep when certain processes, such as hydrogen burns, occur in the problem. They and the edit interval during such processes are discussed in Section 3.2.6.

(4) The problem restart times are shown in Figure 4-2. Restart times may be specified through the TRESTART keyword. Since this keyword is not used in the input used to generate Figure 4-2, the restart times are by default the end times of each time zone.

4.1.1.3 Intercell Flow. (5) As shown in Figure 4-3, the first part of the information from flow input processing describes the flow path arrangements and gives the parameters used in both the explicit and implicit flow solver options. (6) If the implicit flow option is selected, the parameters relevant to that option are given in the second part of the report as illustrated in Figure 4-3. Output similar to that in Figure 4-3 would also be provided for engineered vent flow paths if these had been specified.

4.1.1.4 Global Fission Product Parameters. (7) Fission product half-lives and decay power coefficients are shown for each decay chain in Figure 4-4. The parent-daughter relationships are also indicated. For fission products for which decay power has been specified, as many as four power coefficients may be printed. These coefficients are defined as a_1 through a_4, respectively, in the expression for the specific power given in Equation 2-23. Note that only one coefficient should be used for fission products that represent individual nuclides and not a fission product group.

4.1.1.5 Global Aerosol Parameters. (8) Aerosol modeling parameters are as shown in Figure 4-5. The term "calculated" signifies that the code will calculate the values of that particular parameter using internal analytic expressions.

(9) This block also gives the names of the aerosol materials specified for the problem and the particle size range to be used for each size class.

4.1.2 Cell Level Input Processing

Cell level input processing is done on a cell-by-cell basis. The order in which the cells are processed with respect to input is the order in which the cells are specified in the input file. (However, in the time-dependent calculations, the cells are processed in numerical order.) Figures 4-6 through 4-15 give examples of the output from the input processing of different cell level input blocks within a given cell. An appropriate set of such output will be present for each cell in the problem.

```
****************************************
*                                      *
*                                      *
*          cell input section          *
*              cell no. 1              *
*                                      *
*                                      *
****************************************

control parameters - cell no.    1

     cell number ............................. ncell =   1
     number of heat transfer structures ..... nhtm =   4
     maximum no. of heat transfer nodes ..... mxslab =  10

     number of pool sources .................. nsopl =   0
     no. of points in pool sources ........... nsppl =   0
     number of atmospheric sources ........... nsoatm =  2
     no. of points in atmos sources .......... nspatm =  2
     number of spray sources ................. nsospr =  0
     no. of points in spray sources .......... nspspr =  0
     number of aerosol sources ............... nsoaer =  2
     no. of points in aerosol sources ........ nspaer =  3
     number of fission product sources ....... nsofp =   3
     no. of points in fission product sources .. nspfp =  3

     number of srv atmospheric sources .....nsosat =   0
     no. of points in srv atmospheric tables .. nspsat =  0
     number of srv aerosol sources .....nsosae =   0
     no. of points in srv aerosol tables ..... nspsae =  0
     number of srv fission sources .....nsosfp =   0
     no. of points in srv fission tables ..... nspsfp =  0

     number of engineering systems ........... naensy =  1
     number of engineering sources ........... nsoeng =  1
     no. of points in engineering sources ..... nspeng =  3

     number of concrete layers ............... jconc =   0
     number of intermediate layers ........... jint =   0
     number of pool layers ................... jpool =   0
     number of atmospheric layers ............ jatm =   1

     number of cell level tables ............. numtbc =  0
     maximum no. of table entries (ea table) .. maxtbc =  0

     number of corcon rays  .................. nraycc =  0
     number of vanesa fission products  ..... nvfpsm =  0
```

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Figure 4-6 Cell Control Parameters

```
++++ input (atmos   ) - process cell atmos section.

    atmospheric data in cell no.  1

         number of gases in atmosphere ..... nma =  3
         total mass (kg) ..................... tmgas =  1.50684e+03
         gas temperature (k) ................. tgas =  3.20000e+02
         gas pressure (pa) ................... pgas =  1.20000e+05
         gas heat capacity (j/kg/k) ......... cvgas =  7.69700e+02
         internal energy of gas (j) ......... ugas =  1.44776e+08
         mean molecular weight (kg/kg-mole) ... wtmol =  2.78407e+01
         volume of gas (m**3) ................ volume =  1.20000e+03
         density of gas (kg/m**3) ............ rhogs =  1.25570e+00

++++ input (atmos   ) - cell atmos section completed.

++++ input (source  ) - process cell atmospheric-source section.

     2  gas sources :

    source table for h2ov     with    2 data points

    time (s)     0.000e+00 1.000e+02
    mass (kg/s)  5.000e+00 0.000e+00
    enth (j/kg)  2.547e+06 0.000e+00

                 (source table is a step function)

    source table for h2       with    2 data points

    time (s)     0.000e+00 1.000e+01
    mass (kg/s)  1.000e+01 0.000e+00
    temp (k)     3.000e+02 3.000e+02

                 (source table is a step function)

     2  gas sources :
          h2ov    h2

++++ input (source  ) - cell atmospheric-source section completed.
```

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Figure 4-7 Upper Cell Atmosphere Initial Conditions and Sources

```
++++ input (h-burn  ) - process cell hydrogen-burn section.

    hydrogen burn - initial conditions

         initial cell elevation (m) ..... elev =  0.00000e+00
         cell characteristic length (m) ..... chrl =  1.06266e+01
         propagation delay fraction ..... kprop =  5.00000e-01
         burn time (s) ..... burnt = (calculated)
         fraction of initial combustible ... cfrmng =  1.00000e-02
         flame speed (m/s) ..... flam = (calculated)
         burns will be initiated only after  tactiv =  2.00000e+01
         burns will be suppressed after .....tdeact =  7.00000e+01

         mole fractions for propagation into this cell
                             combustible         oxygen          steam

            spontaneous      1.00000e-03      1.00000e-02      9.90000e-01
            horizontal       6.00000e-02      5.00000e-02      5.50000e-01
            upward           4.10000e-02      5.00000e-02      5.50000e-01
            downward         9.00000e-02      5.00000e-02      5.50000e-01

++++ input (h-burn  ) - cell hydrogen-burn section completed.

++++ input (condense) - process cell condensation section.

    condense option is active

    maximum condensate film depth (m), flmax=  1.00000e-05

++++ input (condense) - cell condensation section completed.

++++ input (overflow) - process fp and aerosol overflow section.

    overflow and runoff are to cell    2 (from cell    1 )

++++ input (overflow) - fp and aerosol overflow section completed
```

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Figure 4-8 Combustion Model Parameters, Condensation Option, and Cell Overflow Option

```
++++ input (engineer) - process engineering systems section.


   an engineered system called :  sprays   is defined comprising  2 component(s) ...

        system source ... originates from cell    1
        system sink ..... terminates in cell    2
        elevation drop (m) ... inlet to outlet =  1.00000e+01


   source table for h2o1     with    3 data points

   time (s)     0.000e+00 1.000e+02 1.500e+02
   mass (kg/s)  0.000e+00 1.000e+02 0.000e+00
   temp (k)     2.830e+02 2.830e+02 2.830e+02

                (source table is a step function)

 1 engineered system sources=   h2o1


        the system includes a containment spray component with the following characteristics ...

             average droplet diameter (m) ........ spdiam =  1.00000e-03
             initial i2 partition coefficient .... sppci2 =  2.50000e+03
             methyl iodide partition coeff ....... sppcmi =  5.00000e+02
             cell pres to initiate spray (pa) .... spstpr =  0.00000e+00
             cell temp to initiate spray (k) ..... spsttm =  0.00000e+00
             spray height above floor (m) ........ sphite =  7.50000e+00

        the system is comprised of  2 components
        system source originates from cell    1
        system sink terminates in cell    2
        elevation drop (m) inlet to outlet   1.00000e+01


++++ input (engineer) - engineering systems section completed.
```

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Figure 4-9 Engineered Systems Parameters

```
++++ input (low-cell) - process lower-cell section.


    lower cell conditions in cell   2     at time =      0.000 (s)

          layer                                  average        materials present
        no   name        kz     depth (m)      temp (k)        mass (kg)   name
      ---------------   ---------------       --------      ------------------------

        3    pool         1  1.00000e-03        280.00        1.00000e+02   h2ol

        2    debris       1  2.55955e-03        900.00        1.00000e+03   fe
                                                             1.00000e+03   ss
        1    concrete     5  4.19174e-03        280.00        2.00000e+01   fe
                                                             1.00000e+03   conc
        1    concrete     4  4.19174e-03        280.00        2.00000e+01   fe
                                                             1.00000e+03   conc
        1    concrete     3  4.19174e-03        280.00        2.00000e+01   fe
                                                             1.00000e+03   conc
        1    concrete     2  4.19174e-03        280.00        2.00000e+01   fe
                                                             1.00000e+03   conc
        1    concrete     1  4.19174e-03        280.00        2.00000e+01   fe
                                                             1.00000e+03   conc

    heat transfer information ...

          layer          x-section     from - to   heat tran coef   heat tran rate                temperature (k)
        no   name        area (m**2)   (l1 - l2)     (w/m**2/k)       (w/m**2)       l#-(    top     middle    bottom)
      ---------------   -----------   ---------   --------------   --------------   ------------------------------

        4    atmos       1.00000e+02     4 -  3      0.00000e+00      0.00000e+00

        3    pool        1.00000e+02     3 -  2      0.00000e+00      0.00000e+00     1-( 280.00    280.00    280.00)

        2    debris      1.00000e+02     2 -  1      0.00000e+00      0.00000e+00     1-( 900.00    900.00    900.00)

        1    concrete    1.00000e+02     1 -  0      0.00000e+00      0.00000e+00     5-( 280.00    280.00    280.00)
                                                                                      4-( 280.00    280.00    280.00)
                                                                                      3-( 280.00    280.00    280.00)
                                                                                      2-( 280.00    280.00    280.00)
                                                                                      1-( 280.00    280.00    280.00)

    cumulative gas-pool exchange amounts

        coolant mass evolved (kg) .....   0.00000e+00
        energy transferred to gas (j) .   0.00000e+00


++++ input (low-cell) - lower-cell section completed.
```

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Figure 4-10 Lower Cell Initial Conditions

```
++++ input (struc   ) - process cell structures section.

   data for heat conduction lump no.    1          structure title = dome

        the structure is a roof     with a shape of a sphere   with   5 nodes
        the outer face of the structure is located in cell no.  0
        the outer face of the structure sees a constant temperature of   280.00 (k)

        node number                          1           2           3           4           5
        compound names                      ss          ss          ss          ss          ss
        node temperatures (k)          2.8000e+02  2.8000e+02  2.8000e+02  2.8000e+02  2.8000e+02
        total masses (kg)              5.0326e+05  5.1332e+05  5.2348e+05  5.3375e+05  5.4411e+05
        interface positions (m)    1.0000e+01  1.0100e+01  1.0200e+01  1.0300e+01  1.0400e+01  1.0500e+01
        surface areas (m**2)       6.2832e+02  6.4095e+02  6.5370e+02  6.6658e+02  6.7959e+02  6.9272e+02

   data for heat conduction lump no.    2          structure title = wall1

        the structure is a wall     with a shape of a slab     with   8 nodes
        the outer face of the structure is located in cell no.  1

        node number                          1           2           3           4           5
        compound names                      fe          fe          fe          fe        conc
        node temperatures (k)          2.8000e+02  2.8000e+02  2.8000e+02  2.8000e+02  2.8000e+02
        total masses (kg)              7.9759e+04  7.9759e+04  7.9759e+04  7.9759e+04  2.4000e+04
        interface positions (m)    0.0000e+00  1.0000e-01  2.0000e-01  3.0000e-01  4.0000e-01  5.0000e-01
        surface areas (m**2)       1.0000e+02  1.0000e+02  1.0000e+02  1.0000e+02  1.0000e+02  1.0000e+02

        node number                          6           7           8
        compound names                    conc        conc        conc
        node temperatures (k)          2.8000e+02  2.8000e+02  2.8000e+02
        total masses (kg)              2.4000e+04  2.4000e+04  2.4000e+04
        interface positions (m)    5.0000e-01  6.0000e-01  7.0000e-01  8.0000e-01
        surface areas (m**2)       1.0000e+02  1.0000e+02  1.0000e+02  1.0000e+02

   data for heat conduction lump no.    3          structure title = wall2

        the structure is a wall     with a shape of a slab.    with   4 nodes
        the outer face of the structure is located in cell no.  1

        node number                          1           2           3           4
        compound names                      fe          fe          fe          fe
        node temperatures (k)          3.2000e+02  3.2000e+02  3.2000e+02  3.2000e+02
        total masses (kg)              3.9791e+04  3.9791e+04  3.9791e+04  3.9791e+04
        interface positions (m)    0.0000e+00  1.0000e-01  2.0000e-01  3.0000e-01  4.0000e-01
        surface areas (m**2)       5.0000e+01  5.0000e+01  5.0000e+01  5.0000e+01  5.0000e+01

   data for heat conduction lump no.    4          structure title = floor1

        the structure is a floor    with a shape of a slab     with   5 nodes
        the outer face of the structure is located in cell no.  2

        node number                          1           2           3           4           5
        compound names                      fe          fe          fe          fe          fe
        node temperatures (k)          3.2000e+02  3.4000e+02  3.6000e+02  3.8000e+02  4.0000e+02
        total masses (kg)              7.1623e+04  7.1544e+04  7.1464e+04  7.1384e+04  7.1304e+04
        interface positions (m)    0.0000e+00  1.0000e-01  2.0000e-01  3.0000e-01  4.0000e-01  5.0000e-01
        surface areas (m**2)       9.0000e+01  9.0000e+01  9.0000e+01  9.0000e+01  9.0000e+01  9.0000e+01

++++ input (struc   ) - cell structures section completed.
```

Figure 4-11 Heat Transfer Structure Parameters

```
++++ input ( fpm-cell ) - process fission product hosting section.


    targeted release map for cell no. 1 rate (per sec) = a * exp[-b/t],t>=threshold
       element      from host --> to host              a             b          threshold t
      no. name      no. name      no. name

        7  orgi132     3  te132-a     1  gas        2.00000e+00   0.00000e+00   0.00000e+00
        2  xe133       6  dome        1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132       6  dome        1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        2  xe133       8  wall1       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        2  xe133       9  wall1       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        2  xe133      10  wall2       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        2  xe133      11  wall2       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132       8  wall1       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132       9  wall1       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132      10  wall2       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132      11  wall2       1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        2  xe133      12  floor1      1  gas        1.00000e+01   0.00000e+00   0.00000e+00
        8  xe132      12  floor1      1  gas        1.00000e+01   0.00000e+00   0.00000e+00

    initial fission product host masses and untargeted release and acceptance fractions
    in cell  1 having 15 hosts

    host no.   3 host name : te132-a
    chain   1  moli133  ---->   xe133    ---->   cs133    ---->
    masses :    0.000e+00        0.000e+00        0.000e+00
    chain   2  cs137    ---->   ba137    ---->
    masses :    0.000e+00        0.000e+00
    chain   3  te132    ---->   orgi132  ---->   xe132    ---->
    masses :    1.000e+00        0.000e+00        0.000e+00
    chain   4  sr90     ---->   y90      ---->   zr90     ---->
    masses :    0.000e+00        0.000e+00        0.000e+00

++++ input ( fpm-cell ) - fission product hosting section completed.
```

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Figure 4-12 Targeted Release and Acceptance Map and Fission Product Initial Masses

```
++++ input (fission ) ++++ input (source  ) - process cell fission-source section.


     3  fission product sources :


    source table for moli133  with    2 data points

    time (s)      0.000e+00 1.000e+02
    mass (kg/s)   1.000e-02 0.000e+00


                (source table is a step function)

    source table for cs137    with    3 data points

    time (s)      0.000e+00 5.000e+01 1.500e+02
    mass (kg/s)   0.000e+00 1.000e-02 0.000e+00


                (source table is a step function)

    source table for sr90     with    3 data points

    time (s)      0.000e+00 5.000e+01 1.500e+02
    mass (kg/s)   0.000e+00 1.000e-02 0.000e+00


                (source table is a step function)

     3  fission product sources :
           moli133 cs137   sr90


++++ input (fission ) ++++ input (source  ) - cell fission-source section completed.
```

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Figure 4-13 Fission Product Sources

```
++++ input (aerosol ) - process cell aerosol section.


    aerosol data in cell no.  1

         aerosol component      initial mass (kg)

            te132-a                1.0000e+02
            h2ol                   1.0000e-02

    source table for cs137-a  with    3 data points

    time (s)      0.000e+00 5.000e+01 1.500e+02
    mass (kg/s)   0.000e+00 1.000e+00 0.000e+00


                (source table is a step function)

    source table for sr90-a   with    3 data points

    time (s)      0.000e+00 5.000e+01 1.500e+02
    mass (kg/s)   0.000e+00 1.000e+00 0.000e+00


                (source table is a step function)

        2 aerosol sources :

              cs137-a sr90-a


++++ input (aerosol ) - cell aerosol section completed.
```

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Figure 4-14 Aerosol Initial Masses and Sources

summary of active global, cell and layer flags ...

	global flags 1 1 1 1 1 1 1 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6	cell flags 1 1 1 1 1 1 1 1 1 1 2 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0	layer flags 1 1 2 3 4 5 6 7 8 9 0
global	s s s s s s s s s s s s		
cell 1		c c c c c c c c c	
cell 2		c c c c c c c c	
layer 4			
layer 3			
layer 2			
layer 1			
cell 3		c	
layer 2			
layer 1			

	global flags 1 1 1 1 1 1 1 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6	cell flags 1 1 1 1 1 1 1 1 1 1 2 1 2 3 4 5 6 7 8 9 0 1 2 3 4 5 6 7 8 9 0	layer flags 1 1 2 3 4 5 6 7 8 9 0

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note : inactive flags (off or false) are not printed in above matrix.

global flags - descriptor

1	flowf	- intercell flow
2	prflf	- intercell flow output
3	prspf	- sodium spray fire output
4	praef	- aerosol output
5	prlcf	- lower cell output
6	prhtm	- heat transfer output
7	prfpf	- fission product output
8	prbrn	- hydrogen burn output
9	nrfast	- fast reactor
10	nfaers	- aerosol model
11	nffis	- fission product model
12	matflg	- material property
13	nrther	- light water reactor
14	prwsp	- inactive
15	preng	- engineered system output
16	pruser	- user output

cell flags - descriptor

1	nfhtxf	- heat transfer module
2	nfspry	- sodium spray fire module
3	lowcel	- lower cell model
4	nfcond	- condensation model
5	nfgasc	- gas source
6	nsfatm	- fission product source for atmosphere
7	nsfspr	- sodium spray source
8	nsfaer	- aerosol source
9	nsffp	- fission product source
10	nfburn	- hydrogen burn
11	hthas	- heat transfer: atmosphere to structure
12	htuply	- h. t.: upper to lower atmosphere
13	htloly	- h. t.: lower to sub-structure
14	htlay	- h. t.: layer to layer
15	htrad	- radiation heat transfer
16	nfchem	- atmosphere sodium & hydrogen chemistry
17	nfengs	- engineered system
18	nfseng	- engineered system source
19	nfspwo	- spray washout of aerosols

Figure 4-15 Summary of Global, Cell, and Layer Flags

The first section in the output for a given cell gives the cell control parameters. The order of subsequent output will depend on the ordering of input blocks in the input file. In general the output will be given in the order that the input blocks are present in the input file. However, as discussed below, output for the FPM-CELL block may be moved to the end of the input processing section.

In processing a given input block, information is often required that is available only after other input blocks have been processed. One input block that has this dependency on other input blocks is FPM-CELL. FPM-CELL may therefore be processed by an initialization routine at the end of all other input processing. If this happens, the input processing information and diagnostic messages for FPM-CELL will be placed at the end of the input processing section.

4.1.2.1 Cell Control Parameters. (10) The cell control parameter information is illustrated in Figure 4-6. These control parameters all have defaults of zero (except "jatm", the atmosphere layer control parameter, which defaults to 1). (Note that even though "jatm" is shown as 1, this value is irrelevant in the case shown since a lower cell is not considered by the code to be present in the cell. Other solid or liquid layers would have to be present for the lower cell to be considered present.)

4.1.2.2 Upper Cell Atmosphere Initial Conditions and Sources. (11) The information from cell atmosphere input processing is illustrated in Figure 4-7. The initial conditions shown follow a convention followed in the time-dependent output; namely, in the case of a saturated atmosphere, the gas density, heat capacity, and molecular weight exclude the contribution of the liquid phase of the condensable. Note also that the internal energy of the cell atmosphere may be negative at low gas temperatures, since the enthalpies of noncondensable gases included in the CONTAIN material library are set to zero at a reference temperature of 273.15 K.

(12) The information about user-specified atmospheric source tables is illustrated in Figure 4-7. The time, mass, and enthalpy (or temperature) points are given for each source table specified in the input block. A message is printed after each source table indicating whether the table is to be interpolated in a step-wise fashion or whether it is to be interpolated linearly.

Note that any number of source tables for the same material may be specified. The effects of the tables will be additive. Also note that aerosol, fission product, lower cell, and engineered system source tables are defined in their own input blocks and should not be specified in the ATMOS block.

4.1.2.3 Hydrogen and Carbon Monoxide Combustion. (13) If the hydrogen and carbon monoxide combustion model has been enabled in a given cell through the H-BURN input block, information similar to that shown in Figure 4-8 will be given. The word "calculated" implies that a default internal analytic expression will be used to calculate values that will vary with conditions.

4.1.2.4 Condensation on Structures.. (14) The input processing information for the CONDENSE input block is illustrated in Figure 4-8. If the FORCED option within CONDENSE had been used, the tabular data associated with this option would also be displayed in this report.

4.1.2.5 Cell Overflow. (15) Information is given if the user has specified the cell OVERFLOW keyword to direct condensate runoff and aerosol mesh losses to a cell different from the cell being processed. This option is intended to redirect condensate runoff and mesh losses from the current cell. Thus, if the user does not explicitly specify a different cell, the output shown will not be present. If the user specifies zero for the overflow cell, a message will be given to indicate that condensate runoff and aerosol mesh losses will be lost from the problem.

4.1.2.6 Engineered Systems. Any number of engineered systems may be specified in a given cell, and each system may be comprised of several components. Each component of each system specified is indicated as illustrated in Figure 4-9. (16) A source table component of an engineered system is described as shown. Note that a source table represents an external source and does not imply that mass is drawn at the specified rate from the cell labeled as the "system source." (17) The principal component of the system, such as spray, is also described. The output may include various parameters characterizing that component. (18) Each engineered system description is concluded by a summary giving the number of components, the source cell (not used by the system shown), and the sink cell (used for collecting spray water in the system shown). The elevation drop, corresponding to the drop in elevation from the bottom of the pool in the source cell to bottom of the pool in the sink cell, is not used by the system shown.

4.1.2.7 Lower Cell. An example of the input processing information for a lower cell input block is illustrated in Figure 4-10. This particular example is taken from a problem that does not use the CORCON/VANESA models. (CORCON/VANESA output is described separately in Section 4.2.)

(19) The first block of information gives the layer arrangement, the initial layer compositions, temperatures, and node sizes. Additional details are given in the second block of information. Three temperatures are shown for each node in the lower cell. Upon initialization, all temperatures in a given node or layer are uniform. As the calculation progresses, however, the concrete and intermediate layers can develop temperature gradients. From left to right the three values shown represent the temperatures at the upper interface, the node center, and the lower interface, respectively. The heat transfer coefficients shown in this output are always zero since they have not been initialized at this point.

If the makeup decay power model had been specified for this cell, a message would be given indicating that this model has been activated. The values of the parameters used in calculating the makeup decay power as a function of time after reactor shutdown would also be given.

4.1.2.8 Heat Transfer Structures. (20) The input processing information for heat transfer structures is illustrated in Figure 4-11. The first few lines of the output for each structure indicate the type (ROOF, WALL,

or FLOOR), shape (SPHERE, CYLINDER, or SLAB), number of nodes, and the outer surface boundary condition of the structure. Note that a cell number of zero for the outer surface implies that the outer boundary condition corresponds either to having the gas adjacent to the surface at constant temperature or to an adiabatic condition. If that cell number corresponds to an actual cell different from the cell being processed, a dry heat transfer coefficient is used for that surface. The remaining portion of the output for each structure gives the compositions, initial temperatures, and geometric data for each node in the structure.

4.1.2.9 Fission Product Initial Conditions and Transport Parameters. This section describes the input processing information given for the FPM-CELL input block, which handles fission product initial conditions and the release and acceptance models. (21) The fission product transfers specified in the targeted release and acceptance (TARGET) model are shown in Figure 4-12. The release and acceptance table is mostly self-explanatory; however, the names specified by the user are translated into the internal representation of hosts and fission products used by code, and that on occasion requires some explanation. First, if both the inner and outer surface of a structure are specified as hosts in the TARGET input, the structure name will appear twice in the table. The two hosts representing the inner and outer surface can be differentiated by the host number; the outer surface of a structure has a host number that is one larger than that of the inner surface. Second, if a generic host name (ROOF, WALL, or FLOOR) is specified in the TARGET input, the actual structures and area-weighted transfer rates will be reflected in the table. Finally, if a fission product belonging to more than one chain is specified, each occurrence of that fission product in the linear chain decomposition will be reflected by a separate entry in the table. The location of the fission product in the linear chain decomposition in that case is indicated by the fission chain element number given in the table.

(22) Also included in the information displayed are the masses of all fission products for each host that has at least one nonzero initial fission product mass. Note that the mass of every element in each chain is given, even if only one element in one of the chains has a nonzero initial mass. If used, the nontargeted release and acceptance transfer rates are also given at this point.

As noted earlier, the FPM-CELL input block may be processed at the end of all other global and cell input processing. In that case, the information discussed above will be placed at the end of the output from all other global and cell level input processing, but before the flag table.

4.1.2.10 Fission Product Sources. (23) The information from the processing of fission product source tables is illustrated in Figure 4-13. The example given in Figure 4-13 is for three fission product source tables. Note that, although specified in the input, the hosts to which the fission products are assigned are not given in this report. Also note that since fission products in CONTAIN do not have heat capacity, an enthalpy or temperature specification is not appropriate for fission product sources and is not reported. Like all other sources in CONTAIN, fission product source tables may be interpolated in a step-wise manner or interpolated linearly. A message after each fission product source table indicates which interpolation method has been chosen.

4.1.2.11 Aerosol Initial Masses and Sources. (24) The information from the processing of aerosol initial conditions and source tables specified in the cell level AEROSOL block is illustrated in Figure 4-14. Each aerosol component with a specified initial mass is included in the first part of the output. Any aerosol sources specified after the AEROSOL keyword will be given in the second part of the output. Like fission products, aerosols in CONTAIN do not have heat capacity; therefore, an enthalpy or temperature specification is not appropriate for aerosol sources and is not reported.

4.1.2.12 Summary of Global, Cell, and Layer Flags. (25) At the completion of the global and cell level input processing, a table of flags for various code options is displayed. This table gives the user a means to check the flags related to single keyword options such as THERMAL and PRAERO, since such options do not generate input processing information blocks of their own. An example of this table is given in Figure 4-15. In addition to the flag values, a key to the flag numbers is also displayed.

4.1.3 Time-Dependent Output

At the completion of the input processing, the code initiates the time-dependent calculations, and time-dependent output is generated. There are two basic types of time-dependent output written to the main output file, the long edits and the short edits. The user can control the frequency of each of these edits through the use of the LONGEDT and SHORTEDT options, respectively. In addition, the presence or absence of much of the long edit output is controlled by the output keywords discussed below.

Because the number of variables calculated by CONTAIN is quite large, a number of output keywords allow the user to control the models represented in the long edits. (They do not, however, affect the information written to the plot file(s).) Upper cell atmospheric conditions are automatically given in each cell. The keywords to use for other types of output are listed below along with the type of output they control. The keyword to use to obtain output similar to that shown in the specific examples below is also indicated in the discussion of each type of output.

- PRAER — Detailed suspended aerosol inventories and aerosol deposition summaries
- PRAER2 — Detailed suspended aerosol and aerosol deposition inventories
- PRBURN — Hydrogen and carbon monoxide combustion model
- PRENGSYS — Engineered systems model
- PRFISS — Fission product mass and decay power summaries
- PRFISS2 — Detailed fission product mass inventories and decay power distributions
- PRFLOW — Intercell flow model
- PRHEAT — Heat transfer structure model
- PRLOW-CL — Lower cell model
- PR-USERO — User-implemented output (requires code updates)

The long edit output is displayed in Figures 4-16 through 4-23 and discussed in Sections 4.1.3.1 through 4.1.3.10. The user should note that much of the information in the long edits is grouped by cell; that is, results from different models are displayed first for one cell, then for the next cell, etc. However, the output from the intercell gas flow model and the fission product model is grouped by model toward the end of each long edit, after the information grouped by cells.

The short edit output is discussed in Section 4.1.3.11. A sample short edit is given in Figure 4-24.

4.1.3.1 Cell Atmospheric Conditions. The output for time-dependent conditions in the upper cell atmosphere is illustrated in Figure 4-16. (26) In the first block, the word "gas" is used to indicate that the quantity involved pertains only to the noncondensible gases and the coolant vapor in the atmosphere. The gas heat capacity shown in the first block is that at constant volume.

The saturation ratio is the ratio of the total mass of coolant (liquid plus vapor) present in the atmosphere to the amount that would be present if the gas temperature corresponded to the dew point, with all other conditions held fixed. Thus, values of the saturation ratio less than one represent a superheated condition, while values greater than one represent saturated conditions with suspended liquid coolant. Liquid water on aerosols is not included in this ratio.

(27) The composition of the atmosphere is given in terms of both the mass of each constituent and the corresponding molar fractions. Gas, liquid, and solid masses are given; however, only gas phase materials are considered in calculating the molar fractions. Liquid water on aerosols is not included in this part of the output but is displayed elsewhere (see Section 4.1.3.2)

(28) The amount of condensate present on the structures is given as part of the upper cell atmospheric conditions. The condensation resulting in these condensate masses is calculated only if the CONDENSE option has been specified for the current cell. In the example shown, the DOME and FLOOR structures have no condensate on their outer surfaces since they are located in another cell. (Other zero values are a consequence of evaporation from the respective structure surfaces.)

When the condensate film thickness reaches a maximum thickness, any additional condensate is considered to drain from the structure surfaces and to flow into the pool in the cell specified through the OVERFLOW keyword. By default, that cell is the cell containing the structures. If a pool is not defined in the cell to which the runoff is diverted, the condensate will be lost from the problem. Whether or not the condensate is lost, the cumulative amount that has drained from the structures in each cell is indicated.

4.1.3.2 Aerosol Airborne Mass Concentrations. (29) The aerosol output illustrated in Figure 4-17 gives the airborne mass concentration for each aerosol component in each size class. The airborne mass concentrations are given if either PRAER or PRAER2 has been specified. The column labeled "net" is the sum of the mass concentrations over all components within the indicated size class. The first row labeled "component total"

```
problem time =    1000.000 (s)                                    cptime =      17.779 on a cray

-----------------------------------      < upper dome >      ----------------------------------------

atmospheric conditions in cell   1          at time =    1000.000 (s)

gas pressure (pa)       =  1.51817e+05     gas temperature (k) =   300.25     total mass of gas (kg)      =  1.33256e+03
internal energy (j)     = -4.68815e+07     saturation temp (k) =   300.25     density of gas (kg/m**3)    =  1.11047e+00
number of gas kg-moles =  7.29772e+01      saturation ratio    =  1.03843     gas heat capacity (j/kg/k) =  1.14283e+03

the following materials are present in the cell atmosphere

     material name        mass          gas molar fraction

       n2              1.16340e+03       0.5694
       o2              8.39277e+01       0.0359
       h2              5.41587e+01       0.3711
       h2ov (vapor)    3.10827e+01       0.0236
            (liquid)   1.19438e+00       0.0000

total condensate film mass on each structure
      num  structure     inner face (kg)     outer face (kg)

        1  dome              6.11748e+00         0.00000e+00
        2  wall1             9.73627e-01         9.73627e-01
        3  wall2             0.00000e+00         0.00000e+00
        4  floor1            0.00000e+00         0.00000e+00

sum of condensate film mass on structures in cell =  8.06473e+00 (kg)

total accumulated overflow mass to lower cell =  3.79652e+02 (kg)
```

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27

28

Figure 4-16 Cell Atmospheric Conditions

```
simple   aerosol conditions in cell   1          at time =    1000.000 (s)

     total density (kg/m**3) =  2.69378e-02
     total mass (kg)         =  3.23254e+01

                              component densities (kg/m**3)
      diameter range (m)        cs137-a   te132-a   sr90-a    h2ol      net
     1.000e-07 to  1.995e-07  0.000e+00 0.000e+00 0.000e+00 9.257e-06 9.257e-06
     1.995e-07 to  3.981e-07  8.530e-09 7.712e-10 6.308e-09 2.288e-04 2.288e-04
     3.981e-07 to  7.943e-07  1.903e-06 1.796e-07 1.412e-06 3.266e-04 3.301e-04
     7.943e-07 to  1.585e-06  6.420e-05 6.851e-06 4.814e-05 3.892e-04 5.084e-04
     1.585e-06 to  3.162e-06  1.013e-03 1.692e-04 8.014e-04 2.676e-03 4.660e-03
     3.162e-06 to  6.310e-06  1.516e-03 2.728e-04 1.221e-03 3.448e-03 6.459e-03
     6.310e-06 to  1.259e-05  1.326e-03 2.445e-04 1.075e-03 2.895e-03 5.540e-03
     1.259e-05 to  2.512e-05  1.088e-03 2.030e-04 8.854e-04 2.343e-03 4.520e-03
     2.512e-05 to  5.012e-05  8.266e-04 1.550e-04 6.737e-04 1.762e-03 3.418e-03
     5.012e-05 to  1.000e-04  2.999e-04 5.689e-05 2.447e-04 6.634e-04 1.265e-03
                              ========= ========= ========= ========= =========

     component total (kg/m**3) 6.137e-03 1.108e-03 4.951e-03 1.474e-02 2.694e-02

     component total (kg)      7.364e+00 1.330e+00 5.941e+00 1.769e+01 3.233e+01


     total deposited mass (kg) over system time step =  4.23782e+00

                               cs137-a   te132-a   sr90-a    h2ol      net (kg)
          total     roof       5.126e-05 5.363e-06 3.837e-05 2.059e-03 2.154e-03
          total     wall       4.794e-03 8.639e-04 3.867e-03 1.131e-02 2.083e-02
          pools +   floor      1.018e+00 1.920e-01 8.307e-01 2.174e+00 4.215e+00
                               ========= ========= ========= ========= =========

     deposited mass (kg)       1.023e+00 1.928e-01 8.346e-01 2.188e+00 4.238e+00


     total cumulative deposited mass (kg) =  1.20403e+02

                               cs137-a   te132-a   sr90-a    h2ol      net (kg)
          total     roof       1.913e+00 1.049e+01 1.745e+00 2.822e-01 1.443e+01
          total     wall       9.002e-01 4.984e+00 8.496e-01 4.812e-01 7.215e+00
          pools +   floor      2.306e+01 5.396e+00 1.937e+01 5.093e+01 9.876e+01
                               ========= ========= ========= ========= =========

     cum deposited mass (kg) = 2.588e+01 2.087e+01 2.196e+01 5.170e+01 1.204e+02
```

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Figure 4-17 Aerosol Airborne Densities and Summary Aerosol Deposition Information (PRAER)

```
detailed aerosol conditions in cell   1          at time =    1000.000 (s)

     total density (kg/m**3) =  2.69378e-02
     total mass (kg)         =  3.23254e+01


     total deposited mass (kg) over system time step =  4.23782e+00

                              cs137-a   te132-a   sr90-a    h2ol      net (kg)
          inner     dome      5.126e-05 5.363e-06 3.837e-05 2.059e-03 2.154e-03
          inner     wall1     3.423e-03 6.168e-04 2.761e-03 8.044e-03 1.484e-02
          outer     wall1     1.372e-03 2.471e-04 1.106e-03 3.263e-03 5.988e-03
          inner     wall2     0.000e+00 0.000e+00 0.000e+00 9.227e-07 9.227e-07
          outer     wall2     0.000e+00 0.000e+00 0.000e+00 9.227e-07 9.227e-07
          inner     floor1    1.018e+00 1.920e-01 8.307e-01 2.174e+00 4.215e+00
                              ========= ========= ========= ========= =========

     deposited mass (kg)      1.023e+00 1.928e-01 8.346e-01 2.188e+00 4.238e+00


     total cumulative deposited mass (kg) =  1.20403e+02

                              cs137-a   te132-a   sr90-a    h2ol      net (kg)
          inner     dome      1.913e+00 1.049e+01 1.745e+00 2.822e-01 1.443e+01
          inner     wall1     3.592e-01 1.788e+00 3.359e-01 2.120e-01 2.696e+00
          outer     wall1     3.270e-01 1.765e+00 3.086e-01 1.649e-01 2.565e+00
          inner     wall2     1.070e-01 7.154e-01 1.026e-01 5.213e-02 9.771e-01
          outer     wall2     1.070e-01 7.154e-01 1.026e-01 5.213e-02 9.771e-01
          inner     floor1    2.306e+01 5.396e+00 1.937e+01 5.093e+01 9.876e+01
                              ========= ========= ========= ========= =========

     cum deposited mass (kg) = 2.588e+01 2.087e+01 2.196e+01 5.170e+01 1.204e+02


     total mass lost from mesh (kg) =  6.75029e+01

                              cs137-a   te132-a   sr90-a    h2ol      net (kg)
          upper bin           1.608e+01 3.412e+00 1.355e+01 3.444e+01 6.748e+01
          lower bin           4.339e-04 1.670e-05 1.633e-02 4.812e-03 2.159e-02


     aerodynamic mass median diameter (m)  =  7.39974e-06
     geometric standard deviation          =  3.09060e+00
     aerodynamic settling diameter (m)     =  2.24879e-05
     mass deposition rate (kg/s)           =  3.77772e-02
```

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Figure 4-18 Detailed Aerosol Deposition Information (PRAER2)

```
structure conditions in cell   1          at time =    1000.000 (s)

     no   name     shape    type       nodes     temperatures (k):

       1  dome     sphere   roof      1 -  10    285.55 281.14 280.14 280.01 280.00    280.00 280.00 280.00 280.00 280.00
       2  wall1    slab     wall      1 -   8    285.14 282.99 281.27 280.51 280.04    280.06 281.22 293.55
       3  wall2    slab     wall      1 -   4    323.96 323.19 323.19 323.96
       4  floor1   slab     floor     1 -   5    334.29 345.01 360.18 375.06 384.50
```

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```
cumulative burn information in cell   1          at time =    1000.000 (s)

     h2 mass burned ..................  3.49999e+01
     co mass burned ..................  0.00000e+00
     o2 mass burned ..................  2.80000e+02
     h2ov mass produced ..............  3.15279e+02
     co2 mass produced ...............  0.00000e+00
     energy released .................  5.00499e+09
```

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```
 conditions of egrspray engineered system at time =  1000.000 (s)

     liquid diverted to or from this or lower numbered cells will not be accounted for until the next system time step.

     notice :    0.00000e+00 (kg) of coolant has overflowed from cell  1 to cell  2 during the last        5.000 (s)

     containment spray information ...
```

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	during past 5.000 (s)	totals thru 1000.000 (s)
vapor mass (kg) from atmosphere	3.21590e-02	4.87010e+02
vapor energy (j) from atmosphere	1.72301e+05	1.43108e+09
liquid mass (kg) out	5.00032e+02	9.99870e+04
liquid energy (j) out	-1.14300e+08	-1.82872e+10

```
     liquid diverted to or from this or lower numbered cells will not be accounted for until the next system time step.

     liquid pumped to heat exchanger in last        5.000 (s)

          from pool of source cell .....  1
          into pool of sink cell .......  1
          mass (kg) of coolant moved ...  5.00000e+02

     heat exchanger system ...

          temperature (k) drop .........  5.00000e+01

     system source information ...

          mass flow rate (kg/s) ........  1.00000e+02
          source temperature (k) .......  2.84026e+02
```

Figure 4-19 Structure Temperatures (PRHEAT), Combustion Model Output (PRBURN), and Engineered Systems (PRENGSYS) Output

lower cell conditions in cell 2 at time = 1000.000 (s)

layer no	name	kz	depth (m)	average temp (k)	materials present mass (kg)	name
3	pool	1	6.04660e-02	357.24	5.85782e+03	h2ol
2	debris	1	2.52051e-03	361.35	1.00000e+03	fe
					1.00000e+03	ss
1	concrete	5	4.19186e-03	362.39	2.00000e+01	fe
					1.00000e+03	conc
1	concrete	4	4.19186e-03	363.91	2.00000e+01	fe
					1.00000e+03	conc
1	concrete	3	4.19186e-03	365.14	2.00000e+01	fe
					1.00000e+03	conc
1	concrete	2	4.19186e-03	365.99	2.00000e+01	fe
					1.00000e+03	conc
1	concrete	1	4.19186e-03	366.43	2.00000e+01	fe
					1.00000e+03	conc

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heat transfer information ...

layer no	name	x-section area (m**2)	from - to (11 - 12)	heat tran coef (w/m**2/k)	heat tran rate (w/m**2)	temperature (k) 1#-(top	middle	bottom)
4	atmos	1.00000e+02	4 - 3	-1.28600e+02	2.16315e+03			
3	pool	1.00000e+02	3 - 2	3.26288e+02	-1.33959e+03	1-(357.24	357.24	357.24)
2	debris	1.00000e+02	2 - 1	1.15854e+03	-1.21007e+03	1-(361.35	361.35	361.35)
1	concrete	1.00000e+02	1 - 0	0.00000e+00	0.00000e+00	5-(362.39	362.39	363.15)
						4-(363.15	363.91	364.53)
						3-(364.53	365.14	365.57)
						2-(365.57	365.99	366.21)
						1-(366.21	366.43	366.43)

cumulative gas-pool exchange amounts

coolant mass evolved (kg) ..... 4.80262e+02
energy transferred to gas (j) . 1.34282e+09

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Figure 4-20 Lower Cell Conditions (PRLOW-CL)

intercell flow conditions at time = 1000.000 (s)

from cell	to cell	flow (kg/s)	area (m**2)
1	2	-5.39050e-02	1.00000e-01
1	3	1.85033e-03	1.00000e-05

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Figure 4-21 Intercell Flow Conditions (PRFLOW)

simple fission product masses (kg) in cell 1 at time = 1000.000 (s)

host	type	name	1 moli133	1 xe133	1 cs133	2 cs137	2 ba137	3 te132
1	gas	gas	2.38197e-01	4.12238e-03	4.06504e-04	0.00000e+00	0.00000e+00	0.00000e+00
2	aerosol	cs137-a	0.00000e+00	0.00000e+00	0.00000e+00	7.25907e-02	3.07242e-02	0.00000e+00
3	aerosol	te132-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	2.34141e-02
4	aerosol	sr90-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
0	total	roof	0.00000e+00	0.00000e+00	0.00000e+00	6.18135e-04	2.67112e-04	4.85769e-04
0	total	wall	0.00000e+00	0.00000e+00	0.00000e+00	1.30719e-03	5.65022e-04	1.18471e-03
0	total	floor	0.00000e+00	0.00000e+00	0.00000e+00	5.08012e-02	2.14727e-02	1.74816e-02
		total	2.38197e-01	4.12238e-03	4.06504e-04	1.25317e-01	5.30290e-02	4.25662e-02

host	type	name	3 orgi132	3 xe132	4 sr90	4 y90	4 zr90
1	gas	gas	2.51497e-04	3.06869e-05	4.51501e-23	6.36060e-26	4.79454e-29
2	aerosol	cs137-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
3	aerosol	te132-a	0.00000e+00	1.98871e-07	0.00000e+00	0.00000e+00	0.00000e+00
4	aerosol	sr90-a	0.00000e+00	0.00000e+00	8.12376e-02	2.09976e-04	2.91585e-07
0	total	roof	1.03355e-06	0.00000e+00	7.30953e-04	1.92840e-06	2.72927e-09
0	total	wall	2.45320e-06	0.00000e+00	1.60826e-03	4.24518e-06	6.01220e-09
0	total	floor	1.13764e-05	0.00000e+00	5.77339e-02	1.49030e-04	2.06667e-07
		total	2.66360e-04	3.08858e-05	1.41311e-01	3.65179e-04	5.06994e-07

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host material information in cell 1 at time = 1000.000 (s)

host	type	name	power (watts)	temperature (k)
1	gas	gas	2.94450e+03	3.00190e+02
2	aerosol	cs137-a	8.51488e+01	3.00190e+02
3	aerosol	te132-a	5.03404e+00	3.00190e+02
4	aerosol	sr90-a	4.48345e+02	3.00190e+02
0	total	roof	4.86615e+00	0.00000e+00
0	total	wall	1.06699e+01	0.00000e+00
0	total	floor	3.81992e+02	0.00000e+00
		total	3.88055e+03	

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Figure 4-22 Fission Product Mass and Decay Power Summaries (PRFISS)

detailed fission product masses (kg) in cell 1 at time = 1000.000 (s)

host	type	name	1 moli133	1 xe133	1 cs133	2 cs137	2 ba137	3 te132
1	gas	gas	2.38197e-01	4.12238e-03	4.06504e-04	0.00000e+00	0.00000e+00	0.00000e+00
2	aerosol	cs137-a	0.00000e+00	0.00000e+00	0.00000e+00	7.25907e-02	3.07242e-02	0.00000e+00
3	aerosol	te132-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	2.34141e-02
4	aerosol	sr90-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
6	inner	dome	0.00000e+00	0.00000e+00	0.00000e+00	6.18135e-04	2.67112e-04	4.85769e-04
8	inner	wall1	0.00000e+00	0.00000e+00	0.00000e+00	2.43023e-04	1.03783e-04	1.42686e-04
9	outer	wall1	0.00000e+00	0.00000e+00	0.00000e+00	5.29903e-04	2.28398e-04	4.30458e-04
10	inner	wall2	0.00000e+00	0.00000e+00	0.00000e+00	2.67130e-04	1.16421e-04	3.05782e-04
11	outer	wall2	0.00000e+00	0.00000e+00	0.00000e+00	2.67130e-04	1.16421e-04	3.05782e-04
12	inner	floor1	0.00000e+00	0.00000e+00	0.00000e+00	5.08012e-02	2.14727e-02	1.74816e-02
		total	2.38197e-01	4.12238e-03	4.06504e-04	1.25317e-01	5.30290e-02	4.25662e-02

host	type	name	3 orgi132	3 xe132	4 sr90	4 y90	4 zr90
1	gas	gas	2.51497e-04	3.06869e-05	4.51501e-23	6.36060e-26	4.79454e-29
2	aerosol	cs137-a	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00	0.00000e+00
3	aerosol	te132-a	0.00000e+00	1.98871e-07	0.00000e+00	0.00000e+00	0.00000e+00
4	aerosol	sr90-a	0.00000e+00	0.00000e+00	8.12376e-02	2.09976e-04	2.91585e-07
6	inner	dome	1.03355e-06	0.00000e+00	7.30953e-04	1.92840e-06	2.72927e-09
8	inner	wall1	2.47876e-07	0.00000e+00	2.84207e-04	7.41418e-07	1.03843e-09
9	outer	wall1	8.90413e-07	0.00000e+00	6.41902e-04	1.68943e-06	2.38581e-09
10	inner	wall2	6.57457e-07	0.00000e+00	3.41075e-04	9.07167e-07	1.29398e-09
11	outer	wall2	6.57457e-07	0.00000e+00	3.41075e-04	9.07167e-07	1.29398e-09
12	inner	floor1	1.13764e-05	0.00000e+00	5.77339e-02	1.49030e-04	2.06667e-07
		total	2.66360e-04	3.08858e-05	1.41311e-01	3.65179e-04	5.06994e-07

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host material information in cell 1 at time = 1000.000 (s)

host	type	name	power (watts)	temperature (k)
1	gas	gas	2.94450e+03	3.00190e+02
2	aerosol	cs137-a	8.51488e+01	3.00190e+02
3	aerosol	te132-a	5.03404e+00	3.00190e+02
4	aerosol	sr90-a	4.48345e+02	3.00190e+02
6	inner	dome	4.86615e+00	2.85548e+02
8	inner	wall1	1.88482e+00	2.85143e+02
9	outer	wall1	4.25886e+00	2.93549e+02
10	inner	wall2	2.26310e+00	3.23965e+02
11	outer	wall2	2.26310e+00	3.23965e+02
12	inner	floor1	3.81992e+02	3.34288e+02
		total	3.88055e+03	

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Figure 4-23 Detailed Fission Product Masses and Decay Powers (PRFISS2)

```
cell  pgas            temperatures                          gas molar                          aerosol mass          flows
                cell  cell  cell  cell  pool          percent          sat        density deposit  to   mdot   to   mdot
                 gas  roof  wall floor  ave   h2    co    o2   h2ov ratio

        time =     900.000 (s)              cptime =      17.665 (s)

# 1 1.513e+05  300   285   298   333     0 37.13  0.00  3.58  2.36  1.03489   2.99e-02 1.16e+02  2-6.78e-02  3 1.84e-03
# 2 1.513e+05  340     0   325     0   357 25.52  0.00  6.56 18.29  1.00520   3.81e-02 6.94e+02  1 6.78e-02  0 0.00e+00
# 3 9.000e+04  285     0     0     0   284  0.00  0.00 19.39  1.54  1.00000   9.83e-12 1.26e-07  1-1.84e-03  0 0.00e+00
```

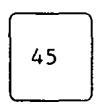

Figure 4-24 A Short Edit

gives the total airborne aerosol mass concentration of each component. The second row has been multiplied by the volume of the cell to give the total airborne aerosol mass of each component.

4.1.3.3 Aerosol Deposition. (30) A summary of the amounts of aerosol deposited on structures and in the pool is given if PRAER is specified. This summary displays the total amount of deposited mass in the indicated locations ("roof", "wall", and "pools + floor"). Presently, with the exception of coolant aerosols, aerosols may end up in the pool only through the depletion caused by engineered systems, through scrubbing processes occurring within the pool, or through aerosol mesh losses. The latter are generated when aerosols grow until they exceed the maximum size allowed in the largest size class or shrink (through evaporation) until they are smaller than the minimum size of the smallest size class. If mesh losses occur, they will be placed either on the floor, in the pool, or in the waste holding location of the cell specified through the OVERFLOW keyword. The specific location is discussed in Section 2.2.4.2. By default, the overflow cell is the cell in which the overflow occurs. If neither a floor nor a pool is present in the overflow cell, the aerosol mesh losses will go to the waste location. If nonzero, the aerosol mass in the waste location will be indicated in the output. Coolant aerosols may end up in the pool of the overflow cell through one additional process if condensation on structures is modeled. In that case any coolant aerosols deposited on structures will be incorporated into the condensate film on the structures. The condensate runoff may then accumulate in the pool of the overflow cell as described in Section 4.1.3.1 above.

(31) A detailed account of aerosol deposited mass is given if the PRAER2 keyword is specified. This output gives the amount of aerosol deposited on each structure surface as well as in the two pool repositories, although the latter are not shown in Figure 4-18 because they have no mass. The first pool repository includes aerosol mesh losses and aerosols removed from the atmosphere by engineered systems. The second pool repository includes aerosols that have been scrubbed within the pool in the SPVENT, SRV, and VANESA models.

(32) The last block of information in the aerosol output is given if either PRAER or PRAER2 is specified. The quantity labeled as "total mass lost from mesh" gives the cumulative amount of losses from the aerosol mesh, as defined above. The label "upper bin" denotes the cumulative amount of aerosols that have become too large, and "lower bin" denotes the cumulative amount that have become too small. Occasionally, very small negative mass values may appear in the lower bin. These negative values are the consequence of small integration errors in the calculation and are not meaningful.

The labels "aerodynamic mass median diameter" and "settling diameter" refer to effective sizes of the aerosols represented by the particle distribution function. The former refers to the size of a spherical particle of unit specific gravity (and unit shape factor) that will settle at the same rate as the geometric mass median particle in the particle distribution; the latter refers to the particle diameter in a mono-disperse distribution of spherical particles of unit specific gravity that would have the same suspended mass and mass settling rate as those of the actual particle distribution.

4.1.3.4 Structure Temperatures. (33) The display of structure temperatures is controlled by the PRHEAT keyword. The output gives the temperatures of each node of each structure, as shown in Figure 4-19.

4.1.3.5 Hydrogen and Carbon Monoxide Combustion. (34) The display of cumulative inventories of materials involved in hydrogen and carbon monoxide combustion is controlled by the PRBURN keyword. The output is illustrated in Figure 4-19. The energy released is the enthalpy of combustion referenced to the liquid state of water.

4.1.3.6 Engineered Systems. (35) A summary of the effects of engineered systems operation is given on a cell-by-cell basis if requested through the PRENGSYS keyword. The output given in Figure 19 is for a spray system with both an injection and a recirculation mode. The output is more complicated than that for a typical system. A common feature of the output from an active engineered system is the vapor/liquid mass and energy transfer information. The label "vapor mass ... from atmosphere" refers to the condensate removed from the atmosphere through the operation of the system. The label "liquid mass out" refers to the condensate removed plus any coolant introduced during the operation of the system. For example, in a spray system the coolant introduced is the spray water and in an ice condenser system is the melted ice. The liquid mass out is directed to the pool of the cell labeled as the "system sink."

If liquid transfer occurs to or from a cell in which an engineered system is defined, or to or from a lower numbered cell as a result of the operation of that engineered system, the pool inventories in those cells may not reflect the transfers that have occurred over the last timestep. (These transfers may result in unprocessed mass in interface arrays at the time of output.) In the example of Figure 4-19, overflow from the pool to a different cell is specified. In addition, the sprays are drawing water from the pool in the present cell in the recirculation mode. Thus two messages about possibly unprocessed mass transfers are given.

4.1.3.7 Lower Cell Conditions. (36) If PRLOW-CL is specified, lower cell conditions are given as shown in Figure 4-20. The first part of the output indicates the lower cell configuration, including the name, height, average temperature, and composition of each layer. If a concrete layer is specified, it can be divided into a number of nodes. The default number of concrete nodes is five, as indicated in this example. All other layers have a single node. An atmosphere layer is automatically defined whenever a lower cell is specified.

The "heat transfer information" block gives the cross-sectional area of the layers and the layer interface conditions. The heat transfer coefficient and heat transfer rate between adjacent layers, respectively, are given. Note that if the CONDENSE option has been specified, the heat transfer coefficient given between the pool and the atmosphere is an effective one taking into account both sensible heat and mass transfer. Under some conditions, this effective heat transfer coefficient can be negative.

Three temperatures are shown for each node. The three values shown represent the temperatures at the node upper interface, the node center, and the lower interface, respectively.

If the makeup decay power model had been activated, the decay power distribution among the lower cell layers would also be displayed.

(37) The "cumulative gas-pool exchange amounts" block gives the net condensation on or vaporization of coolant from the pool for all processes involving the direct exchange of vapor between the pool and a gas phase. The amounts reflect boiling and condensation and evaporization both at the top surface and at bubble surfaces if gases are bubbling through the pool. A positive sign for the coolant mass evolved means that the net amount of vapor produced from the pool is positive. The amounts do not reflect direct exchange of liquid, liquid sources to the pool, or indirect exchange of vapor. Examples of indirect exchange of vapor include condensate runoff from structures that accumulates in the pool and condensate on spray drops that enter the pool. Note that the BOIL keyword must be specified in the pool PHYSICS input block to obtain this output block.

4.1.3.8 Intercell Flow Conditions. If requested through the PRFLOW keyword, the intercell gas flow conditions are displayed after the time-dependent output that is grouped by cells. (38) As shown in Figure 4-21, these conditions consist of the flow rates between various cells and the current flow path areas. A positive sign for the flow rate means the flow direction is the direction implied by the FROM and TO labels. A negative sign implies the converse. The flow rates correspond to those present at the end of the previous system timestep, whereas the flow areas correspond to those at the beginning of the next timestep. (A discontinuous change in the flow area may result from a flow path opening at the time of edit.) Figure 4-21 gives the conditions for regular flow paths. The output for engineered vents and the BWR suppression pool vent is similar to that for the regular flow paths.

4.1.3.9 Fission Product Inventories. If requested, information about fission product inventories and host temperatures and powers is displayed after the time-dependent output from different models that is grouped by cells. The fission product output is illustrated in Figures 4-22 and 4-23. Like the aerosol output, fission product output may be displayed at two levels of detail. At the simple level requested by PRFISS, for the purposes of reporting fission product masses and host power, structure surfaces serving as hosts are grouped into the three categories of ROOF, WALL, and FLOOR. Lower cell layers are also grouped into one category. At the more detailed level requested by PRFISS2, the corresponding quantities are reported for individual hosts. Only those hosts with no fission products are not listed at the detailed level of output. The resulting automatic suppression of zeros can save considerable space in the detailed output.

(39,41) The fission product output is given on a cell-by-cell basis. The first two blocks of output in Figures 4-22 and 4-23 illustrate the listing of the fission product masses in a particular cell. The number to the left of each fission product name listed across the top indicates the decay chain to which that fission product belongs. The columns on the left list the hosts on which the fission products reside. The host number for the ROOF, WALL, and FLOOR hosts in Figure 4-22 is zero, since these labels represent generic and not actual fission product hosts.

(40,42) The third block of output in Figures 4-22 and 4-23 shows the amount of decay power and the temperature associated with the hosts in a particular cell. The values shown reflect the decay power generated by the individual fission products. For lower cell layer hosts, they do not reflect any makeup decay power added to the layers, which is displayed separately. Also shown in this block are the temperatures of various hosts. Temperatures for generic hosts are shown as zero.

The makeup decay power model is not invoked in the problem generating the output in Figures 4-22 and 4-23. If the makeup decay power model had been invoked, the amount of makeup power added to a particular lower cell would be given at the very end of the fission product output for that cell.

4.1.3.10 User-Implemented Output. The user may wish to implement his or her own coding for output in the USERO subroutine. Output may be written from the USERO subroutine to either the main output file, the plot file(s), or the user output file discussed in Appendix B. The call to the USERO subroutine is controlled by the PR-USERO output keyword and occurs once every plot, or edit, timestep, unlike the calls to most of the formatted-output routines, which occur once every long edit timestep. If written to the main output file in conjunction with a long edit, the output from the USERO subroutine will appear after the regular CONTAIN output that is grouped by cell. The user may access both global and cell level variables from the USERO subroutine.

4.1.3.11 Short Edits. A short edit is illustrated in Figure 4-24. CONTAIN will write a short edit at a frequency controlled by the SHORTEDT option. The default frequency is every system timestep. As shown in Figure 4-24 a single line is displayed for each cell in a short edit.

(43) The "roof", "wall", and "floor" temperatures are the area-weighted surface node temperatures for the corresponding structure surfaces within a particular cell. Each structure surface located within the cell in which the structure is defined is taken into account in these temperatures. The pool temperature shown is that of the pool or coolant layer in the lower cell model. If no pool is present, the value shown will be zero.

(44) The gas molar percentages for the gases H2, CO, O2, and H2OV are printed. The saturation ratio, discussed in Section 4.1.3.1 in conjunction with the upper cell atmosphere output, is also included.

(45) The aerosol mass deposited is the cumulative mass deposited in all repositories located in the cell, including the structure surfaces and the two pool repositories. The output under the label "flows" gives the mass flow rate for the regular flow paths with the two largest rates. The integer prefixing each flow value given under the label "mdot" corresponds to the cell that is nominally receiving the flow from the cell numbered on the extreme left under the label "cell." A minus sign indicates the flow is actually in the opposite direction. A zero flow rate value may mean that the pressure difference between the two cells is negligible or that the flow path is closed.

4.2 CORCON and VANESA Output

The CORCON output is in the same basic form as is found in the stand-alone CORCON MOD-2 output. The order in which various parts of the input processing is reported is different from that of the stand-alone code but the same information is presented. This information is explained in the CORCON MOD-2 manual [Col84].

As shown in Figure 4-25, the VANESA input processing information appears in the middle of two sections of the CORCON input processing. In the VANESA input processing, information is first given about the values of parameters that may be set by the user. The initial material inventories as specified by the user and as modified by VANESA are then given. Finally, the mapping between VANESA constituents and CONTAIN aerosol components and fission products is given.

CORCON time-dependent output is presented in two places in the CONTAIN output. The first is in the lower cell section of each long edit. The average CORCON layer temperatures and the interface temperatures are reported in the values associated with the CORCON intermediate layer. Also, a summary of cumulative CORCON results is given. An example is shown in Figure 4-26.

CORCON output is also given in CORCON edits that appear independently of the CONTAIN long edits. The frequency of the CORCON edits is controlled by the TIMES input specified in the CORCON section of the lower cell input. This output is exactly the same as the output from the stand-alone CORCON code [Col84] and is not shown here.

VANESA time-dependent output is given in VANESA edits that appear independently of the CONTAIN long edits. The frequency of these is controlled by the EDITDELT keyword in the VANESA section of the lower cell input. An example of this output is shown in Figure 4-27. Information about the gas flow rates provided to VANESA is given, as well as the cumulative releases of the VANESA constituents. Also given is the current VANESA material inventory. VANESA output is described in more detail in Reference Pow86.

4.3 Diagnostic Output

The user will inevitably make errors in writing input datasets. In addition, the code will often encounter abnormal conditions during the calculation of the time-dependent results. To assist the user in understanding and correcting such problems, the code will write diagnostic messages either to the main output file or the error file. These messages all will be prefixed with the readily identifiable pattern:

```
   >
>>>>>  (diagnostic message to the user)
   >
```

The above pattern is also used in the output file to prefix messages regarding events, such as hydrogen burns, that are not usually reasons

++++ input (low-cell) - process lower-cell section.

corcon time control parameters in cell 2

dtmin	dtmax	edit interval	to time
30.000	30.000	180.000	2.160e+04

*** corcon geometry specification ***
ray center coordinates

r0 = 0.000000 z0 = 0.500000

concrete cavity geometry

right cylinder

nrays - number of rays = 95

zt - z-coordinate of top = 0.000000

rad - cylinder radius (m) = 3.00000

hit - cylinder height (m) = 5.00000

radc - corner radius (m) = 0.100000

nbot - number of bottom points = 10

ncorn = number of corner points = 10

* * * corcon concrete specifications * * *

non-standard concrete, user defined

rhoc (kg/m3)	rbr (kg/kg c)	si (-)	tsol (k)	tliq (k)	tic (k)	tw (k)	delh (j/kg)	ew (-)
2.340000e+03	1.350000e-01	2.763040e-01	1.350000e+03	1.650000e+03	3.500000e+02	1.550000e+03	2.928921e+06	9.000000e-01

species name	mass fr.(kg/kg c)	molecular wt.
sio2	0.3590	60.0843
cao	0.3637	56.0794
al2o3	0.0010	101.9613
co2	0.2023	44.0098
h2oevap	0.0400	18.0152
h2ochem	0.0340	18.0152

*** corcon flags and parameters ***

*** flags ***				*** control parameters ***	
ilyr = 0	icool = 0	igeom = 2	icon = 0	timeo = 0.00 (sec)	deltim = 30.0000 (sec)
igas = 0	ifp = 0	isur = 1	iabl = 0	timend = 21600.00 (sec)	
isplsh= 0	ipinc = 0	iflor = 0	irstrt = 0	dprin = 0.00 (sec)	tprin = 0.00 (sec)
imov = 1	ipg = 0	israbl = 0	iaopac = 0		

Figure 4-25 CORCON and VANESA Parameters

```
      ++++ input (vanesa ) - model parameters in cell     2


the concrete weight fractions are:
                              cao         3.63696e-01
                              al2o3       1.00000e-03
                              na2o        0.00000e+00
                              k20         0.00000e+00
                              sio2        3.59000e-01
                              feo         0.00000e+00
      the weight fractions sum to:      7.23696e-01              the rebar mass fraction     :      1.35000e-01
vanesa parameter values:
      vanesa time step/corcon time step ...    5.00000e-01
      diffusion coefficient(m**2/s) .......    1.00000e-08
      bubble diameter(m) ..................    1.00000e-02
      particles/bubble ....................    1.00000e+00
      particle diameter(m) ................    1.00000e-06

initial melt fission product inventory

           cesium                          0.00000e+00 kg
           iodine                          0.00000e+00 kg
           xenon                           0.00000e+00 kg
           krypton                         0.00000e+00 kg
           te                              2.09000e+01 kg
           ba                              5.66000e+01 kg
           sn                              1.52000e+02 kg
           ru                              1.27000e+02 kg
           uo2                             9.84130e+04 kg
           zr                              7.57500e+03 kg
           zro2                            1.70600e+04 kg
           fe                              8.54000e+04 kg
           feo                             6.00000e+03 kg
           mo                              1.72000e+02 kg
           sr                              5.27000e+01 kg
           rb                              0.00000e+00 kg
           y                               2.82000e+01 kg
           tc                              4.54000e+01 kg
           rh                              2.56000e+01 kg
           pd                              6.43000e+01 kg
           la                              7.68000e+01 kg
           ce                              1.62000e+02 kg
           pr                              6.26000e+01 kg
           nd                              2.10000e+02 kg
           sm                              4.19000e+01 kg
           pu                              5.78000e+02 kg
           cr                              3.68200e+03 kg
           mn                              1.92000e+02 kg
           ni                              2.03900e+03 kg
           ag                              1.11200e+03 kg
           sb                              2.80000e-01 kg
           nb                              0.00000e+00 kg
```

Figure 4-25 CORCON and VANESA Parameters (continued)

modified initial melt inventory

fe	8.54000e+04 kg
cr	3.68200e+03 kg
feo	6.00000e+03 kg
cr2o3	0.00000e+00 kg
ni	2.03900e+03 kg
mo	1.72000e+02 kg
ru(rh,pd,tc)	2.60045e+02 kg
sn	1.52000e+02 kg
sb	2.80000e-01 kg
te	2.09000e+01 kg
ag	1.11200e+03 kg
mn	1.92000e+02 kg
uo2	9.84130e+04 kg
zro2	1.70600e+04 kg
cs2o(rb)	0.00000e+00 kg
bao	6.31936e+01 kg
sro	6.23230e+01 kg
la2o3(pr,nd,sm,y)	4.96533e+02 kg
ceo2(pu02)	6.13515e+02 kg
nb2o5	0.00000e+00 kg
csi	0.00000e+00 kg
zr	7.57500e+03 kg

the vanesa constituents will be assigned to the following aerosol components

constituent name	aerosol comp number	aerosol name
fe	5	mgo
cr2o3	5	mgo
ni	5	mgo
mo	4	mmo
ru	4	mmo
sn	4	mmo
sb	4	mmo
te	3	u
ag	5	mgo
mn	5	mgo
cao	5	mgo
al2o3	5	mgo
na2o	5	mgo
k2o	5	mgo
sio2	5	mgo
uo2	5	mgo
zro2	5	mgo
cs2o	2	pu
bao	4	mmo
sro	4	mmo
la2o3	4	mmo
ceo2	4	mmo
nb2o5	4	mmo
csi	1	uo2

Figure 4-25 CORCON and VANESA Parameters (continued)

```
 12 vanesa constituents will be tracked individually as fission products

vanesa con. name     no. of f.p.        f.p. name        frac. assigned        host name

    csi                  2
                                        i                4.89000e-01         uo2
                                        cs               5.11000e-01         uo2

    cs2o                 1
                                        cs               9.44000e-01         pu

    te                   1
                                        te               1.00000e+00         u

    sb                   1
                                        rf               1.00000e+00         u

    sro                  1
                                        rf               8.48000e-01         u

    bao                  1
                                        rf               8.96000e-01         u

    la2o3                1
                                        rf               8.53000e-01         u

    ceo2                 1
                                        rf               8.53000e-01         u

    nb2o5                1
                                        rf               7.03000e-01         u

    ru                   1
                                        rf               1.00000e+00         u

    mo                   1
                                        rf               1.00000e+00         u

    zro2                 1
                                        oth              2.40000e-03         mno

 ++++ input(vanesa ) - model parameters completed

                                melt fission product inventory
                    based on  9.00000e+01 metric ton uranium core operated at  3.40000e+03 mw(thermal)
                  melt contains  8.67402e+01 metric tons uranium, corresponding to  96.38 percent of core

       elements, retained fractions (**denotes user input, others from wash 1400), and gram-atoms in melt

  mo  (0.970)  5.6716e-01     tc  (0.970)  1.4511e-01     ru  (0.970)  3.5968e-01     rh  (0.970)  6.5533e-02
  sb  (0.850)  1.9558e-03     te  (0.850)  5.0694e-02     sr  (0.900)  1.8927e-01     ba  (0.900)  1.6596e-01
  zr  (0.990)  7.0765e-01     ce  (0.990)  3.7026e-01     np  (0.990)  3.6650e-02     cm  (0.990)  1.5315e-03
  nb  (0.990)  1.0850e-02     pu  (0.990)  6.7696e-01     am  (0.990)  4.8777e-03     y   (0.990)  1.0633e-01
  la  (0.990)  1.5919e-01     pr  (0.990)  1.3840e-01     nd  (0.990)  4.4451e-01     sm  (0.990)  5.2084e-02
  eu  (0.990)  1.5484e-02     rb  (0.190)  1.5147e-02     cs  (0.190)  6.8875e-02     br  (0.100)  5.1290e-04
  i   (0.100)  3.0360e-03
```

Figure 4-25 CORCON and VANESA Parameters (continued)

```
                                fission products grouped as 4 pseudo-species

 1.19013e+00 gram-atoms of fpm      with atomic fractions
      mo  4.76552e-01          tc  1.21930e-01          ru  3.02216e-01          rh  5.50639e-02      sb  1.64339e-03
      te  4.25853e-02

 3.08001e+00 gram-atoms of fpox     with atomic fractions
      sr  6.14511e-02          ba  5.38829e-02          zr  2.29756e-01          ce  1.20214e-01      np  1.18992e-02
      cm  4.97248e-04          nb  3.52284e-03          pu  2.19792e-01          am  1.58367e-03      y   3.45213e-02
      la  5.16855e-02          pr  4.49356e-02          nd  1.44321e-01          sm  1.69103e-02      eu  5.02712e-03


 8.40218e-02 gram-atoms of fpalkmet with atomic fractions
      rb  1.80272e-01          cs  8.19728e-01

 3.54890e-03 gram-atoms of fphalogn with atomic fractions
      br  1.44524e-01          i   8.55476e-01

          initial power at start of corcon, 1.07141e+04 sec after scram is 2.03909e+07 watts
              representing   0.62 percent of operating power of fraction of core in melt


                                        *** corcon melt layer specification ***
                                  initial corcon core melt constituent masses (kg)and temperatures
0                  oxides              spemw          coninp          metals              spemw          coninp

                   feo          7.1846400e+01   6.0000000e+03          fe          5.5847000e+01   8.5400000e+04
                   uo2          2.7002780e+02   9.8413000e+04          cr          5.1996000e+01   3.6820000e+03
                   zro2         1.2321880e+02   1.7060000e+04          ni          5.8710000e+01   2.0390000e+03
                   fpox         1.3716610e+02   1.3843823e+03          zr          9.1220000e+01   7.5750000e+03
                   fpalkmet     1.3300000e+02   3.6618506e+01          fpm         9.8338300e+01   3.8350772e+02
                   fphalogn     1.2700000e+02   1.4769115e+00

initial temperature (t0) in degrees k =    2.5000000e+03

initial temperature (tm) in degrees k =    2.5000000e+03

initial mass of oxides =    1.2289548e+05

initial mass of metals =    9.9079508e+04


     source table for h2ol     with    3 data points

     time (s)     0.000e+00 1.071e+04 1.072e+04
     mass (kg/s)  0.000e+00 1.832e+04 0.000e+00
     enth (j/kg)  0.000e+00 2.000e+05 0.000e+00

                  (source table is a step function)
```

Figure 4-25 CORCON and VANESA Parameters (continued)

```
lower cell conditions in cell   2     at time =     102.010 (s)

      layer                                average        materials present
   no   name          kz    depth (m)      temp (k)       mass (kg)   name
  ---------------    ---------------      --------      ------------------------

   3   pool           1      none
   2     corcon         3  0.00000e+00      2522.84       8.59569e+02    lcclox

   2     corcon         2  5.06808e-01      2564.16       9.87100e+04    lccmet

   2     corcon         1  5.22663e-01      2492.53       1.23404e+05    lcchox


heat transfer information ...

      layer            x-section     from - to    heat tran coef    heat tran rate                temperature (k)
   no   name          area (m**2)    (l1 - l2)     (w/m**2/k)        (w/m**2)          l#-(     top    middle   bottom)
  ---------------    -----------    ---------    --------------    --------------     ------------------------------

    4    atmos        2.82743e+01      4 -  2      7.52751e+00      -1.49971e+04

    3    pool              none
    2    corcon       2.73476e+01      2 -  0      5.00000e+19       0.00000e+00       3-(2400.74  2522.84  2378.35)
                                                                                        2-(2378.35  2564.16  2500.00)
                                                                                        1-(2500.00  2492.53  2493.30)


cumulative gas-pool exchange amounts

     coolant mass evolved (kg) .....    1.00000e+01
     energy transferred to gas (j) .    3.03833e+07


corium concrete interaction results (cumulative)

     mass (kg) of co2 liberated ...    1.02295e-06
     mass (kg) of h2o liberated ...    6.39727e-04
     mass (kg) of co  liberated ...    2.33355e-02
     mass (kg) of h2  liberated ...    4.65367e-01
          (previous corcon cycle)

     decay heat source (w) ........    2.46378e+08
     chemical reaction source (w) .    0.00000e+00
     heat loss to concrete (w) ....    8.67150e+07
     heatup ablation prods (w) ....    0.00000e+00
     heat loss melt surface (w) ...    4.13185e+07
     zr mass in melt (kg) .........    7.57500e+03
     c  mass in melt (kg) .........    0.00000e+00
     maximum cavity radius (m) ....    3.00922e+00
     maximum cavity depth  (m) ....    5.00889e+00
```

Figure 4-26 CORCON Time-Dependent Output

```
                                        vanesa version 1.00.01
  step start time =    280.10          vanesa edit time =    310.10
                      zion plant ( 2 cell )  tmlb
                            case 2a


 ----------------------------------          corcon/vanesa standard probl      ----------------------------------------
   values received from corcon:

flow rate of gas (STP,m**3/sec ) passing through melt ...   5.30646e+00
temperature oxide layer 1 ..............................   2.51905e+03
temperature oxide layer 2 ..............................   2.51905e+03
concrete addition rate (kg/sec) to debris ..............   4.49501e+01
floor area covered by debris (m**2) ....................   2.82743e+01
steam passing through melt (kgmoles/sec) ...............   1.82989e-01
co2 passing through melt (kgmoles/sec) .................   3.39004e-02


       vanesa results integrated over an interval of   3.00000e+01 (sec)
                          in steps of   1.50000e+01 (sec)

 vaporization aerosol (kg/m**3 of gas, ambient) .........  1.99894e-02
 mechanical aerosol (kg/m**3 of gas, ambient) ...........  7.31207e-09
 total aerosol (kg/m**3 of gas, ambient) ................  1.99894e-02
 total aerosol (kg/m**3 of gas, 1 atm, 298 K) ...........  1.68974e-01
 gas flow rate (kgmoles/sec) ............................  2.19600e-01
 aerosol mass source rate (kg/sec) ......................  9.07404e-01
 aerosol density (kg/m**3) ..............................  3.93631e+03
 mean aerosol size (microns) ............................  9.30318e-01


                                  aerosol composition
                          ------- averaged over last vanesa interval ------
      constituent name          percent composition          source rate (kg/sec)          accumulated release(kg)

          fe                          13.72                    1.24533e-01                    2.22366e+01
          cr2o3                        0.00                    2.88045e-05                    4.61487e-03
          ni                           0.69                    6.28013e-03                    1.07980e+00
          mo                           0.00                    1.81967e-08                    3.06248e-06
          ru                           0.00                    1.37807e-07                    2.32069e-05
          sn                           0.40                    3.65110e-03                    6.38238e-01
          sb                           0.00                    3.77517e-07                    6.70232e-05
          te                           0.70                    6.39536e-03                    1.15677e+00
          ag                          22.23                    2.01680e-01                    3.56055e+01
          mn                           6.16                    5.59183e-02                    9.97758e+00
          cao                         14.26                    1.29413e-01                    1.96620e+01
          al2o3                        0.86                    7.79447e-03                    1.04789e+00
          na2o                         0.00                    0.00000e+00                    0.00000e+00
          k2o                          0.00                    0.00000e+00                    0.00000e+00
          sio2                        29.09                    2.64002e-01                    4.26431e+01
          uo2                          1.74                    1.57995e-02                    2.81344e+00
          zro2                         0.02                    1.74734e-04                    3.19980e-02
          cs2o                         0.00                    0.00000e+00                    0.00000e+00
          bao                          1.61                    1.46369e-02                    3.03485e+00
          sro                          3.26                    2.96088e-02                    6.25528e+00
          la2o3                        2.09                    1.89453e-02                    3.45282e+00
          ceo2                         3.15                    2.85428e-02                    5.53362e+00
          nb2o5                        0.00                    0.00000e+00                    0.00000e+00
          csi                          0.00                    0.00000e+00                    0.00000e+00
```

Figure 4-27 VANESA Time-Dependent Output

total mass released (kg) = 1.55274e+02

gas composition
------- averaged over last vanesa interval ------

gas name	percent composition	source rate (kg/sec)	accumulated release(kg)
h2o	0.08	1.06953e-03	1.90833e-01
h2	27.53	3.63304e-01	7.05797e+01
h	0.41	5.46439e-03	9.93480e-01
oh	0.00	8.13742e-13	1.32565e-10
o	0.00	2.25939e-06	3.54550e-04
o2	0.00	3.27317e-11	4.83716e-09
co2	0.01	7.89189e-05	7.11918e-03
co	71.96	9.49516e-01	8.88143e+01

melt composition

melt component	mass(kg)
fe	8.65769e+04
cr	3.68199e+03
ni	2.03793e+03
mo	1.72000e+02
ru	2.60045e+02
sn	1.51369e+02
sb	2.79934e-01
te	1.97572e+01
ag	1.07683e+03
mn	1.82143e+02
cao	3.15289e+03
al2o3	7.68726e+00
na2o	0.00000e+00
k2o	0.00000e+00
sio2	3.08922e+03
uo2	9.84101e+04
zro2	1.94420e+04
cs2o	0.00000e+00
bao	6.01954e+01
sro	5.61433e+01
la2o3	4.93122e+02
ceo2	6.08048e+02
nb2o5	0.00000e+00
csi	0.00000e+00
feo	5.97253e+03
cr2o3	0.00000e+00
zr	5.81155e+03

Figure 4-27 VANESA Time-Dependent Output (continued)

for aborting but may be difficult to detect. Some but not all event information is also written to the event summary file. The user should note that the pattern ">>>>>" is unique to diagnostic and other special messages.

When input datasets are processed, numerous tests for errors are conducted. If the code detects an error, a diagnostic message is written to the error file. The code then attempts to finish processing the input dataset; however, in some instances the remainder of the input will not be processed sensibly after the error has occurred. In such cases, fixing one error may cause the other apparent input errors to disappear. After a certain number of errors, or after the processing of a dataset with errors is completed, the code will abort by calling the nonexistent routine EREXIT from the subroutine ABORT. (If the former routine exists in the system library, the user should either change the name of EREXIT or write a separate EREXIT routine to control the abort.) This method of aborting has been chosen since it causes a subroutine traceback in most systems.

A diagnostic message issued during the time-dependent calculations may or may not lead to an immediate abort. In general the diagnostics written to the output file either concern special events or reflect conditions that may impact the calculation but not invalidate it. In general, the diagnostics for obviously serious abnormal conditions, including those that lead to an immediate abort, or for conditions that may be serious, but whose severity cannot be determined by the code, are written to the error file. Included in the latter type of conditions are those that are created by non-upward-compatible changes. (After such a change, the same input will still be accepted by the code but may lead to a different action from that intended by the user.) Because of the existence of the latter types of changes, it is recommended that the user always scan the error file for diagnostic and warning messages, even if the calculation does not abort. If scanning the error file does not sufficiently identify a particular problem, the user should also scan the output file. The unique pattern ">>>>>" may be used to search for diagnostic messages.

5. PRACTICAL AND CAUTIONARY ADVICE TO THE USER

Much of this manual has focused on what CONTAIN is designed to do and how to implement its features. There is also a need to discuss the limitations of the models in order to help the analyst understand the types of problems for which the code is suited and is not suited. One of the purposes of this section is to identify and briefly discuss some of these limitations (with no attempt at treating the subject comprehensively).

A second purpose of this section is to offer some practical suggestions about how to run the code. These comments are based on a substantial body of experience gained in applying CONTAIN to a wide variety of severe accident scenarios. In some cases, the suggestions are oriented towards increasing the efficiency of the process of producing useful calculations. In other cases, the idea is to caution against avoidable errors or pitfalls that have been encountered in the past. Finally, there are some suggestions about how to overcome some of the limitations of the code by simulating an effect not explicitly modeled. Such suggestions apply to manipulations of the code through input; modifications to the code itself lie beyond the scope of this document.

Such a discussion can never be complete. Furthermore, it is not essential in learning to run CONTAIN. Therefore, this section is more loosely organized than the rest of the User's Manual. It is intended that as more experience is gained with the code and feedback from the user community is obtained, additional material will be incorporated into this section.

The rest of this section is organized into three parts. Section 5.1, "Key Simplifying Assumptions in CONTAIN," addresses general limitations that are inherent in the CONTAIN modeling approach. These limitations are not expected to change with near-term improvements to the code.

Section 5.2, "Specific Model Limitations," is concerned with more detailed discussions of assumptions and approximations in individual models. Many of these deficiencies are expected to be resolved in future modifications to the code.

Section 5.3, "Practical Suggestions," lists suggestions that should be of use to the analyst in running the code and in getting as much useful information from it as possible. Problems and pitfalls to avoid are discussed, but there are also some ideas on how to make the code do things not obviously included in its nominal range of capabilities.

5.1 Key Simplifying Assumptions in CONTAIN

- Well-Mixed Atmosphere. The atmosphere physics modeling in CONTAIN assumes that the atmosphere within a given cell is well-mixed. The atmosphere is taken to be uniform both in temperature and in material concentrations. This assumption may not be appropriate in many cases. During many accident scenarios, it is possible that the cell atmospheres may experience thermal stratification and/or concentration gradients. On the other hand, most severe accident scenarios involve large sources and

sinks of heat and/or mass, resulting in substantial convection. The resulting mixing may overcome natural tendencies towards stratification or nonhomogeneity.

Several phenomena that are related to ESFs may be affected by the well-mixed atmosphere assumption. Depending upon conditions, each of the three systems (containment spray, fan cooler, and ice condenser) removes some combination of the following from the atmosphere: steam, energy, aerosols, and fission products. The effect of these systems in reality may be to set up gradients of these quantities that would subsequently affect the performance of the system. Such a heterogeneity in cell properties is not treated in CONTAIN.

One way to evaluate the importance of the well-mixed assumptions is to nodalize open volumes into a larger number of nodes. If important stratification effects are observed, the implication is that the coarser nodalization is inadequate. However, even if there appears to be little effect, it cannot be assured that the well-mixed assumption is justified, since buoyant plume behavior requires a finely resolved finite difference treatment of the momentum equation for a completely accurate treatment. The CONTAIN flow equation does not include the momentum convection terms in the momentum transport equation. (See Section 5.2.3.)

- Feedback on Primary System Neglected. CONTAIN is designed to be an analytical tool for assessing accident events occurring within the containment of nuclear power plants. Because the primary system is not modeled, there is no feedback in terms of how events and conditions in the containment will affect conditions in the primary system. Such effects could be important if, for example, the pressure buildup in the containment building could influence the rate at which coolant, hydrogen, aerosols, or radionuclides were lost from a breach in the primary system. Although nothing prevents the user from defining additional cells to represent primary system volumes, CONTAIN models were not developed with primary system conditions in mind, and it would be up to the user to assess their validity for such applications. The steam equation of state assumed would, for example, be grossly inaccurate for many typical primary system conditions.

5.2 Specific Model Limitations

Specific model limitations and assumptions are discussed below. The organization of the discussions is as follows:

Fission Product Modeling
Aerosol Modeling
Atmosphere Physics Modeling
Heat Transfer
Lower Cell Modeling
ESF Modeling

5.2.1 Fission Product Modeling

- No Spray Washdown of Fission Products from Walls. If containment sprays are activated, fission products that are deposited on structure surfaces might reasonably be expected to wash off these surfaces. Even though CONTAIN does provide a semi-mechanistic model for washdown of fission products with condensate runoff, such a model does not exist for spray washoff of fission products. This might however be simulated nonmechanistically with the targeted release formalism, i.e., by using it to transfer fission products from the wall to the pool (or to other locations).

- Gamma and Beta Heating Effects. The heat given off by many radionuclides as they decay often includes a significant fraction of gamma-ray emission energy. Much of this gamma energy is absorbed in solid objects within containment, such as walls and equipment. Relatively little would be absorbed by the gases present. Therefore, a significant fraction of the energy given off by fission products decaying in the atmosphere will not be absorbed by the atmosphere, as is assumed in the CONTAIN modeling. Similarly, some of the gamma heating from fission products deposited on structure surfaces would be radiated away from the surface and absorbed by other structures. Much of the gamma energy would be absorbed well below the structure surfaces, not in the surface node as is assumed in CONTAIN. Furthermore, when fission products are deposited upon structure surfaces, a significant fraction of their beta energy may still be deposited in the cell atmosphere rather than in the structure. These effects are not modeled in CONTAIN. The implications of some of these effects are explored further in Reference Wil87a.

- No Scrubbing of Gaseous Fission Products in Pools. The suppression pool SRV and vent models evaluate scrubbing of aerosols, and hence fission products hosted to aerosols. However, no modeling is provided for the scrubbing of gaseous or vapor phase fission products such as elemental iodine and other gaseous iodine species. To a limited degree, this effect can be simulated using targeted release and acceptance; see Section 5.3.

5.2.2 Aerosol Modeling

- Assumption That All Aerosol Particles of a Given Size Have the Same Water Content. The aerosol module assumes that all particles within a given size class have the same composition. To do otherwise would require the code to maintain a three-dimensional mesh of composition/size information, in place of the current two-dimensional mesh, with significant increases in complexity and computational cost. However, under certain conditions involving condensation/evaporation, significant error can result in the aerosol calculation. Suppose, for example, that gas containing water aerosols flows into a cell that contains solid aerosols, and suppose further that the cell atmosphere is superheated so that the water aerosols quickly evaporate before they agglomerate significantly with the solids.

In reality, the evaporation of the water would have no effect upon the solids. In CONTAIN, if the solid and water aerosol size distributions overlap, all particles in the overlapping size region will be assumed to have the average composition for that size and thus will be assumed to be part water and part solid. When the water is evaporated, the solid residue will therefore be shifted down in size. In one extreme case of this kind, an aerosol component with a mass median diameter of ten microns was found to be shifted down to the one micron size range.

A somewhat similar problem can arise when a large amount of water first condenses upon solid aerosols, and subsequently re-evaporates. Since condensation acts to make the smaller particles grow more (in a relative sense) than the large ones, it acts to collapse the size spectrum into a smaller number of size classes. The resulting loss of size resolution is irreversible, and the initial size distribution is not fully recovered when the water evaporates. In some cases, some of the aerosol particles will be calculated to be smaller than the smallest allowed size after evaporation and will be lost from the mesh (see Sections 2.2.4.2 and 3.3.1.11).

- Aerosol-Atmosphere Thermal Equilibrium. The aerosols are assumed to be at the same temperature as the atmosphere. Because the mass of the suspended solid aerosols is assumed to be small compared with the total atmosphere mass, such aerosols do not contribute to the total atmosphere heat capacity. This simplifying assumption is expected to be valid for most applications, but in extreme cases it could lead to heat transfer errors. Because of the large masses involved, water is treated in a special special way for LWR analyses; when water condenses onto or evaporates from aerosols, the saturated liquid enthalpy is removed from or added to the atmosphere. However, this quantity is evaluated at the current atmosphere temperature. The energy associated with the change in sensible heat of the liquid between the temperature at which condensation occurs and that at which evaporation occurs is neglected. This can result in errors, but they are expected to be negligible in most instances.

- No Aerosol Deposition in Flow Paths. Current models do not allow for aerosol deposition processes in flow paths. Deposition occurs only in cells. It is possible to model a flow path as a cell, in which case the aerosol behavior would be calculated. However, effects due to bulk movement of the gases in the path, such as impaction of aerosols on the surfaces of the flow path, would not be accounted for. Also, the efficiency of the flow solvers may be adversely affected by a relatively small cell in the flowpath.

- No Insulating Effect Due to Aerosol Plateout and Buildup. As aerosols plate out on surfaces, they may well act as an insulating blanket. In dry environments, aerosol deposits have been shown to be light and fluffy, so that the aerosol layer has a high void fraction and, thus, a high gas fraction. The conductivity of the layer, therefore, could be quite low. In many LWR

accident scenarios, condensed water films are expected to substantially reduce this effect.

Certain nuclear plants rely on external cooling of the containment shell to remove heat from containment following a severe accident. An aerosol deposit on the inside of the containment shell will serve to insulate the shell to some extent, reducing the effectiveness of the external cooling system. This would likely result in somewhat higher internal temperatures and pressures. For LMRs, this effect has been found to be potentially significant. For LWRs, degradation of heat transfer at fan cooler surfaces due to aerosol deposition could also be important. The insulating effects of aerosol deposits on surfaces are not modeled in CONTAIN.

5.2.3 Atmosphere Physics Modeling

- Hydrogen Burn Model. The model in CONTAIN for combustion of hydrogen (and carbon monoxide) is essentially the same as that in the HECTR code and is believed to be a reasonably good one for many purposes. However, there are some uncertainties associated with its results, and the user should take them into account in evaluating any results that might be sensitive to these limitations, e.g., in applications assessing whether pressurization due to burns poses a threat to containment integrity.

  The default burn model uses correlations for the flame speed which depend on the initial hydrogen and steam concentrations, with high steam concentrations yielding low flame speeds and, hence, long burn times (up to several tens of seconds). These long burn times permit substantial gas-structure heat transfer during the burn, which can result in considerable mitigation of the peak pressure due to the burn. There are only limited experimental data available at high steam fractions to support these correlations, and the data show much scatter, with some data supporting the low speeds predicted by the CONTAIN default model while other results imply less retardation due to steam than is predicted. Hence, in any application for which the peak pressure is of importance, the user should explore the sensitivity to the burn time by varying either of the parameters "burnt" or "flam" in the hydrogen burn input (Section 3.3.1.7).

  In the default burn model, combustion ceases once the oxygen mole fraction drops to 0.005. Since the initial oxygen mole fraction is typically of the order 0.05 to 0.2, this limit means that up to 10% of the oxygen initially present will not be available for combustion in scenarios in which oxygen, rather than hydrogen, is the limiting reactant. This limit may be unrealistic in some cases, especially when strong burns are expected; the user can set it to any desired value through the input parameter "mormng".

  The default burn correlations for flame speed, flammability limits, and propagation are based upon experimental results in

which the initial temperatures are relatively low, generally not far above the saturation temperature. If initial temperatures are much higher than this, it is expected that flammability regions will extend over a broader range than predicted by the default model, and flame speeds will be higher than predicted. CONTAIN does not include any modeling for these dependencies upon the initial temperature. The user may investigate the possible implications of these effects by varying the appropriate parameters in the hydrogen burn input block (Section 3.3.1.7).

Note, also, that all combustion events are evaluated as deflagrations that yield only static loads due to the pressure rise associated with the atmospheric heating. There is no modeling for accelerated flames, detonations, or the dynamic loads that would result from these phenomena.

- No Deposition or Heat Loss in Flow Paths. Currently no provision exists for removal of mass, energy, or fission products within a flow path. The atmosphere gases, aerosols, and fission products cannot be deposited on the flow path walls. Sensible heat from the gas, furthermore, cannot be transferred to the flow path walls. The flow rate may be determined to some extent by viscous losses. In this case, any heating resulting from viscous effects is assumed to be retained in the flowing material. If either the flow path inventories or heating effects are important, they must be modeled through an intervening cell.

- Flow Paths as Virtual Boundaries Between Cells. The intercell flow modeling may be used to describe both orifices or flow channels and lumped parameter flow resistances. The lumped parameter flow resistances are appropriate to the case in which the cell boundary does not correspond to a physical boundary but is drawn within an open volume. The user should be aware of the limitations of the CONTAIN modeling for situations in which the flow areas are comparable to the cell cross-sectional area, as in the case of a virtual boundary. First, not all processes important to transport between cells are modeled, and some of these, such as countercurrent flow and turbulent diffusion may be more important for large flow areas than for small flow areas. Also, in the momentum equation it is assumed that the momentum and kinetic energy of the flow is dissipated completely in the downstream cell. In reality, the dissipation may occur over a number of cells; that is, momentum convection may be important. Because of this assumption, care should be used in setting the flow coefficient to obtain the proper overall flow particularly if the nodalization is fine. (If the flow coefficient is held constant for each virtual boundary while the nodalization is refined without limit, the gas transport in the problem will go to zero!)

  Carryover of aerosols and fission products from cell to cell due to convection and settling (in the case of aerosols) is modeled. However, spray droplets introduced in one cell are not allowed to fall through a cell boundary to another cell.

- Equation of State for Steam. CONTAIN assumes an ideal gas equation of state for water vapor and also assumes the specific energy is not a function of pressure. Consequently, close to the saturation line, small errors (up to 10%) may occur in the vapor density and other properties at pressures typical of containment applications ($P < 10^6$ Pa); well above saturation, errors are expected to be negligible. If the code is applied to scenarios with pressures above those typical of containment applications, larger errors are possible.

5.2.4 Heat Transfer

- Aerosols Treated as Pure Absorber/Emitters. The treatment of aerosol emissivity in CONTAIN is derived for absorbing aerosols that produce negligible scattering. The user should be cautioned that if this condition is not satisfied the aerosol cloud may scatter effectively and significantly reduce the radiative heat transfer or emissivity of a hot gas radiating to cold walls. This effect and others that arise in the presence of significant scattering are not taken into account in CONTAIN, and this omission may lead to calculated gas pressures and temperatures that are too low. To some extent the user can explore the importance of the effect of aerosol emissivity on the problem by varying the "kmx" or "absorb" parameters (Sections 2.3.1.5.2, 3.3.1.5), or by omitting aerosols from the radiation modeling. However, there is no direct means of forcing the emissivity of the gas-aerosol cloud to be less than the emissivity calculated for the gas alone.

- No Water or Carbon Monoxide Release from Heated Concrete. Significant quantities of water can be released from heated concrete even below the ablation temperature. This release is of particular importance in LMRs where the released water can react with sodium coolant. Both hydrogen and heat are produced by this reaction. CONTAIN does not model the release of water or gases from heated concrete, except during the concrete ablation resulting from direct contact of core debris with concrete. Thus, gas release due to radiant heating of concrete structures above a molten pool is not modeled. These releases can be simulated by using source tables for the materials given off. However, the actual release is a function of the temperature of the concrete. Source tables used for this purpose, therefore, should be carefully developed so that both the quantity and timing of the releases reflect the anticipated concrete heatup characteristics.

5.2.5 Lower Cell Modeling

- No Conduction Heat Transfer to Walls in Lower Cell. There is no heat transfer from the lower cell layers to the surrounding wall structures via conduction through these layers and the structures in contact with them. This might be significant in a system that has high conductivity walls, such as the steel liners one might find in an LMR system.

- Lower Cell Nodalization. The model used to describe phenomena in the lower cell assumes that all materials within a given node are in thermal equilibrium and homogeneously distributed. The intermediate layers and the pool layer each consist of one node, whereas the concrete layer may have five or more nodes. If necessary, the material in the intermediate layer can be separated out to different individual layers.

- ANSI Makeup Decay Power Remains in Cell. The lower cell model allows the user to distribute makeup decay power, as defined by the ANSI standard, in all layers of the cell being modeled (see Section 2.3.2.2), including the atmosphere layer. The power attributed to the atmospheric layer by the ANSI model will not, however, flow with the atmospheric gases. The makeup decay power will always remain in the cell for which it was originally defined. Mobile heat sources should be modeled explicitly with fission products or fission product groups.

- Gas Generation From Core-Concrete Interactions. In the CORCON model, it is assumed that the thermal attack of concrete is sufficient to produce gas generation rates high enough to sustain a gas film between the concrete layer and the overlying hot solid or melt that is attacking the concrete. The heat transfer coefficient implied by this assumption has been a matter of some controversy which may be resolved through ongoing experimental research.

- CORCON Layer Flip. The CORCON model assumes that the core debris initially segregates into a metal layer which is located above a heavy oxide layer. Ablation is assumed to furnish light oxide products to the lower layer until its density is less than the metal layer and "layer flip" occurs. The heavy oxide layer materials are then assumed to join the light oxide layer materials atop the metals. There is some doubt about the validity of this scenario, since the metal layer may have metallic uranium mixed with lighter metals, so that the initial configuration may have the metal layer on the bottom. Furthermore, agitation by gases passing through the melt may be sufficient to cause considerable interlayer mixing. Again, ongoing experimental research should help resolve these issues.

- CORCON Fission Product Inventories. Fission products are added to the CORCON inventories whenever UO_2 is included among the materials being introduced into CORCON. The reason for this addition is that CORCON computes the radionuclide inventory based on the user-specified mass of uranium in the core and the values of the retention factors for fission products. Thus the CORCON system is keyed to the amount of UO_2 in a given mass of core debris. The fission products added in association with the added UO_2 will affect the decay heat computation.

  There will also be an effect on the VANESA model. The added fission products will be used to modify the VANESA inventories. However, the reverse coupling is not yet implemented. Radionuclides which VANESA calculates as being released from the core debris are not removed from the CORCON inventories of fission

products. Such a treatment awaits the work being done by the CORCON/VANESA development group to produce an integrated version of the two models.

5.2.6 Engineered System Modeling

- No Carryover of Containment Spray from Cell to Cell. There may be instances in which the user desires to model the upper region of the containment, where the spray nozzles are located, as a single cell, and subdivide the lower region into one or more cells. The CONTAIN spray model does not treat a spray falling from one cell into another cell or set of cells. If the spray carryover is perceived to be important in the lower region (e.g., with respect to aerosol scrubbing), this situation may be simulated by specifying individual spray systems originating in the lower region.

- Calculational Sequence Effects. CONTAIN performs its major blocks of calculations in sequential order. Lower cell calculations are performed first, then upper cell calculations, and finally, ESF calculations. Because the coupling among these models is largely explicit, for some calculations time delays in the effects of one model on another may occur. For example, mass added to a lower cell pool by an engineered system (e.g., sprays) will show up in the output delayed by a timestep. This happens because the lower cell calculations are carried out before those for the engineered systems. Similarly, cell calculations are performed in sequential order according to cell number. Events occurring in higher-numbered cells that affect lower-numbered cells will not show up until the next system timestep. Users should be aware of these time-delay effects in interpreting CONTAIN output. Rerunning the problem with a reduced timestep will usually reveal whether such effects are important.

5.3 Practical Suggestions

Many lessons have been learned through the exercise of CONTAIN for specific applications (see Appendix A for relevant publications). Some of the more universally applicable suggestions are included below.

- Optimizing Multicell Calculations. The flow option of choice for all but the most restrictive flow areas is the IMPLICIT = "nimpli" option, where "nimpli" is the number of cells to be solved by the implicit technique. If "nimpli" is less than "ncells", the cells not solved implicitly are solved by a simple Euler explicit method. Stability considerations preclude the use of explicit cells which are not relatively large in volume or not coupled to other cells entirely through highly restrictive flow paths. The explicit cells in practice are likely to be environment cells with very large volumes (of order 10^{10} m^3). By excluding the environment cells from the implicit solver matrix, the overhead due to multiple environment cells is

reduced considerably. Robustness of the implicit solver is also improved.

It is difficult to give general guidelines on improving the convergence of the implicit solver. Shorter system timesteps often help, as will larger than default values for the "pvtmin" parameter. Cell level models which act as strong sources or sinks may cause problems if the sources or sinks cause a change in the mass of a cell by more than 20% per system timestep. User-specified sources may also cause problems. The source mass should be limited to 20% of the cell mass per system timestep. If actually a sink, the source should not be allowed to drive any of the atmosphere component masses negative.

The QUASI flow option and especially the REDUCE option within the QUASI option should be considered obsolete. The default explicit inertial flow option, using the Runge-Kutta solver, may be of interest with regard to very fast transients or because of the integration error control. However, the models available with the explicit inertial flow option are not as extensive as those available with the IMPLICIT option.

- Choked Flow at Less Than the Critical Pressure Difference. To model choked flow, CONTAIN limits the flow velocity in flow paths to the local sound speed, using the standard expression for the limiting flow rate of an ideal gas assuming adiabatic flow. However, under certain conditions the user may find that choking arises at pressure differences less than the expected critical value for choked flow. The most likely cause is the specification of an unrealistically small value of the turbulent flow coefficient discussed in Section 3.2.3. For an orifice, this coefficient should be of order unity. If a much smaller value is used, the flow velocities calculated for a given pressure difference will be too large, and the pressure difference at which choking begins will be too small. For realistic values of the flow coefficient, the onset of choking in the calculation will occur at approximately the correct value of the pressure difference.

- Upward Compatibility Issues. Every effort has been made to make the CONTAIN 1.1 input compatible with existing input decks for prior code versions. In some instances, however, the models and/or code architecture have undergone such severe modifications that intelligent translations of old input options are not possible. In other instances, the old input format is accepted by CONTAIN 1.1 but the action taken may differ from the action that the user originally intended. A warning message is always written to the error file when the latter condition is encountered. Therefore, the error file should always be checked for the message: ">>>>> warning". Appendix D summarizes the major instances in which the action taken has been substantially. One of these instances of loss of upward compatibility, aerosol behavior in cells without floors, is important enough to be discussed below.

- Aerosol Gravitational Settling Without Floors. In code versions prior to CONTAIN 1.1, a default floor with an area equal to "volume"/"height" is automatically defined in cells without heat transfer structures. This is incompatible with the new aerosol fall-through model and the new aerosol deposition and fission product host architecture. Therefore, a default floor is not created in cells without structures in CONTAIN 1.1. As a result, aerosol gravitational settling in cells without structures can only occur with respect to flow paths. Such settling is activated with the FPCOSN or VCOSN keywords in the FLOWS or ENGVENT input. In the absence of floors or the above model, gravitational settling is not considered present. Unless other processes remove aerosols, the aerosols will remain airborne until agglomeration causes the aerosols to be lost from the size mesh (i.e., exceed the particle sizes allowed in the largest size class). Aerosols which are lost from the mesh will be immediately removed from the atmosphere and placed either in the pool or in the waste holding array (see Section 2.2.4.2). It is possible that quite unrealistic aerosol behavior in the atmosphere will be calculated in such cases.

- No Aerosol Settling on Pools. As in previous versions of CONTAIN, direct gravitational settling onto pool surfaces is not modeled in CONTAIN 1.1. If a floor is included, the fission products hosted to the aerosols settling on the floor can be transferred from the floor to the pool using the targeted release and acceptance formalism.

- Modeling the Outside Environment. The outside environment can be modeled as a very large cell (volume > 10^{10} m^3). The quantities of aerosols leaked to the environment can be readily determined as long as no structures, which tend to remove aerosols, are defined in the environment cell. (CONTAIN 1.1 does not define a default floor for aerosol gravitational settling in cells without structures.) Aerosol mesh losses for the environment cell should be checked when settling of aerosols is not permitted.

- Mass Transfers by Negative Mass Tables. Mass transfer among cells can be simulated by defining source tables that are positive in one cell and negative in the other. Such user-controlled transfers are not mechanistic, but they can be useful in cases when adequate models in CONTAIN do not exist. A similar approach may be used to bring about mass transfers within a cell, e.g., between layers in the lower cell. It is up to the user to assure that the inventories of the quantity transferred do not go negative.

- Lower Cell Heat Conduction And User-Defined Materials. With the inclusion of two new capabilities in CONTAIN 1.1, it should now be possible to obtain realistic results for heat conduction in the lower cell layers. The new heat conduction algorithm is a major improvement over the method that was used previously. However, if it is desired to employ this model with realistic concrete properties, it may be necessary to use the user-defined material option also. The concrete layer material is often the

standard CONTAIN material named CONC. Should an application require accurate modeling of heat transfer into the concrete and the concrete is well characterized, a user-defined material for that concrete should be specified and used in the concrete layer definition. The tables associated with user-defined materials allow the appropriate properties to be specified. All materials specified in the concrete layer will contribute to the bulk layer properties for conduction, so iron reinforcement, if present, may be specified separately from the concrete material (see Section 2.3.2.1).

- Fission Product Mass Effects. Fission products are treated as being massless in terms of their effects on processes such as intercell flow and aerosol dynamics. This treatment may not be appropriate for certain types of problems. Fission product masses could, for example, significantly influence the behavior of their aerosol hosts. Thus, the user should attempt to minimize the discrepancy between the fission product masses and the aerosol masses. For example, if a fission product attached to an aerosol host is introduced via source tables, the mass of the aerosol host should be increased by the corresponding amount through source tables. If possible, the size of the aerosol particles should also reflect the presence of the fission product mass.

- Simulation of Pool Scrubbing of Elemental Iodine. The CONTAIN 1.1 models for BWR vents and SRVs do not include scrubbing of gaseous fission products such as elemental iodine. If it is acceptable to assume that iodine will be in equilibrium between the pool and the atmosphere, a simulation of the net effect may be defined using the targeted release and acceptance formalism. Let the partition coefficient, K, be defined to be the ratio of the aqueous concentration to the atmospheric concentration at equilibrium. To simulate the equilbrium behavior, the user can define both pool-to-gas and gas-to-pool transfers, with the (gas-to-pool)/(pool-to-gas) release rate ratio being equal to $K*V_1/V_2$, where V_1 and V_2 are, respectively, the volumes of the pool and of the atmosphere. (Inclusion of V_1 and V_2 is necessary because a mass release rate is proportional to the total quantity of a fission product associated with a host, while the partition coefficient is defined in terms of concentrations.) The sum of the release rates governs the rate of approach to equilibrium. Thus, if K is 20 and the atmosphere volume is 10 times the pool volume, and an approach to equilibrium with a time constant of 33.3 seconds is desired, this could be achieved by the following FPM-CELL input:

```
FPM-CELL
  TARGET
    MOLI2  0.02  0.0  0.0  FROM GAS   TO LAYER POOL
    MOLI2  0.01  0.0  0.0  FROM LAYER POOL  TO GAS
  EOI
EOI
```

Temperature-dependent release rates may be specified in order to simulate the temperature dependence of the partition coefficient. Since the pool temperature would presumably govern the gas-to-pool transfer, it should be redefined as a pool-to-gas transfer with a negative rate. The reader should refer to Equation 2-20 to see how a negative rate is interpreted.

It should be noted that the assumption of rapid equilibrium is likely to be invalid for some accident scenarios. Equally important, aqueous iodine chemistry is actually very complex and will include many dependencies that cannot be simulated using the release and acceptance formalism as presently implemented. The partition coefficient, as defined above, will depend upon pH, total iodine concentration, and possibly the amounts of the many other chemical species that might be present in the pool during a severe accident. In addition, slow iodine reactions such as hydrolysis to iodide and iodate can cause a time-dependent change in the effective value of the partition coefficient. To a limited degree, this effect could also be simulated by defining additional interhost transfers. Radiation chemistry effects can introduce additional complexities.

- Multiple Sources for a Single Species. Use of CONTAIN for the analysis of LWR accidents usually requires that sources of water, steam, and hydrogen be defined as part of the input to the code. These sources may come from design-basis-accident codes or other codes that model core and reactor coolant system transport of liquids, vapors, and gases. More than one source table for the same material can be specified in the input. The fact that the effects of such tables are additive gives the user flexibility in combining sources that may have been generated by different codes.

- Simulating Quenching Phenomena. To simulate a quenching process in a pool, the user may exercise the HT-COEF option to define an enhanced heat transfer coefficient between a hot intermediate layer and the coolant layer. The heat transfer coefficient should be set to a low value or to zero until the time the hot material is actually injected into the coolant, and then increased to a high value. The numerical solvers for the lower cell system are sufficiently robust to handle the situation in which large amounts of energy are dumped into a layer in a short time. The energy being added per timestep can be of the order of tens of percent of the layer's total energy. Steam spikes due to molten fuel dropping into water in the cavity have been effectively simulated in this way (see Section 6.3 for an example). The important thing to remember is that the heat transfer coefficient specified in the HT-COEF option is associated with the nominal area of the layer. To simulate an enhanced heat transfer area (due to fuel fragmentation, for example), it is necessary to multiply the heat transfer coefficient desired by the ratio of the true heat transfer area to the nominal layer area. Similarly, the steady-state behavior of a porous debris bed can be simulated with the same option.

- Structure Noding Considerations. In modeling a composite structure, neighboring nodes in different materials should be about the same size. Otherwise, the effects of the different node sizes may swamp the effects of the different conductivities of the materials.

  Note also that the condensation model does not take into account the resistance of the half-node between the point at which the first node temperature is calculated and the structure surface. The surface node thickness should be kept fairly small so that the structure surface temperature and the surface node temperature do not differ greatly. In cases where condensation on structures is a key phenomenon, the user should check the sensitivity of the results to varying surface node thicknesses. Note that, as discussed in Section 2.3.1.3.1, node thicknesses should not be changed too much from one node to the next.

- Restarts. Long-running jobs can be efficiently handled using the restart option. Each restart file should be saved under a file name that is different from the name of any previously generated restart files. Such a backup avoids the loss of previous restart information should an error or system problem occur during the run.

- Output Handling. When a user is first getting acquainted with the code or is running a new problem, it is desirable initially to run a job for only a few "long-edit" cycles to test the quantity of output being generated. The quantity of output may require microfiche rather than hard copy or the judicious use of the LONGEDT and SHORTEDT output options.

- Annotated Input. Users are encouraged to add comments to their input files. This is accomplished using the && sign, followed by a blank and then the appropriate comments.

  Comments at the beginning of an input file describing the nature of the file, the particular circumstances being modeled, etc., are useful for later referral. One can also use the TITLE option. However, titles cannot be put at the very beginning of a deck, as can comment lines. On the other hand, titles are printed at the beginning of each long edit and become part of the plot file. They are therefore convenient for labeling the output.

6. SAMPLE PROBLEMS

This section deals with four sample problems. A brief description of each problem is given, followed by annotated input descriptions and examples of the calculated results for these problems. The sample problems emphasize different capabilities of CONTAIN but are not intended to be comprehensive. They are included here to illustrate some of the CONTAIN features and to guide the user in setting up input datasets.

The sample problems deal with the following phenomenological areas:

- atmosphere thermodynamics and heat transfer during a steam blowdown into an LWR containment building,
- fission product decay and transport via intercell flow and aerosol settling,
- lower cell thermodynamics and heat transfer during a steam spike resulting from large heat transfer rates between a pool and a hot solid layer, and
- BWR suppression pool vent and SRV behavior.

6.1 LWR Steam Blowdown into Containment

This sample problem illustrates the capability of CONTAIN to perform blowdown calculations. The geometry is typical of a reactor containment building. A blowdown source is specified for the first 23 s. The passive heat sinks are lumped into five structures. For the sake of illustration, forced-convection/condensation heat transfer to two of these structures is activated 40 s into the problem. Prior to that time, natural convection is assumed. A convection velocity of 3 m/s is specified for structure number 1 and 10 m/s for structure number 4. Figure 6-1 shows the containment pressure response to the blowdown and the subsequent condensation onto the structures as predicted by CONTAIN. Also shown is the cumulative mass of vapor condensed on structure number 4. The effect of the activation of forced convection at 40 s is barely perceptible on the pressure trace but is readily apparent on the condensation curve. The input for this problem, together with comments, is shown in Figure 6-2.

6.2 Fission Product Intercell Transport

The CONTAIN treatment of fission products allows for their transport from one cell to another. This movement is dictated by the intercell flow of fission product hosts. In this sample problem, four fission products in two decay chains are used. Chain 1 consists of fission products DUM1 and DUM2; DUM1 decays to DUM2. Similarly, chain 2 consists of fission products DUM3 and DUM4; DUM3 decays to DUM4. Note that in this example, DUM2 and DUM4 also decay, although their daughters are not explicitly specified.

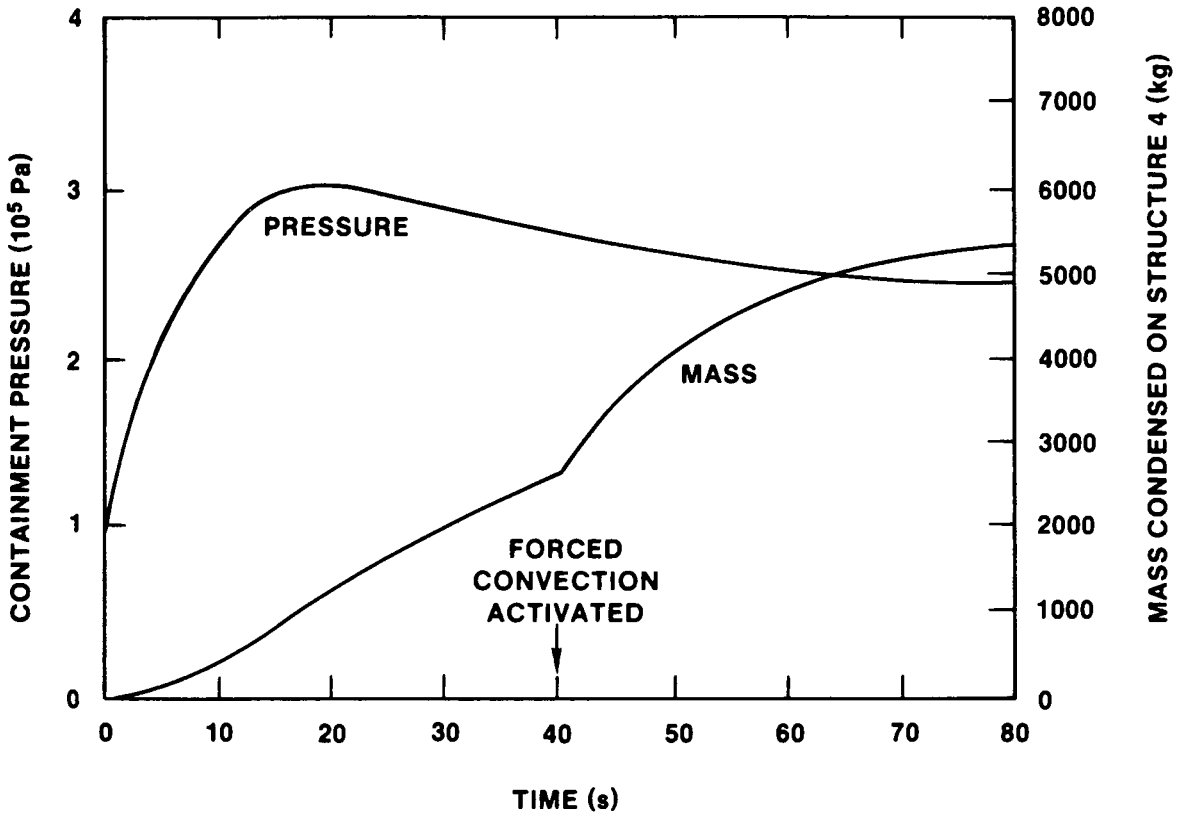

Figure 6-1. Containment Pressure Response

This problem specifies two cells that are interconnected by a flow path and contain heat sinks to maintain nearly isothermal conditions. Cell 1 is initially at a higher pressure than cell 2. The atmosphere gas is the host for the fission products in chain 1. The aerosol NA2O2 is the host for the fission products in chain 2. All the fission products and aerosols are initially in cell 1. Each fission product has an initial mass in cell 1 of 1.0 kg.

The initial pressure differential between the two cells is quite small, and the total mass transferred from cell 1 to cell 2 is only about 5% of the initial mass in cell 1. Hence, only a small amount of fission product mass is transferred.

Figures 6-3 and 6-4 show the fission product masses transported into cell 2. Figure 6-3 gives the masses for DUM1 and DUM2. Each has an initial mass of 1.0 kg, and both are transported by the gas. With the flow characteristics used in this problem, the cell pressures have essentially equalized at about 80 s, and the flow becomes negligible at that time. The difference in the behavior of the fission product masses with time is due to decay and to settling. Figure 6-4 shows that some of DUM3 and DUM4 has been deposited as a result of their host aerosol settling.

The annotated input for this sample problem is shown in Figure 6-5.

```
CRAY                                              ← machine type

CONTROL
  NCELLS=1 NTITL=2 NTZONE=2                       ← global control block
EOI

MATERIAL                                          ← material specification
  COMPOUND N2 O2 H2O1 H2OV CONC FE

TIMES 59. 0.0 0.2 5.0 40.0                        ← times block with default
              1.0 5.0 80.0                          cell time fraction

TITLE
  CONDENSATION MODEL TEST - FORCED                ← problem title
  CONVECTION AFTER 40 SECONDS

THERMAL                                           ← reactor type

THERMO                                            ← thermodynamics and mass
                                                    accounting

PRHEAT                                            ← structure print flag

CELL=1
CONTROL
  NHTM=5 MXSLAB=5
  NSOATM=1 NSPATM=14                              ← cell control block
  NUMTBC=2 MAXTBC=2
EOI

GEOMETRY 5.95E4 48.                               ← cell volume and height

STRUC

  NAME=ROOF TYPE=ROOF SHAPE=SPHERE
  NSLAB=5 TUNIF=300. TOUTER=300.
  CHRLEN=19.8
  X=10.8 19.81 19.83 19.86 19.92 20.6
  COMPOUND=FE FE CONC CONC CONC
  EOI

  NAME=FLOOR TYPE=FLOOR SHAPE=SLAB
  NSLAB=4 SLAREA=1.2E3 TUNIF=300.
  TOUTER=300. CHRLEN=19.8                         ← three of five structures
  X=0. .005 1.33 2.67 4.
  COMPOUND=CONC CONC CONC CONC
  EOI

  NAME=WALL TYPE=WALL SHAPE=CYLINDER
  NSLAB=5 CYLHT=76. TUNIF=300
  TOUTER=300. CHRLEN=38
  X=19.8 19.81 19.83 19.86 19.92 20.6
  COMPOUND=FE FE CONC CONC CONC
  EOI
```

Figure 6-2. Annotated Input for Steam Blowdown

```
  NAME=SINK1 TYPE=WALL SHAPE=SLAB
  NSLAB=3 IOUTER=1 SLAREA=1.4E4
  TUNIF=300. CHRLEN=10.
  X=0. .005 .300 .305
  COMPOUND=CONC CONC CONC
  EOI

  NAME=SINK2 TYPE=WALL SHAPE=SLAB
  NSLAB=3 IOUTER=1 SLAREA=4.E4
  TUNIF=300. CHRLEN=10.
  X=0. .001 .003 .0038
  COMPOUND=FE FE FE
  EOI
```

← two more structures

```
ATMOS=3
```

← atmosphere input

```
  1.003E5 294.
```

← pressure and temperature

```
  N2=.795 O2=.195 H2OV=1.E-5
```

← 3 materials present

```
SOURCE=1
  H2OV=6
  IFLAG=1
  T= 0.   0.2    0.7   1.2   2.2
     3.2  4.2    8.2  10.2  15.2
    20.2  22.7  23.2  24.0
  MASS=0.69E4 2.97E4 2.71E4 2.45E4 1.96E4
       1.69E4 1.51E4 0.96E4 0.82E4 0.38E4
       0.21E4 0.01E4 0.     0.
  ENTH=1.13E6 1.12E6 1.12E6 1.13E6 1.11E6
       1.11E6 1.10E6 1.14E6 1.13E6 1.10E6
       0.69E6 0.45E6 0.     0.
  EOI
```

← atmosphere source table

```
CONDENSE
```

← structure condensation activated

```
  FORCED=2
  VAR-X=CTIME    X=2 40. 80.
  VAR-Y=VELOCITY Y=2 3.  3.
  EOI
  VAR-X=CTIME    X=2 40.  80.
  VAR-Y=VELOCITY Y=2 10.5 10.5
  EOI
```

← forced convection velocity tables

```
  STR-COND 2 1,1 4,2
```

← pair first table with first structure; second table with fourth structure

```
  EOF
```

← end of input data

Figure 6-2. Annotated Input for Steam Blowdown (continued)

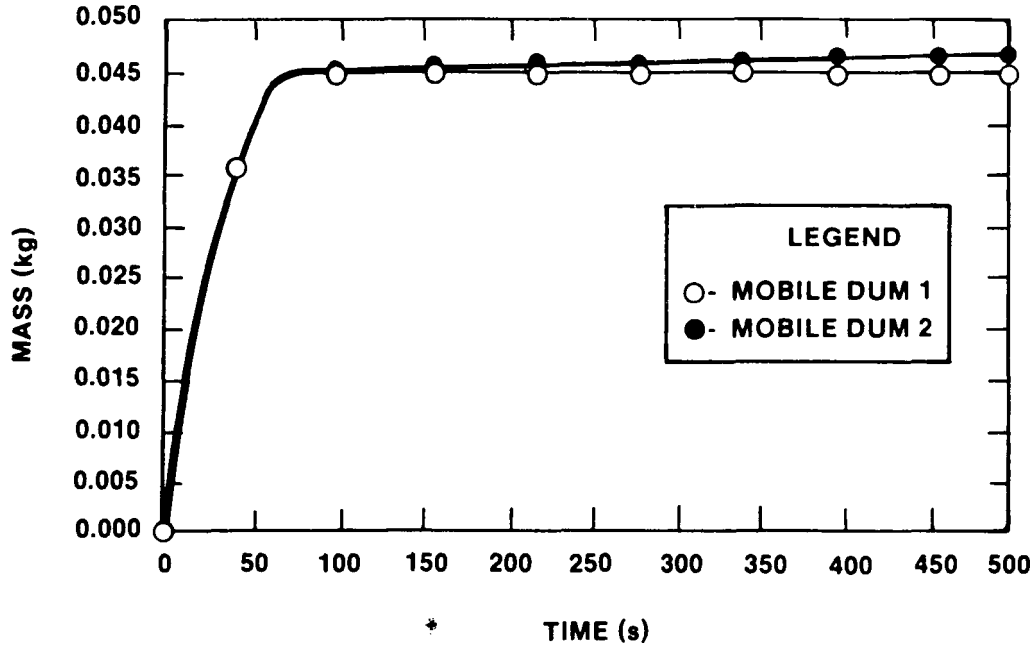

Figure 6-3. Mass of Fission Products DUM1 and DUM2 Transported into Cell 2

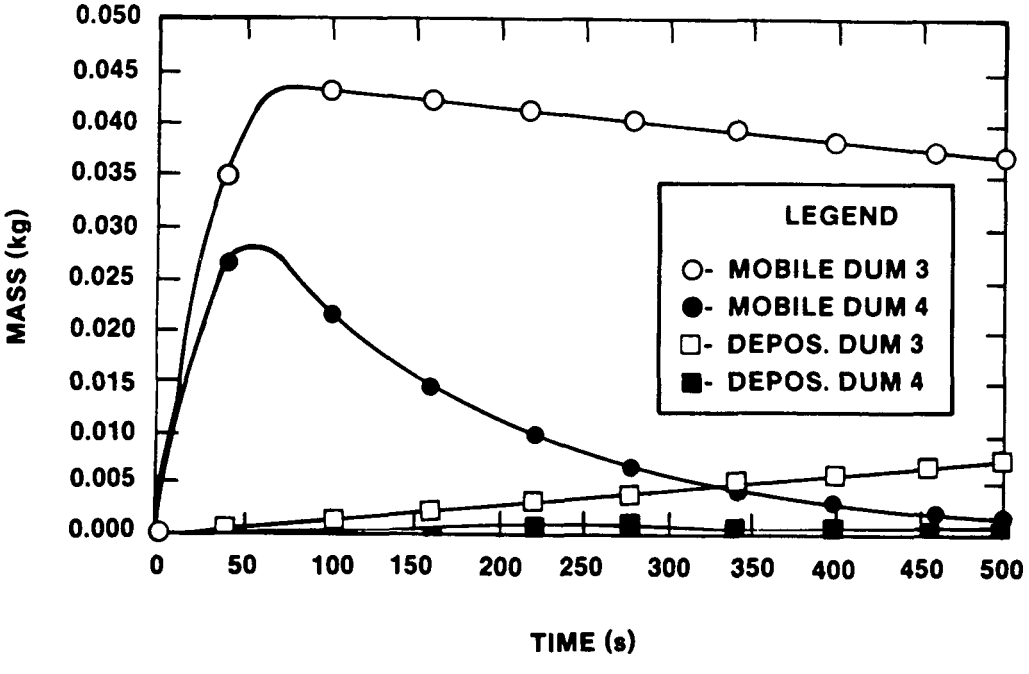

Figure 6-4. Mass of Fission Products DUM3 and DUM4 Transported into Cell 2

```
CRAY                                          ← machine specification
CONTROL
  NCELLS=2 NTITL=2
  NCHAIN=2 NFCE=4                             ← global control block
  NAC=2    NSECTN=20
  NTZONE=2
EOI

MATERIAL
  COMPOUND N2 FE CONC K2O MGO                 ← material, aerosol, and
  FP-NAMES DUM1 DUM2 DUM3 DUM4                  fission product names

TIMES 60.0 0.0
  0.1  5.0 20.0                               ← times block
  1.0 10.0 500.0
  1.0  1.0

FLOWS IMPLICIT
  AREA(1,2)=0.02 AV1(1,2)=0.05                ← flow path characteristics
  CFC(1,2)=2.0 TOPEN(1,2)=0.0

PRFLOW PRFISS2 PRAER2                         ← detailed print options

FISSION
  NFPCHN=2
    FPNAME   DUM1   DUM2
    HFLIFE   1.0E4  0.9E4                     ← fission product
    POWER    1.0    1.0                       characteristics
  NFPCHN=2
    FPNAME   DUM3   DUM4
    HFLIFE   1.1E4  1.0E2
    POWER    1.0    1.0
EOI

AEROSOL
  K2O  2.0E-6 0.693                           ← aerosol characteristics
  MGO  1.0E-6 0.693

THERMAL                                       ← reactor type

TITLE
TEST PROBLEM FT02 - VERSION 1.1               ← problem title
FISSION PRODUCT TRANSPORT AND DECAY

CELL=1
CONTROL NHTM=2 MXSLAB=3 EOI                   ← cell control block

TITLE
  HIGH PRESSURE CELL (#1)                     ← cell title

GEOMETRY 1.000.0 10.0                         ← cell volume and height
```

Figure 6-5. Annotated Input for Fission Product Intercell Transport

```
ATMOS-1
1.1E5 300.0                                  ← initial pressure, temperature,
N2 1.0                                         and composition of atmosphere

STRUC
  NAME-HEATSINK
  TYPE-WALL SHAPE-SLAB
  NSLAB-3   CHRLEN-1.0  SLAREA-1.0E5
  IOUTER-1  TUNIF-300.0
  x         = 0.0   0.005 0.010 0.015
  COMPOUND  = FE    FE    FE
  EOI                                        ← structure definition
  NAME-DEFFLOOR
  TYPE-FLOOR  SHAPE-SLAB
  NSLAB-3     CHRLEN-1.0 SLAREA-100.0
  TOUTER-300.0 TUNIF-300.0
  X         = 0.0   1.0   2.0  3.0
  COMPOUND  = CONC  CONC  CONC
  EOI

FPM-CELL
  HOST-GAS           1.0 1.0 0.0 0.0      ← initial fission product masses
  HOST-AEROSOL MGO   0.0 0.0 1.0 1.0
EOI

AEROSOL-2
  K2O-1.0 MGO-1.0                          ← aerosol initial masses

CELL-2
CONTROL NHTM-2 MXSLAB-3 EOI                ← cell control block

TITLE
  LOW PRESSURE CELL (#2)

GEOMETRY 1000.0 10.0

ATMOS-1
1.0E5 300.0 N2 1.0

STRUC
  NAME-HEATSINK TYPE-WALL SHAPE-SLAB
  NSLAB-3 CHRLEN-1.0 SLAREA-1.0E5 IOUTER-1 TUNIF-300.0
  X         = 0.0   0.005 0.010 0.015
  COMPOUND  = FE    FE    FE
  EOI
  NAME-DEFFLOOR TYPE-FLOOR SHAPE-SLAB
  NSLAB-3 CHRLEN-1.0 SLAREA-100.0 TOUTER-300.0 TUNIF-300.0
  X         = 0.0   1.0   2.0  3.0
  COMPOUND  = CONC  CONC  CONC
  EOI

EOF                                        ← terminate input file
```

Figure 6-5. Annotated Input for Fission Product Intercell Transport (continued)

6.3 Steam Spike

The purpose of this example is to illustrate the ability of the CONTAIN pool boiling model to treat an energetic steam spike. The physical problem being modeled is the mixing and quenching of molten debris that has been injected into a water pool. As discussed in Section 5.3 under "Simulating Quenching Phenomena," the enhanced heat transfer area resulting from the fragmentation of the debris can be simulated with an enhanced time-dependent heat transfer coefficient. This is implemented by means of the HT-COEF table option in the lower cell. The lower cell configuration used to simulate the steam spike consists of a 10-cm deep water pool, initially near saturation at 372 K, resting on a high temperature intermediate layer that is initially at 2500 K. The steam spike is initiated at 10 s and terminated at 15 s by the HT-COEF option. The atmosphere initially contains nitrogen with saturated water vapor at 372 K and 0.1 MPa total pressure. Heat transfer structures, simulating a wall and a roof, tend to cool the atmosphere through heat transfer and condensation.

Figure 6-6 shows the thermal response of the atmosphere and pool as well as the heat input rate resulting from the steam spike. Heat and mass balances between the pool and the atmosphere agree well with analytically derived values (which are not shown here). On the time scale shown, the structure heat transfer has relatively little effect upon the system temperatures. The annotated input is shown in Figure 6-7.

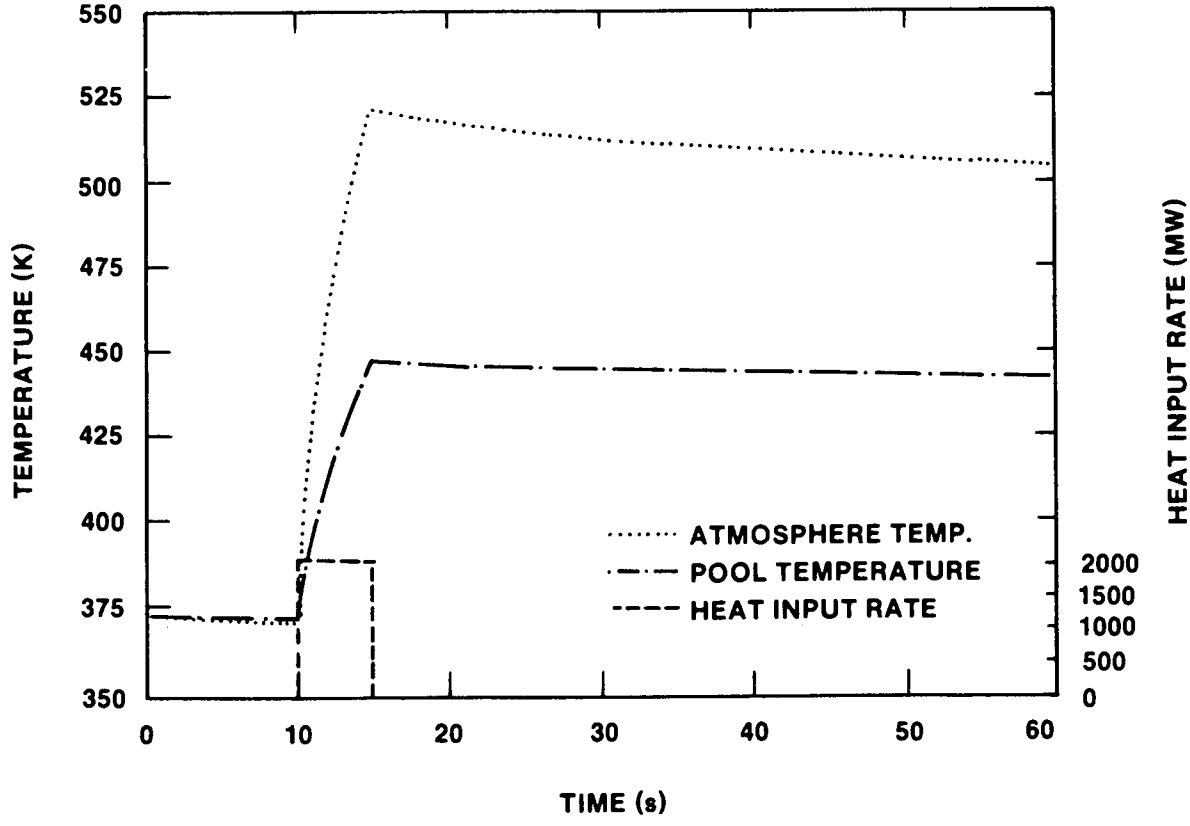

Figure 6-6. Containment Response to Steam Spike

```
CRAY                                          ← machine

CONTROL
  NCELLS=1 NTITLE=3 NTZONE=3                  ← global control block
EOI

MATERIAL
  COMPOUND N2 O2 H2O FE FEL CONC              ← material names

TIMES 50.0  0.0
  2.0  2.0 10.0                               ← time zones with default
  1.0  1.0 30.0                                 cell timestep fraction
  2.0  2.0 60.0

THERMO                                        ← thermodynamics and mass
                                                accounting
PRLOW-CL                                      ← lower cell print
                                                requested

TITLE
  LOW-CELL BOILING MODEL                      ← problem title
  STEAM SPIKE - POOL ON HOT SURFACE
  STRUCTURES ADDED, CONDENSATION ON

THERMAL                                       ← thermal reactor

CELL=1
CONTROL
  NHTM=2  MXSLAB=7
  JINT=1  JPOOL=1                             ← cell control block
  NUMTBC=1  MAXTBC=4
EOI

GEOMETRY  1000.0  10.0                        ← cell volume and height

ATMOS=2  1.E+5 372.0                          ← atmosphere initial
  H2OV=0.001  N2=1.                             conditions

HT-TRAN  ON OFF ON OFF OFF                    ← heat transfer flags set

CONDENSE                                      ← structure condensation
                                                enabled
```

Figure 6-7. Annotated Input for Steam Spike

```
STRUC

  NAME=WALL TYPE=WALL SHAPE=CYLINDER
  NSLAB=7 CHRLEN=15.0 IOUTER=2
  CYLHT=15.0 TUNIF=320.0 IOUTER=2
  COMPOUND=CONC CONC CONC CONC CONC
    CONC CONC
  X=5.64 5.65 5.67 5.70 5.80 5.90
    6.00 6.14
  EOI

  NAME=ROOF TYPE=ROOF SHAPE=SLAB
  NSLAB=7 CHRLEN=30.0 IOUTER=320.0
  SLAREA=30.0 TUNIF=320.0 TOUTER=320.0
  COMPOUND=CONC CONC CONC CONC CONC
    CONC CONC
  X=0.0  0.01 0.02 0.04 0.08 0.16
    0.32 0.50
  EOI                                   <- structure input block

LOW-CELL                                <- start of lower cell input

  GEOMETRY 100.0

  INTERM
    LAY-NAM=METAL
    TEMP=2500.0
    COMPOS 1 FEL=76170.0
    PHYSICS
      HT-COEF
      NAME=POOL
      FLAG=1                            <- intermediate layer with
      VAR-X=TIME                           time-dependent heat
      X=4  0.0 10.0 15.0 1.5E4             transfer coefficient to
      VAR-Y=COEF                           pool
      Y=4  0.0 1.E4  0.0  0.0
      EOI
    EOI
  EOI

  POOL
    TEMP=372.0
    COMPOS 1 H2O1=100000.0              <- pool layer with boiling
    PHYSICS BOIL EOI
  EOI

  BC  2500.0                            <- substrate temperature

EOI

EOF                                     <- end of input data
```

Figure 6-7. Annotated Input for Steam Spike (continued)

6.4 BWR Sample Problem

The last sample problem illustrates the use of two BWR-specific models, the suppression pool vent flow path model and the SRV discharge model. These models are discussed in Sections 2.2.3.4.1 and 2.3.4, respectively. The pressure in primary containment for this problem is shown in Figure 6-8, the suspended aerosol masses are shown in Figure 6-9, and input data set is shown in Figure 6-10.

The suppression pool vent modeling is specified through the SPVENT input block in Figure 6-10; the SRV modeling is specified through the SRVSOR input block. Another feature, the vacuum breaker between the drywell and wetwell, is modeled through the variable flow area (VAR-AREA) table in the FLOWS input block.

In order to simplify the input data set, the problem spans only a short period of time around the time of reactor pressure vessel failure. The primary containment, composed of the drywell and the wetwell of a BWR, is

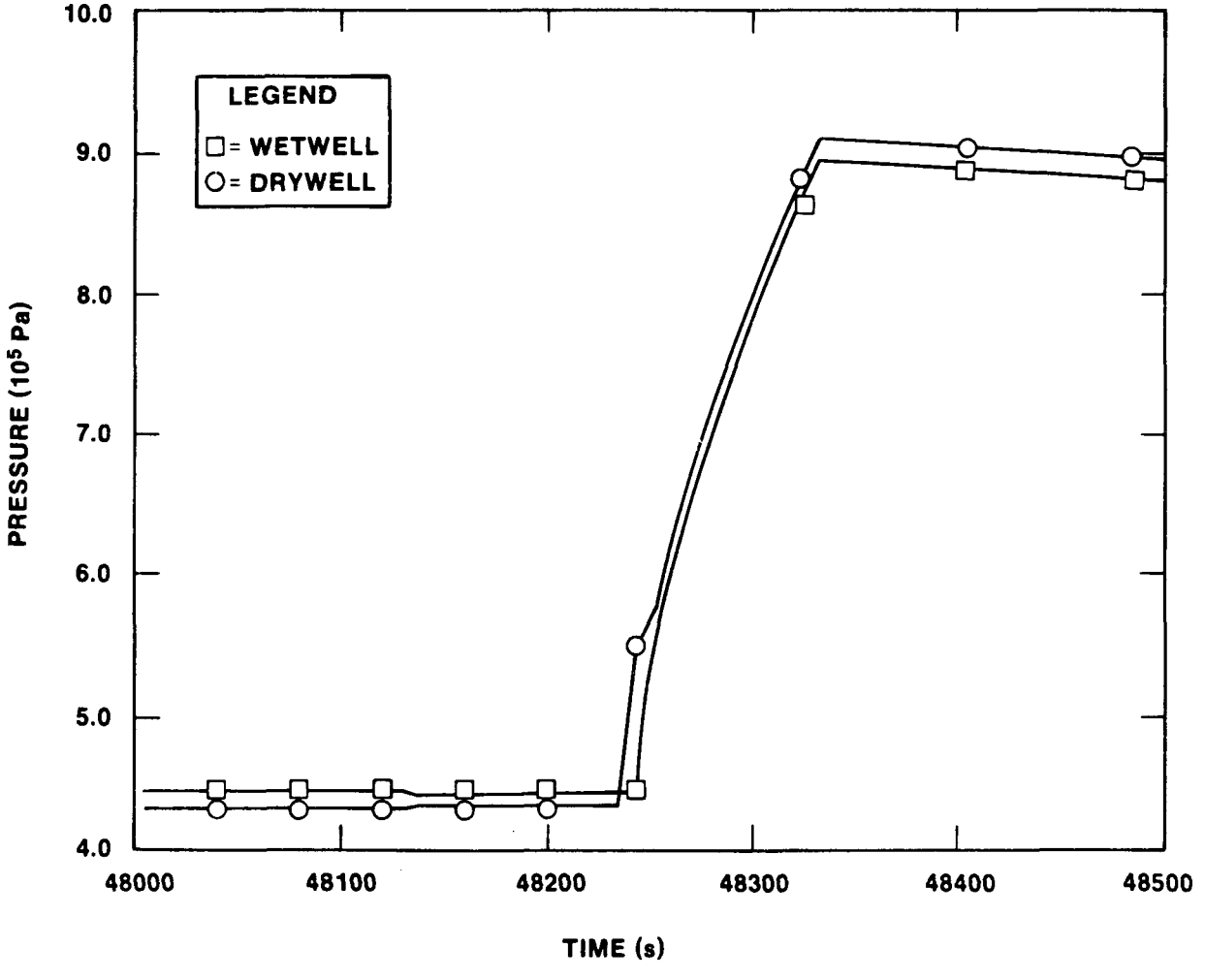

Figure 6-8. Drywell and Wetwell Pressures

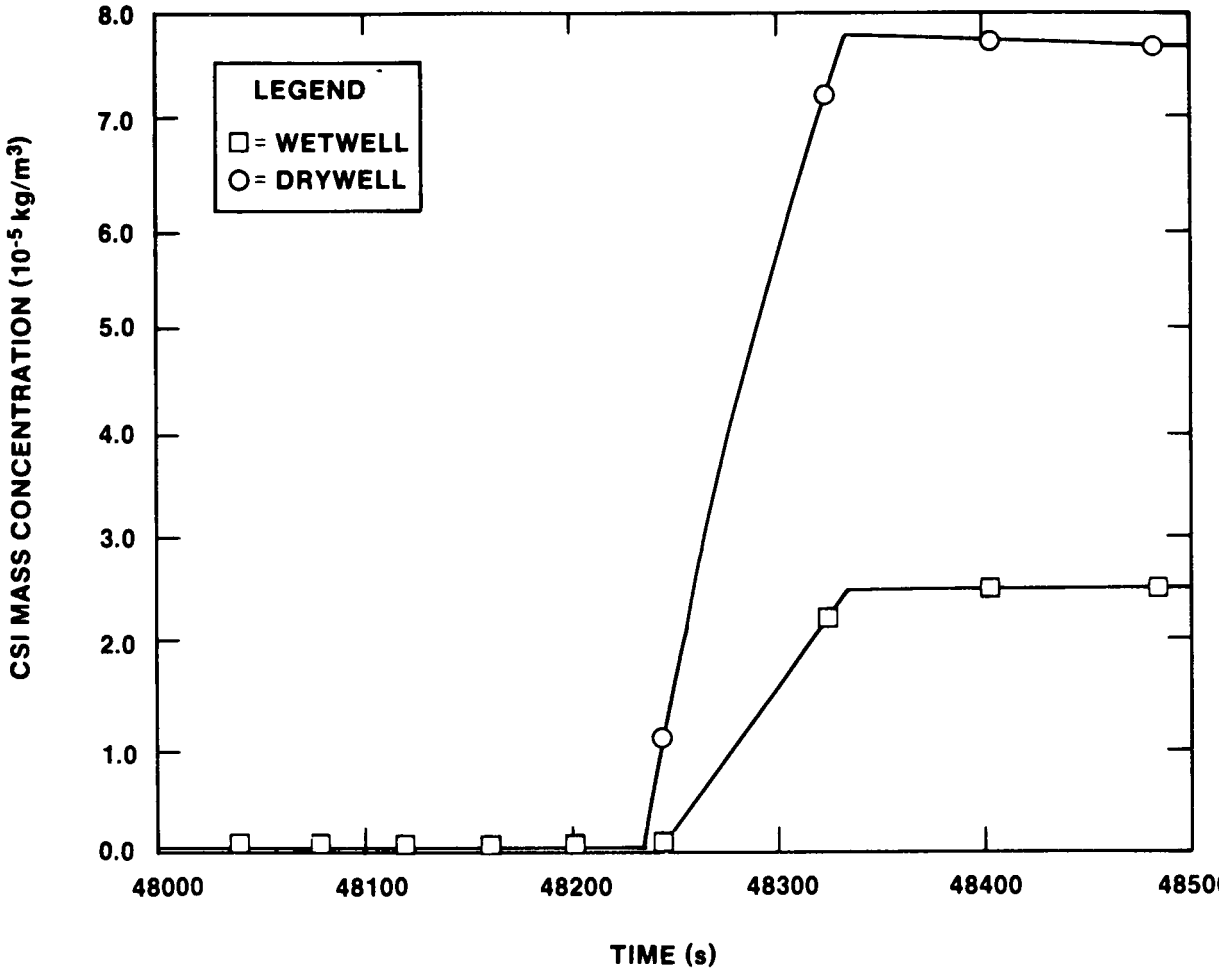

Figure 6-9. Drywell and Wetwell Aerosol Mass Concentrations

assumed not to be breached during this period. The two cells in the problem represent the drywell and wetwell. For simplicity, heat transfer structures are not modeled, although the initial conditions in the problem are taken from a calculation with structures present. To realistically extend the problem to later times, both heat transfer to structures and core-concrete interactions should be modeled.

Between the start of the problem and the time of vessel failure at 48234 seconds, the SRVs vent steam and hydrogen into the suppression pool in the wetwell (cell 1). The cell atmosphere gas compositions in the ATMOS input block reflect the fact that this venting process has been going on for some time. The ratio of steam to hydrogen in the SRV flow specified in the SRVSOR input block is large; therefore, the steam is almost completely condensed in the subcooled pool. The vacuum breakers between the wetwell and drywell normally would open and close to allow the gases and vapor leaving the top surface of the suppression pool to enter the drywell (cell 2). However, the flow at the top surface is extremely low at this point in time; therefore, as shown in Figure 6-8, the drywell and wetwell are not being pressurized. In fact, because of the convective

```
CRAY

CONTROL NCELLS=2 NTITL=1 NTZONE=3
  NAC=2 NSECTN=10 NUMTBG=1 MAXTBG=4      ← global control block
EOI

MATERIAL
  COMPOUND  H2 O2 CO CO2 H2OL H2OV       ← material input
  AERNAMES CSI

TITLE
  BWR PRIMARY CONTAINMENT PROBLEM        ← title

TIMES 36000. 48000.
      5. 5. 48234                        ← times input block
      10. 10. 48334.
      10. 10. 48500.

PRLOW-CL PRFLOW PRAER                    ← print flags on

THERMAL                                  ← reactor type

SPVENT   FDW=1. FWD=1. NWET=1 NDRY=2
  NSVNTS=8 ELEVNT=2.6 VNTLEN=4.5
  DPDRY=1.E4 DPWET=1.E4 AVNT=3.32        ← suppression pool vent
  SPARC EOI                                parameters
EOI

FLOWS  IMPLICIT
  AVL(1,2)=1.0 CFC(1,2)=0.5
  VAR-AREA(1,2) FLAG=2
  VAR-X-DELTA-P                          ← flows input block
  X=4 -1.E9 1.277E4 2.277E4 1.E9
  VAR-Y=AREA
  Y=4 0. 0. 6.4 0. EOI

AEROSOL
  CSI=  1.0E-6   0.7                     ← global aerosol input
  H2OI= 1.0E-8   0.405

CELL=1

CONTROL
  JPOOL=1 NSOSAT=2 NSPSAT=2              ← cell level control
  NSOSAE=1 NSPSAE=2
EOI
```

Figure 6-10. Annotated Input For the BWR Sample Problem

```
TITLE
  WETWELL CELL WITH WATER POOL ONLY

GEOMETRY 3041. 3.0

ATMOS=3 0.0 393.                                  ← atmosphere initial
N2=758. H2=406. H2OV=3278.                           conditions

SRVSOR                                          ┐
  ATMOS SOURCE=2                                │
  H2OV=2 IFLAG=2                                │
  T=    48000. 48234.                           │
  MASS= 40.0 0.                                 │
  ENTH= 2.95E6 2.95E6                           ├  ← srv atmosphere source
  EOI                                           │
  H2=2 IFLAG=1                                  │
  T=    48000. 48234.                           │
  MASS= .011 0.                                 │
  TEMP=600. 600.                                │
  EOI                                           ┤
  AEROSOL SOURCE=1                              │
  CSI=2 IFLAG=1                                 │
  T=    48000. 48234.                           ├  ← srv aerosol source
  MASS= 2.971E3 0.                              │
  EOI                                           │
EOI                                             ┘

LOW-CELL                                        ┐
  GEOMETRY  1020.                               │
  POOL TEMP=394. COMPOS=1 H2OL=3.98E6           ├
    PHYSICS BOIL EOI                            │  ← suppression pool
  EOI                                           │
  BC=300.0                                      │
EOI                                             ┘

HT-TRAN ON OFF ON ON ON                         ← turn off pool bottom
                                                   heat transfer

CELL=2

CONTROL
  NSOATM=2 NSPATM=2 NSOAER=1 NSPAER=2
EOI

TITLE
    DRYWELL CELL

GEOMETRY  4718  30.
```

Figure 6-10. Annotated Input For the BWR Sample Problem (continued)

```
ATMOS=3 0.0 383.
  N2=7590. H2=311. HTOV=3791.

  SOURCE=2                          )
  H2OV=2  IFLAG=1                   |
  T=48234. 48334.                   |
  MASS=140. 0.                      |
  ENTH=3.12E6 3.12E6 EOI            } ← vessel steam and hydrogen
  H2=2 IFLAG=1                      |   to drywell atmosphere
  T=48234. 48334.                   |
  MASS=.04 0.                       |
  TEMP=600. 600. EOI                )

AEROSOL SOURCE=1                    )
  CSI=2 IFLAG=1                     } ← vessel aerosol source to
  T=48234. 48334.                   |   drywell atmosphere
  MASS=.0053 0. EOI                 )

EOF
```

Figure 6-10. Annotated Input For the BWR Sample Problem (continued)

heat transfer between the wetwell atmosphere and the pool surface, the pressure is actually slightly decreasing.

In contrast to the inventories of gases, which reflect SRV venting prior to the start of the problem, the aerosol inventories reflect only the sources introduced after the start of the problem. The CsI aerosols specified in the SRVSOR input block are carried by the steam and hydrogen flowing through the SRV's. These aerosols are almost completely scrubbed out in the suppression pool because of the large amount of steam condensation. Consequently, the suspended mass concentrations of aerosols plotted in Figure 6-9 show almost no contribution from the SRV's.

At 48234 seconds, the drywell begins to be pressurized by steam and hydrogen from the pressure vessel, which is assumed to fail at this time. The blowdown from the pressure vessel is assumed to last for 100 seconds. The drywell pressure increases for one (ten-second) timestep, as shown in Figure 6-8, before the pressure rise is evident to the vent clearing model. After this delay of one timestep, vent clearing takes only a fraction of a second. After clearing, the pressurization rate of the drywell is decreased because of the flow of steam and noncondensable gases into the wetwell.

The aerosols introduced to the problem upon vessel failure are comparable in amount to those introduced through the SRV's. Because of the fact that the relative amount of steam to noncondensable gases in the suppression pool vent flow is much lower than in the SRV flow, the scrubbing of the vent flow is not nearly as efficient as that for the SRV flow. As shown in Figure 6-10 an appreciable amount of aerosols from the drywell enters the wetwell atmosphere. The average decontamination factor from the scrubbing of the vent flow is relatively small.

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APPENDIX B

MACHINE CONTROL AND FILE SPECIFICATION INPUT

1. CONTAIN File Usage

The files used by CONTAIN are listed in Table B-1. The internal file designators, default logical unit numbers, default file names, and file descriptions are also given in that table. Those files marked with an asterisk may be specified through the machine control input, as described in Section 2 of this Appendix. In Table B-1 and elsewhere in this Appendix, the prefix UNIT- appearing in a file name indicates that the file will take on the default name associated with a logical unit number. For example, the file UNIT-10 will be named FOR010.DAT on a VAX and TAPE10 on the CRAY CTSS system with Los Alamos libraries.

2. Machine Control and File Specification Input

The first line of any input dataset must be a machine name. Current options are CRAY and CDC.

Following the machine designation, the user may specify separate plot files for the plot data in any of six categories. By default, the plot data in any of these six categories will be written to the main plot file, PLTFIL. Note that if the separate plot file option is used, either

Table B-1 CONTAIN Data Files

File Designator	Default Logical Unit	Default Name	File Description
nplt	1	PLTFIL	Main plot file
nin	5	INPUT	Input file
nout	6	OUTPUT	Main output file (in printer carriage control format)
ndsk	10	UNIT-10	Restart file
nerr	17	UNIT-17	Error file (formatted)
natap	20	UNIT-20	Aerosol database file
nsumm	21	UNIT-21	Event summary file (formatted)
nusero*	22	UNIT-22	User output file (requires coding)
nccp	30	UNIT-30	CORCON cavity-shape plot file
n11*	1	PLTFIL	Cell atmosphere plot file
n12*	1	PLTFIL	Lower cell plot file
n13*	1	PLTFIL	Structure plot file
n14*	1	PLTFIL	Aerosol plot file
n15*	1	PLTFIL	Fission product plot file
n16*	1	PLTFIL	Engineered systems plot file

the name or the unit number should be specified for a separate plot file but not both. Also, data in different categories cannot be combined on one plot file unless it is the default file. For example, the atmospheric and aerosol plot data cannot be combined by specifying the same file for the variables "atmfil" and "aerfil" discussed below, unless PLTFIL is specified.

Certain file names and logical unit numbers are reserved for CONTAIN's use and may not be specified in the separate plot file option. The reserved file names are INPUT, OUTPUT, UNIT-10, UNIT-17, UNIT-20, UNIT-21, UNIT-30. Reserved logical unit numbers are 5, 6, 10, 17, 20, 21, and 30.

****

```
(CRAY or CDC)
  [[(PLTATM = atmfil or N11 = nn)]      && Atmosphere plot file
  [(PLTLCL = lclfil or N12 = nn)]       && Lower cell plot file
  [(PLTHTR = htrfil or N13 = nn)]       && Structure plot file
  [(PLTAER = aerfil or N14 = nn)]       && Aerosol plot file
  [(PLTFIS = fisfil or N15 = nn)]       && Fission product plot file
  [(PLTENG = engfil or N16 = nn)]       && Engineered systems plot file
  [NUSERO = nn]                         && User output file
  [(SCM or LCM or DISK)]                && Data storage options
EOI]
```

****

CRAY or CDC — machine type specification. IBM machines have also been used to run CONTAIN. However, installation-specific modifications may be required.

PLTATM = atmfil — file name for the atmosphere plot file. This file includes data such as cell atmosphere temperatures and pressures, the fractions and masses of all gases and vapors present, the mass of condensate on cell structures, atmospheric source table information, intercell flow path areas, and intercell flow rates. If "atmfil" is specified and is not the name PLTFIL, unit 11 will be reserved for writes to that file. If neither a name "atmfil" different from PLTFIL or a unit "n11" different from 1 is specified, then PLTFIL and unit 1 will be used.

N11 = n11 — unit number for the atmosphere plot file. Specify either "atmfil" for this file or a unit number but not both. If "n11" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "atmfil" or "n11" is specified then PLTFIL and unit 1 will be used for the atmospheric data.

PLTLCL = lclfil — file name for lower cell plot file. This file includes data such as layer names, layer or node interface positions and thicknesses, layer temperatures, sources to the lower cell layers, and heat transfer coefficients. If "lclfil"

is specified and is not the name PLTFIL, unit 12 will be reserved for writes to that file. If neither a name "lclfil" different from PLTFIL or a unit "nl2" different from 1 is specified, then PLTFIL and unit 1 will be used.

N12 = nl2 — unit number for the lower cell plot file. Specify either a filename for this file or a unit number but not both. If "nl2" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "lclfil" or "nl2" is specified then PLTFIL and unit 1 will be used.

PLTHTR = htrfil — file name for the structure plot file. This file includes information such as the material names specified for each node in each structure, the node interface positions and interface areas, and the node temperatures. If "htrfil" is specified and is not the name PLTFIL, unit 13 will be reserved for writes to that file. If neither a name "htrfil" different from PLTFIL or a unit "nl3" different from 1 is specified, then PLTFIL and unit 1 will be used.

N13 = nl3 — unit number for the structure plot file. Specify either a filename for this file or a unit number but not both. If "nl3" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "htrfil" or "nl3" is specified then PLTFIL and unit 1 will be used.

PLTAER = aerfil — file name for the aerosol plot file. This file includes such information as the aerosol masses by size and component, mass deposition by component, and aerosol source information. If "aerfil" is specified and is not the name PLTFIL, unit 14 will be reserved for writes to that file. If neither a name "aerfil" different from PLTFIL or a unit "nl4" different from 1 is specified, then PLTFIL and unit 1 will be used.

N14 = nl4 — unit number for the aerosol plot file. Specify either a file name for this file or a unit number but not both. If "nl4" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "aerfil" or "nl4" is specified then PLTFIL and unit 1 will be used.

PLTFIS = fisfil — file name for the fission product plot file. This file includes fission product masses and decay powers for various hosts. If "fisfil" is specified and is not the name PLTFIL, unit 15 will be reserved for writes to that file. If neither a name "fisfil" different from PLTFIL or a unit "nl5" different from 1 is specified, then PLTFIL and unit 1 will be used.

N15 = nl5 — unit number for the fission product plot file. Specify either a file name for this file or a unit number but not both. If "nl5" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "fisfil" or "nl5" is specified then PLTFIL and unit 1 will be used.

PLTENG = engfil — file name for the engineered systems plot file. This file includes information about the performance of engineered safety features as well as about the redistribution of coolant among lower cell pools. If "engfil" is specified and is not the name PLTFIL, unit 16 will be reserved for writes to that file. If neither a name "engfil" different from PLTFIL or a unit "n16" different from 1 is specified, then PLTFIL and unit 1 will be used.

N16 = n16 — unit number for the engineered systems plot file. Specify either a file name for this file or a unit number but not both. If "n16" is equal to 1, then the name associated with that unit will be PLTFIL. If neither "engfil" or "n16" is specified then PLTFIL and unit 1 will be used.

NUSERO = n22 — unit number to be used for user-implemented output as described in Section 3.2.7.2. In addition to coding the appropriate statements in the USERO subroutine, the user should also open and close UNIT-"n22" in the main program. Default = 22.

SCM, LCM, or DISK — keywords to designate the storage option appropriate for the user's computer system. If SCM is specified, all data is retained in central memory. LCM and DISK refer to large-core memory and a disk file, respectively. These options may be useful when the computer has too little central memory for a given problem. Because the LCM and DISK options are specific to the computer type and installation, code modifications are required for use of these options. SCM is the default and is always used for single cell problems.

EOI — terminating keyword. If any of the above keywords other than the computer type are given, the input block should be terminated with an EOI.

APPENDIX C

THE REDUCE OPTION

This appendix discusses the REDUCE option, which may be useful if the user encounters stiffness in the quasi-steady (QUASI) flow option but requires that option to assess integration errors. This appendix also discusses formulas which can be used to assess the degree of stiffness present and the improvement in efficiency expected from the REDUCE option. Note that for most applications, the use of the implicit method discussed in Section 2.2.3 will be more efficient than REDUCE.

1. Removing Stiffness with the REDUCE Option

Under some conditions, stiffness may prevent the Runge-Kutta integrator in the quasi-steady flow option from integrating the flow equations properly once the flow rates have dropped below a certain point. This occurs because the flow rates must be high enough to cause changes in the solution vector per timestep that are larger than the error tolerance asked of the Runge-Kutta solver. With stiffness, the Runge-Kutta timestep (by definition) is much smaller than necessary to resolve the time variations of interest, and therefore the change per timestep can drop below the error tolerance. After this point, the solution becomes noisy because any change is accepted as an accurate integration of the flow equations. (In the quasi-steady flow option, the errors in the flow rates are not controlled by the error tolerances specified for the integration of the flow ordinary differential equations with respect to time. Such error tolerances apply only to dynamic variables, such as cell masses, whose time derivatives constitute the set of ordinary differential equations. In the quasi-steady flow option, the flow rates are state functions, not dynamic variables.) The REDUCE option removes stiffness from the problem in a manner that may result in less noise and more accurate flow rates. One drawback is that one can no longer track pressure differences between cells once these differences are on the order of "dpref," which is a characteristic pressure difference discussed in Section 2.2.3.2.2.

When stiffness makes the quasi-steady flow calculations very slow, the user has the option of specifying REDUCE = "nred", which will instruct the code to reduce flow areas artificially by a factor of up to $2^{\text{"nred"}}$ when pressure differences are less than "dpref". These restrictions are made in a way that attempts to preserve the flow distributions, or flow splits, in the possible parallel paths. The restrictions, if they are substantial, tend to drive the pressure differences between cells up to a value on the order of several times "dpref", where the effect of the linear flow resistance term is small. Therefore, the flow distribution in parallel paths with REDUCE turned on may be less sensitive to "dpref" than with REDUCE turned off.

In the REDUCE option, the network of cells and flow paths is examined to determine the connectivity in terms of serial and parallel paths. Figure C-1 shows such a network. A path is indicated by a pair of numbers (i,j). In Figure C-1, (1,2) and (4,5) are serial paths. In addition,

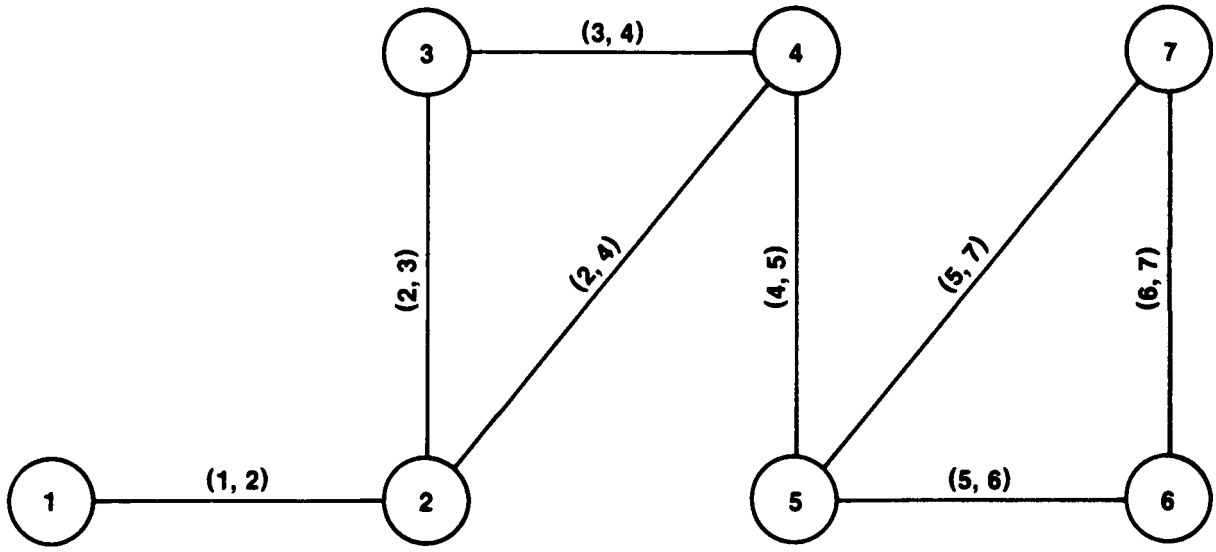

Figure C-1. Network of Cells Connected By Series and Parallel Paths

two sets of parallel-connected paths are available: (2,3), (2,4), (3,4) and (5,6), (5,7), (6,7).

The flow areas of serial flow paths are adjusted independently. However, the flow areas of a parallel-connected set are all adjusted by the same factor. The adjustment is made at each Runge-Kutta timestep. The criteria for adjustment are based on an absolute value of pressure difference $|\Delta P|$, which for a serial path is just the absolute value of the pressure difference across the path and for a parallel-connected set is the maximum pressure difference across any of the paths in the set. The prescription at each timestep is

- If $|\Delta P| <$ "dpref", decrease flow area by a factor of 2
- If "dpref" $< |\Delta P| <$ 3"dpref", keep the areas the same
- If 3"dpref" $< |\Delta P|$, increase flow area by a factor of 2

The areas are reduced at most by a factor of $2^{\text{"nred"}}$ where "nred" is specified as the value supplied immediately following the REDUCE keyword (REDUCE = "nred"). The default value for "nred" is zero. The areas are not increased beyond their normal size.

The user should set "nred" so that the delay time for dilation of the areas up to normal size is acceptable. This delay time is "nred" Runge-Kutta timesteps. The next section provides some quantitative tools for estimating the Runge-Kutta timesteps and for choosing a conservative value for "nred". In practice, however, the best way to determine the acceptability of REDUCE for any particular choice of "nred" for a given problem is to test the quantities of interest for sensitivity to changes in "nred".

2. Formulas for Analyzing Stiffness

The analyst interested in studying the numerical stability and stiffness aspects of the flow equations should be concerned with the time constants associated with intercell flow. The Runge-Kutta timestep controlling the intercell flow of gases is automatically chosen to satisfy internally set relative and absolute error tolerances. Because the Runge-Kutta method is explicit, the maximum timestep that can be taken is a small multiple of the smallest intrinsic time constant in the problem. This is the case even if the behavior associated with this time constant does not manifest itself in the solution being calculated. For example, the small time constant behavior may have died out, and the solution may be extremely close to the steady state solution. However, in an explicit method one cannot take timesteps much larger than the smallest intrinsic time constant. Otherwise, the solution will be unstable. The smallest time constant therefore limits the timestep. This limitation on the timestep during periods when behavior on the time scale of the smallest time constant does not manifest itself is defined as stiffness. In this section, expressions are given so that the user may evaluate the limiting time constant and assess the relative efficiency of both the inertial and quasi-steady flow calculations. Note that the limiting time constant discussed here pertains to the Runge-Kutta method. The implicit method also has limiting time constants from stability, but these are related to convection velocities and are typically much larger.

2.1 Limiting Time Constant in Inertial-Flow Option. Two time constants are of interest in this option. The first is the response time t_r for the flow rate. The response time is applicable to the regime where pressure differences between the upstream and downstream cells are reasonably large. It is defined as the recovery time or rise time for the flow after a sudden perturbation. The second is the oscillation period t_o for the gas in the flow channel. The oscillation time constant comes into play near the point of pressure equilibration. The time constant that will limit the Runge-Kutta timestep for a given flow path depends on the pressure difference for that path. In practice, both time constants should be evaluated, and the smaller should be assumed to be the one that limits the Runge-Kutta timestep. Except for flows occurring at large pressure differences or along extremely short flow path lengths, the oscillation period is generally a more severe constraint on the Runge-Kutta timestep.

The response time is conveniently discussed in terms of two cells, i and j, each sufficiently large so that the pressure difference remains fairly constant while the flow is accelerating after the flow path opens. The flow velocity will rise from zero to a steady state value

$$v_{ss} = \left[\frac{\Delta P_{ij}\rho_{ij}}{\rho_u^2 C_{FC}}\right]^{1/2} \tag{C-1}$$

where ρ_u is the upstream cell gas density. The notation for other quantities is given under Equation (2-3). The response time for turbulent flow is

$$t_r = \frac{L_{ij}\ \rho_{ij}}{4C_{FC}\ v_{ss}\rho_u} \tag{C-2}$$

The oscillation period is discussed for the situation in which one of the cells (say, i) is much smaller than the other. Its pressure (P_i) consequently controls the oscillation period.

When little or no pressure difference exists between the two cells, the inertia of the flow can result in low amplitude oscillations with a half period approximated by

$$t_o = \pi[V/(A_{ij}L_{ij})]^{1/2}t_s \tag{C-3}$$

where V is the smaller of the two cell volumes, and t_s is essentially the time required for sound to travel the length of the flow path:

$$t_s = \frac{L_{ij}}{B^{1/2}} \tag{C-4}$$

For the purpose of making simple estimates, B is the square of the speed of sound. For more precise calculations, the exact expression for B is

$$B = \left[\frac{\partial P}{\partial \rho}\right]_T - \frac{(\partial u/\partial \rho)_T(\partial P/\partial T)_\rho}{C_v} + \frac{(H - u)(\partial P/\partial T)_\rho}{\rho C_v} \tag{C-5}$$

where u is the specific internal energy, C_v is the specific heat, P is the pressure, ρ is the density, and T is the temperature. In general, these quantities are defined with respect to cell i. H, however, is the mean specific enthalpy associated with the flow, i.e.,

$$H = H_{ij} \tag{C-6}$$

where H_{ij} is equal to the specific enthalpy of the upstream cell for the flow between cells i and j.

In general, the derivatives with respect to density in Equation (C-5) should be interpreted as the derivatives corresponding to adding material to the cell according to the flow rates present. If material is flowing into the cell and has a different composition from that of the material in the cell, then such derivatives do not have their usual thermodynamic interpretation. If the flows are entirely into i, then $(dP/d\rho)_T$ should be evaluated as the isothermal change in pressure in cell i per unit mass caused by adding material of the composition coming into the cell. If the flow is entirely out of the cell, then $(dP/d\rho)_T$ has its usual meaning. Also, B becomes somewhat simpler because H becomes the specific enthalpy of cell i, and $H - u = P/\rho$. In this case, the expression for B reduces to the square of the speed of sound in cell i: $B = v_s^2$.

2.2 Limiting Time Constant for Quasi-Steady Flow. The quasi-steady flow model is defined by the relationship in Equation (2-9). The transport equations in the quasi-steady flow model are inertialess and behave in a parabolic fashion, much like the heat conduction equation. One can infer some of the features of the solution by analogy. In particular, no propagating solutions with a finite wave speed exist; there is only diffusive behavior.

Because no propagating solutions exist, the timestep is not limited by the transit time for a sound wave to cross a flow path, as it is in the inertial flow calculation. Rather, the timestep is limited by the pressure relaxation time t_p for a cell, which is analogous to the temperature relaxation time for a node in the finite differenced heat conduction equation.

Generally, the shortest pressure relaxation time occurs in a cell with relatively small volume and relatively large flow areas connecting it with the other cells. Therefore, attention is focused on the cell with the largest flow area to cell volume ratio, and the rest of the cells are treated as having constant pressures. Furthermore, it is assumed that the pressure differences across all flow paths out of the cell in question are either all greater than "dpref" or all less than "dpref", i.e., that the flow laws are the same for all of these paths.

In the following expression for t_p, the cell which is limiting the timestep is i, and the cells connected to it are labeled j. The expression is

$$t_p = \begin{cases} V(C_{LFC})_C/B & \text{for all } \Delta P_{ij} \ll \text{"dpr"} \\ 2V((\Delta PC_{FC}/\rho A^2)_C)^{1/2}/B & \text{for all } \Delta P_{ij} \gg \text{"dpr"} \end{cases} \qquad \text{(C-7)}$$

where V is the volume of cell i, C_{LFC} is defined in Equation (2-9), and the quantities with subscript C are composite quantities defined in terms of sums over flow paths. The quantity B is usually well approximated by the square of the speed of sound, but a more exact formula is given by Equation (C-5), with H defined as the mean specific enthalpy of the flow:

$$H = \sum_j H_{ij} W_{ij} / \sum_j W_{ij} \qquad \text{(C-8)}$$

The other expressions appearing in Equation (C-7) are given by

$$1/(C_{LFC})_C = \sum_j 1/C_{LFC}(i,j) \qquad \text{(C-9)}$$

$$1/\left|(\Delta PC_{FC}/\rho A^2)_C\right|^{1/2} = \sum_j A_{ij}(\rho_{ij})^{1/2}/\left|\Delta P_{ij} C_{FC}(i,j)\right|^{1/2} \qquad \text{(C-10)}$$

Here $C_{LFC}(i,j)$, $C_{FC}(i,j)$, A_{ij}, and ρ_{ij} are the linear flow coefficient, the turbulent flow coefficient, the normal flow area, and the average of the densities of cells i and j, respectively.

These expressions are quite complicated, but in many cases only an estimate of the relaxation time is needed, and it is possible to disregard Equations (C-9) and (C-10) and use Equation (C-7) with a much simpler prescription: A representative value of C_{LFC} or C_{FC} should be used, the sum of all flow path areas should be used for A, and B should be set equal to the square of the speed of sound.

These formulas can be used to analyze the optimum choice of the "nred" parameter when the REDUCE option is used. The timestep is limited by the shortest cell pressure relaxation time in the problem, as given by Equation (C-7). The cell to which this belongs is typically the cell with the largest ratio of total flow area to volume. Because the areas are variable in the REDUCE option, it is not possible to calculate the actual dilation time a priori. However, one can obtain a conservative dilation time in the following manner: The smallest cell pressure relaxation time expected in the problem for normal-size flow areas should be calculated from Equation (C-7). The ΔP in the equation should be set to 3"dpref", because (according to the prescription given above) that is when dilation starts. This time should then be scaled by "nred"*2**"nred" to estimate the dilation time, which can then be compared with time scales of physical interest. Note that this time assumes the Runge-Kutta timestep is being limited by a cell with fully constricted flow paths. That cell is taken to be the cell that would limit the timestep for normal-sized flow paths. In practice, the constriction may not be the maximum, or the timestep may be limited by a different cell with flow areas constricted to a lesser degree. In that case, the actual dilation time can only be shorter than the time estimated above.

APPENDIX D

ALTERNATIVE INPUT FORMATS AND UPWARD COMPATIBILITY

As the CONTAIN code has evolved through several versions, an attempt has been made to keep the structure of the input the same. In some cases, however, input changes were made. Generally, the old input format has been maintained, so that old input files are still upward compatible. This section describes all such alternative formats for input. Readers of Reference Sci84, "Testing of the CONTAIN Code," will notice that the input files listed in that document use a number of these alternative formats.

A number of the alternate input formats allow the user to specify a series of numerical values for the control parameters following the keyword CONTROL. The code assigns values to the control parameters according to the sequence indicated.

1. Global Control Alternative Input Format

CONTROL number (ncells ntitl ntzone nfce nchain nsectn nac nhm numtbg maxtbg)

number	the number of global control values to follow
ncells	number of cells (maximum of 20)
ntitl	number of title lines (maximum of 80 characters/line)
ntzone	number of time zones
nfce	number of fission product chain elements
nchain	number of fission product chains
nsectn	number of aerosol particle size classes (20 recommended)
nac	number of aerosol components
nhm	number of additional fission product host materials (besides the atmosphere gas, all aerosols, floors, walls, and roofs)
numtbg	number of times a global table is used
maxtbg	maximum number of entries used in any global table option

If any value is to be specified, all values preceding it must also be specified. For example, if "nac" is the last value to be specified, then "number" = 7 and seven values are specified, corresponding to the first seven variables in the control block; the default value of 0 will be automatically used for "nhm", "numtbg", and "maxtbg". The default value is 0 for all of the above control parameters.

2. Cell Control Alternative Input Format

CONTROL number (nz nreg nhtm mxslab nsopl nsppl nsoatm nspatm nsospr nspspr nsoaer nspaer nsofp nspfp nstrlw naensy nsensy nchmre nsoeng nspeng jconc jint jpool numtbc maxtbc nraycc nvfpsm)

number	number of cell control values to follow
nz	indexing variable; use value of 1
nreg	indexing variable; use value of 1
nhtm	number of heat transfer structures in the cell

mxslab	maximum number of nodes in any heat transfer structure
nsopl	number of lower cell source tables
nsppl	maximum number of entries in lower cell source tables
nsoatm	number of external atmosphere sources
nspatm	maximum number of entries in atmosphere source tables
nsospr	number of external spray fire sources
nspspr	maximum number of entries in spray fire source tables
nsoaer	number of external aerosol sources
nspaer	maximum number of entries in aerosol source tables
nsofp	number of external fission product sources
nspfp	maximum number of entries in fission product source tables
nstrlw	indexing variable; use value of 0
naensy	number of engineering systems to be defined in atmosphere
nsensy	indexing variable; use value of 0
nchmre	indexing variable, use value of 0
nsoeng	number of engineered system sources
nspeng	maximum number of entries in engineered system source tables
jconc	designator indicating presence of concrete layer in lower cell; the possible values and their meanings are described in Section 3.3
jint	number of intermediate layers in lower cell
jpool	designator indicating presence of pool layer in lower cell; 1 if pool layer present, 0 if not present
numtbc	number of times a cell level table option is used for this cell
maxtbc	maximum number of entries used in any table option within this cell
nraycc	number of rays used to model the CORCON cavity; allows use of the CORCON option in this cell
nvfpsm	number of individually tracked VANESA fission products

If any value is to be specified, all variables preceding it in the above list must also be given. For example, if "nspspr" is the last value to be specified, then "number" = 10 and ten values are specified, corresponding to the first 10 variables in the control block. The default value of 0 will be automatically set for the remaining variables "nsoaer", "nspaer", "nsofp", "nspfp", "nstrlw", "naensy", "nsensy", "nchmre", "nsoeng", "nspeng", "jconc", "jint", "jpool", "numtbc", "maxtbc", "nraycc", and "nvfpsm."

3. Global Aerosol Alternative Input Format

AEROSOL [newcof diam1 diam2 tgas1 tgas2 pgas1 pgas2] [keyword=value]
(mapaer amean avar)

newcof	flag for calculating aerosol coefficient sets (default=1)
diam1	lower diameter limit (m) (default = 1.0E-7 m)
diam2	upper diameter limit (m) (default = 1.0E-4 m)
tgas1	lower temperature limit (K) (default = 273 K)
tgas2	upper temperature limit (K) (default = 673 K)
pgas1	lower pressure limit (Pa) (default = 5.0E4 Pa)
pgas2	upper pressure limit (Pa) (default = 8.0E5 Pa)

The parameter string "newcof diam1 diam2 tgas1 tgas2 pgas1 pgas2" is optional, but if used should be placed before any of the keyword entries.

If a keyword entry redefines any of the parameters in the parameter string, the redefined value will be used. A zero value for a parameter in the string implies the default value for that parameter. The allowable keywords are those identified in Section 3.2.4.

4. Fission Product Names Alternative Input Format

The keyword FISSION can be used in place of the keyword FP-NAMES in the global MATERIAL block. All else remains as described in Section 3.2.1. Thus, the input specifying fission product names would appear as follows using this alternate keyword:

FISSION (names)

names fission product names to be used in the problem

5. Fission Product Alternative Input Formats

Several alternate input options and formats are available for specifying fission product input parameters in the global FISSION input block. First, the decay chain structure and decay power coefficients may be specified with the alternate format shown below at the beginning of the FISSION block. Second, the FPM-CELL blocks may be specified at the global level as shown below. This is true regardless of the format used to specify other fission product input parameters in the FISSION block. If these blocks are placed at the global level then the FPM-CELL keyword must be followed by the cell number for which the following parameters are to apply. Also, global FPM-CELL keyword blocks do not end with an EOI; rather, they end with the next FPM-CELL keyword or the EOI for the entire FISSION block. Third, in place of (or in addition to) the TARGET keyword, RELEASE and ACCEPT may be used as shown below to activate the nontargeted release and acceptance model. It should be noted that this model is entirely different from and less flexible than the TARGET model. Also note that when ACCEPT is given, 1+"nac"+3+"nhc" values for each host are expected to follow even though this number in general will not be the proper number of hosts for the cell in CONTAIN 1.1 (in older versions of CONTAIN, this is the number of hosts in a given cell). The code will automatically reassign the acceptance fractions to the actual CONTAIN hosts in the cell. Fourth, in place of actual structure names, the "hname" following the HOST keyword may be ROOF, WALL, or FLOOR. In this instance, mass will be distributed among structure surfaces of the appropriate type according to surface area. If no surfaces of the specified type exist in the cell, then the mass will be diverted to a waste holding location. Fifth, extra material hosts ("ehnames") are accepted as input; however, any reference to such hosts will be assumed to apply to the DUMMY host, unless the extra material host name matches that of the coolant (H2OL or NAL). Any reference to coolant extra hosts are assumed to apply to the pool as opposed to the DUMMY host, if a pool is defined. If extra material hosts are specified, then the keyword NHM must also be specified in the global CONTROL block as follows:

NHM = nhm total number of extra material hosts in all cells. Even though extra materials are no longer hosts in CONTAIN, this parameter must be entered accurately if the old FISSION

format is used and extra material hosts are defined in the FISSION block

The alternate FISSION block input format is given below. The format shown below assumes that the FPM-CELL blocks are at the global level.

```
FISSION
  (nhc (ehnames)) (nfpchn) (fpnames) (hl)
  [ [FGPPWR=ndpcon] (fpq) ]

  FPM-CELL=1
    (HOST = hname (masses) [RELEASE (fpname = rate) EOI])
    [ACCEPT (fpname (fractions)) EOI]

  FPM-CELL=2
    (HOST = hname (masses) [RELEASE (fpname = rate) EOI])
    [ACCEPT (fpname (fractions)) EOI]
    .
    .
    .

  FPM-CELL=ncell
    .
    .
    .
EOI
```

nhc — number of obsolete extra material fission product hosts in each cell. Specify "ncells" values, one for each cell. The sum of "nhc" over all cells must equal "nhm" in the global CONTROL block even though the code no longer uses extra material hosts.

ehnames — names of the extra material hosts. Specify "nhc" names for each value of "nhc" that is nonzero. If "nhc" is zero for a cell, then no names should be entered for that cell. These extra host names must come from the names of the materials listed in the COMPOUND block in order for CONTAIN to properly reassign the extra host references to the DUMMY host.

nfpchn — number of fission products in each chain ("nchain" values must be specified). The sum of "nfpchn" over all chains must be equal to "nfce" in the global CONTROL block. Unlike hosts, fission product chains are common to all cells.

fpnames — names of fission products in the order of appearance in the decay chains. Specify "nfce" values for all chains.

hl — half-lives corresponding to each of the fission products named above.

FGPPWR — initializes input of "ndpcon". If this keyword is not given, then "ndpcon" will have the value of 1.

ndpcon — number of decay power coefficients per nuclide. All nuclides must have the same value of "ndpcon" when using this old input format.

fpq — the power coefficients. Specify "ndpcon" values for each fission chain element. The definition of the coefficients is given in Section 3.2.5. (W/kg or s^{-1})

HOST — initializes input for specification of initial fission product mass. Note that this keyword must be given if the nontargeted release model is to be used, even if no initial mass specification is desired (zeros should be given in such a case for the masses).

hname — is either a single word or several words that identify a CONTAIN host in the specified cell. The valid host names are described in Section 3.3.1.10. In addition to those names, the generic structure names, ROOF, WALL, and FLOOR may also be given to automatically distribute mass among structure surfaces of the specified type.

masses — is exactly "nfce" initial fission product masses for the host specified. (kg)

RELEASE — initiates specification of nontargeted release rates for fission products hosted to the previously specified "hname" host.

fpname — one of the names given in the FP-NAMES block. All fission chain elements having this name will release at the specified rate from the "hname" host in the cell.

rate — is a constant release rate for the "fpname" fission product chain elements. Note that in the nontargeted release model this release rate need not necessarily equal the sum of the acceptance rates of the various hosts. (See the ACCEPT input below.) (s^{-1})

ACCEPT — initializes input for the host acceptance fractions in the cell. If this keyword is omitted, the acceptance fraction for all hosts will be zero except for that for the GAS, which will be unity.

fpname — one of the names given in the FP-NAMES block. All fission chain elements having this name will be accepted by the various hosts in the cell according the fractions described below.

fractions — exactly 1 + "nac" + 3 + "nhc" values representing the fraction of the released fission product accepted by each host. Note that in the nontargeted release model, mass will not be conserved if these fractions do not sum to unity

NOTE: If the first quantity following the FISSION keyword is a numerical value (i.e., the first "nhc" value), then the old input format described above will be assumed. Otherwise, the keyword formats described in Sections 3.2.5 and 3.3.1.10 will be assumed. Mixing of the two formats is not allowed with the exception that the FPM-CELL blocks may be placed at either the global or cell level regardless of the format used for the rest of the FISSION block.

6. Alternate Structure Input Format

An alternative format for specifying structures under the STRUC keyword discussed in Section 3.3.1.3 is as follows:

(name istr ishape nslab ibc tint chrl vufac [bctr] [heit] (x) (names))

The following group of variables is repeated for each structure:

name	arbitrary name with eight or fewer characters for the structure.
istr	structure type (ROOF, WALL, or FLOOR).
ishape	structure shape (SLAB, CYLINDER, or SPHERE).
nslab	number of nodes in structure.
ibc	number of the cell adjacent to outer face of structure.
tint	initial temperature of structure. (K)
chrl	characteristic length of structure for condensation model. (m)
vufac	a value which depends on the emissivities of the structure surfaces and the uppermost lower cell layer, and on their geometric relationships. (Must be ≤1; see Eq. 2-60.)
bctr	outer face boundary temperature. (K)
heit	if the structure is a SLAB, "heit" is the surface area (m^2); if the structure is a CYLINDER, "heit" is the height (m); if the structure is a SPHERE, "heit" is ignored and must be omitted.
x	node interface positions relative to the inner face of a SLAB or to the center of curvature of a CYLINDER or a SPHERE. (Specify "nslab" + 1 values, starting at inner face.) (m)
names	material name for each node (specify "nslab" names).

This block provides the characteristics of the structures modeled in the cell. Three structural shapes are allowed: slabs, cylinders, and spheres. Cylinders and spheres are actually half-cylinders and

hemispheres whose inner surfaces act as roofs, walls, or floors for aerosol deposition. Thus, to model a whole cylinder or a complete sphere, two structures are required. When "ibc" is a valid cell number (1 ≤ "ibc" ≤ "ncells"), "bctr" must not be present. When "ibc" is not a valid cell number, "bctr" is used as the temperature seen by the outer boundary; if "bctr" is zero, an adiabatic (insulated) outer boundary is assumed. An invalid cell number is one that is greater than the maximum number of cells specified for the problem, i.e., it corresponds to a "fictitious" cell. Radiative heat transfer from the lower cell to the outer face is not currently modeled, regardless of the location of the face. Neither condensation nor aerosol deposition is included on the outer face if the face is in another cell.

The alternate input format may be used in conjunction with the format presented in Section 3.3.1.3. However, the format in Section 3.3.1.3 must always follow the alternative format above.

7. Radiation Alternative Input Format

The RADIAT keyword and the associated alternative radiation input format may be used in place of the keyword RAD-HEAT to activate the radiation model. This alternate input format is capable of activating only the simple gas-structure radiation model. In order to use the net enclosure model, the RAD-HEAT input block must be used.

```
RADIAT
  BEAML (beaml)
  EMSVT (emsvt)
  [PBEAML pbml  PEMSVT pevt]
  [MODAK]
EOI
```

The BEAML and EMSVT keywords are always followed by only "nhtm" values (one for each structure in the cell). The beam length and emissivity of the topmost lower cell layer (usually the pool) are input via the keywords PBEAML and PEMSVT. The beam lengths in this input block are the same as the geometric beam lengths given under the GEOBL keyword in the RAD-HEAT block and should not be confused with the net enclosure inter-surface beam lengths. Also note that when using the RADIAT input, the Cess-Lian correlation is used by default for the gas mixture emittance calculations. The MODAK keyword is used to override this default. Use of the RADIAT input format is discouraged as new options are not accessible within this format.

APPENDIX E

PLOT FILE OUTPUT

CONTAIN places control parameters, calculated results, and other information onto the file(s) associated with unit numbers "nl1", "nl2", "nl3", "nl4", "nl5", and "nl6". The default is 1 for all six unit numbers; however, they may be specified by the user as described in Appendix B. The manner in which the various data are divided among the six units is also discussed in Appendix B. The files associated with these units are often referred to as "plot files" for the reasons described below. Information is written to the unit(s) at an edit frequency defined by the "edtdto" and "edmult" parameters in the TIMES block (see Section 3.2.6). Note that this frequency is not affected by either the LONGEDT or SHORTEDT option.

The primary purpose of writing data to the plot files is to provide an efficient interface between calculated results and separate postprocessing and plotting programs. Such a program is the POSTCON postprocesser and unit conversion program for CONTAIN.[Was87] The table generating and plotting capabilities of POSTCON are extensive, and its use is highly recommended. The plot files may also be postprocessed by other user-defined postprocessing programs. In order to write such programs, the user must have a complete understanding of the structure and contents of the data records written to the plot files. This information is provided in Table E-1. If the user wishes to write a postprocessing program, it may be useful to consult the CONTAIN source listing to ensure that the READ statements used are consistent with the WRITE statements in CONTAIN. Most of the time-dependent plot file output is generated in subroutines CPLOT and GPLOT. The plot file output of control parameters is generated primarily in subroutines IGLOBL and ICAM.

The information on the plot files is in binary form and consists of records with two different formats:

```
oflag,  oblank, value1, value2
oblank, oblank, (variable(i),i=1,n)
```

Most of the data is written in groups of two or more records, with the first record of each group being the first type shown above. The records that follow are mostly the second type given above, with a few exceptions as noted in Table E-1. The first record type consists of a character flag, "oflag", a character blank, "oblank", and two values. The "oflag" character is used to define the type of information to follow. In general, "value1" is the cell number with which the information is associated. Again, there are exceptions, as noted in Table E-1, in which "value1" is either an integer or real zero or other descriptive information. "Value2" is either a calculated result, such as a cell pressure, or a real zero. Normally when "value2" is zero, the data associated with "oflag" is written as a vector in the next record.

The second record type consists of two character blanks followed by a vector of data. The length of the vectors written are either fixed or stored in the plot file as control information. A vector of data is always preceded by two character*8 blanks. This vector may consist of

such data as aerosol densities within a size class at a given time or a series of control words required to process other data records.

Table E-1 shows the information written to the plot file(s). It indicates the flag number, the number of records associated with that flag, the number of words in the record, and a description of the actual data written to the files(s).

Table E-1. Plot File Contents

Flag	Rec	No. of Words	Description
10	2	11	Global control information
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		1	number of cells
		1	number of materials
		1	number of title cards
		1	number of global tables
		1	maximum number of entries in global tables
11	2	6+nm	Material compound names for use in problem
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		nm	material names
12	1	4	Coolant material number and coolant name
	#1	2	character flag, character blank
		1	coolant material number
		1	coolant material name
15	2	6+10*ntitl	Problem title information
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		10*ntitl	title information
20	2	21	Cell level control information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	number of aerosol sources
		1	number of aerosol source points in tables
		1	number of atmospheric sources
		1	number of points in atmospheric source tables

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
20	2	21	Cell level control information (continued)
		1	number of engineering sources
		1	number of points in engineering source tables
		1	number of fission product sources
		1	number of points in fission product source tables
		1	number of lower cell sources
		1	number of points in lower cell source tables
		1	number of spray sources
		1	number of points in spray source tables
		1	number of cell level vector tables
		1	maximum number of entries in cell vector tables
		1	number of heat transfer structures
25	2	16	Cell name/title
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		10	cell name or cell title
100	1	4	Time mark separating transient information
	#1	2	character flag, character blank
		1	real zero
		1	system timestep end point
101	1	4	Atmospheric temperature in cell
	#1	2	character flag, character blank
		1	cell number
		1	cell atmosphere temperature
102	1	4	Atmospheric pressure in cell
	#1	2	character flag, character blank
		1	cell number
		1	cell atmosphere pressure

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
103	2	8	Atmospheric coolant vapor mass and vapor fraction
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	cell coolant vapor mass
		1	cell coolant vapor fraction
		1	cell saturation ratio
104	2	6+nm	Atmospheric mole fractions
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nm	cell mole fractions
105	2	6+nm	Atmospheric mass composition
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nm	cell masses
106	1	4	Total condensate on structures in cell
	#1	2	character flag, character blank
		1	cell number
		1	mass of condensate on structures
107	1	4	Total condensate runoff from structures in cell
	#1	2	character flag, character blank
		1	cell number
		1	mass of condensate runoff
108	2	8	Condensate on individual structures
	#1	2	character flag, character blank
		1	cell number
		1	structure number
	#2	2	two character blanks
		2	condensate mass on each face of structure

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
125	3	11+3*nsp	Atmospheric source table information
	#1	2	character flag, character blank
		1	cell number
		1	number of sources to atmosphere
	#2	2	two character blanks
		1	source table flag
		1	number of entries in source table ("nsp")
		1	name of material source
	#3	2	two character blanks
		3*nsp	source table, consisting of "nsp" time points, "nsp" mass source rates, and "nsp" energy or temperature values
126	3	11+3*nsp	Atmospheric spray source table information
	#1	2	character flag, character blank
		1	cell number
		1	number of spray sources to atmosphere
	#2	2	two character blanks
		1	source table flag
		1	number of entries in source table ("nsp")
		1	name of material source
	#3	2	two character blanks
		3*nsp	source table, consisting of "nsp" time points, "nsp" mass source rates, and "nsp" energy or temperature values
200	2	6+nc2	Intercell flow areas
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		nc2	flow areas ("nc2" = "ncells" * "ncells")
205	2	6+nc2	Intercell flow rates
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		nc2	flow rates ("nc2" = "ncells" * "ncells")

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
210	2	6+nengv	Engineered vent flow areas
	#1	2	character flag, character blank
		2	integer zero, real zero
	#2	2	two character blanks
		nengv	engineered vent flow areas
215	2	6+nengv	Engineered vent flow rates
	#1	2	character flag, character blank
		2	integer zero, real zero
	#2	2	two character blanks
		nengv	engineered vent flow rates
220	2	11	Suppression pool data
	#1	2	character flag, character blank
		2	integer zero, real zero
	#2	2	character blanks
		1	suppression pool flow rate
		4	real zeros (reserved for future use)
310	2	11	Sodium pool fire transient information
	#1	2	character flag, character blank
		1	cell number
		1	zero
	#2	2	two character blanks
		1	mass of oxygen consumed in burn
		1	mass of sodium consumed in burn
		1	mass of peroxide generated in burn
		1	mass of monoxide generated in burn
		1	energy associated with combustion reaction
320	2	8	Pool mass and energy loss (boiling, evaporation, and vaporization)
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	mass of coolant leaving pool (cumulative)
		1	energy carried with coolant mass (cumulative)

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
340	2	9	Timestep control and run time information
	#1	2	character flag, character blank
		1	system timestep end point (real value)
		1	real zero
	#2	2	two character blanks
		1	calculation cycle number
		1	current system timestep size
		1	CPU time utilized in past system timestep
350	2	12	CORCON ablation products, metal mass
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	cumulative mass of CO2 liberated
		1	cumulative mass of H2O liberated
		1	cumulative mass of CO liberated
		1	cumulative mass of H2 liberated
		1	mass of Zr in metal layer
		1	mass of C in metal layer
351	2	11	CORCON heat sources
	#1	2	character flag, character blank
		1	cell number
		1	zero
	#2	2	two character blanks
		1	total decay heat
		1	heat of reaction
		1	heat of ablation
		1	heatup of ablation products
		1	surface heat loss

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
352	2	42	CORCON layer properties
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		36	six sets of values of layer temperature, mass, density, void fraction, lower interface temperature, lower interface heat flux. The first set corresponds to the heavy oxide layer, the third set to the metal layer and the fifth set to the light oxide layer. The sixth set's interface values refer to the top of the light oxide layer, i.e. the top of the CORCON model.
353	2	8	CORCON cavity information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	maximum cavity radius
		1	maximum cavity depth
354	2	31	CORCON layer crust information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		25	five sets of values of radial and axial liquid center temperature, thicknesses of the bottom crust, radial crust and top crust. The first set corresponds to the heavy oxide layer, the third set to the metal layer and the fifth set to the light oxide layer.

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
360	2	12	Hydrogen and CO burn data (cumulative)
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	H2 mass burned
		1	Co mass burned
		1	O2 mass burned
		1	H2OV mass produced
		1	CO2 mass produced
		1	energy liberated by burning
400	2	11	Lower cell control information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	number of concrete layers
		1	number of intermediate layers
		1	number of pool layers
		1	number of atmospheric layers
		1	total number of lower cell layers
401	2	6+nreg	Nodes per lower cell layer
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nreg	number of nodes in each lower cell layer
402	2	6+nreg	Beginning node in each lower cell layer
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nreg	first node number in each lower cell layer

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
405	2	8	Layer names
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		1	generic name of layer
		1	user or default name of layer
410	2	6+nnp	Node thicknesses for each layer
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		nnp	thickness of each node in layer ("nnp" = number of nodes in layer)
415	2	6+nm*nnp	Masses of each lower cell node
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		nm*nnp	component masses of each node in layer ("nnp" = number of nodes in layer)
420	2	6+3*nnp	Temperatures of each lower cell node
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		3*nnp	top, middle, and bottom temperature of each node
425	3	11+3*nsp	Lower cell layer source table information
	#1	2	character flag, character blank
		1	layer number
		1	number of sources to lower cell layer

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
425 (continued)			
	#2	2	two character blanks
		1	source table flag
		1	number of entries in source table ("nsp")
		1	name of material source
	#3	2	two character blanks
		3*nsp	source table, consisting of "nsp" time points, "nsp" mass source rates, and "nsp" energy or temperature values
426	3	13+2*ntb	Lower cell layer heat transfer coefficient tables
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		1	name of table
		1	name of independent variable
		1	name of dependent variable
		1	table interpolation flag, integer 0 or 1
		1	number of data points in vector
	#3	2	two character blanks
		ntb	independent variable vector
		ntb	dependent variable vector ("ntb" = number of data points in vector)
427	3	13+2*ntb	Lower cell layer volumetric heat sources
	#1	2	character flag, character blank
		1	cell number
		1	layer number
	#2	2	two character blanks
		1	name of table
		1	name of independent variable
		1	name of dependent variable
		1	table interpolation flag, integer 0 or 1
		1	number of data points in vector
	#3	2	two character blanks
		ntb	independent variable vector
		ntb	dependent variable vector ("ntb" = number of data points in vector)

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
500	1	4	Aerosol control information
	#1	2	character flag, character blank
		1	number of aerosol sections ("nsectn")
		1	number of aerosol components ("nac")
510	2	6+nac	Aerosol component names
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		nac	names of aerosol materials
520	2	6+nsectn+1	Aerosol size boundaries
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		nsectn+1	diameters of interfaces between size classes
525	3	11+3*nsp	Aerosol source table information
	#1	2	character flag, character blank
		1	cell number
		1	number of aerosol sources to atmosphere
	#2	2	two character blanks
		1	source table flag
		1	number of entries in source table ("nsp")
		1	name of material source
	#3	2	two character blanks
		3*nsp	source table, consisting of "nsp" time points, "nsp" mass source rates, and "nsp" energy or temperature values
530	2	6+n	Aerosol airborne density
	#1	2	character flag, character blank
		1	cell number
		1	zero
	#2	2	two character blanks
		n	densities of each component in each size class ("n" = "nsectn"*"nac")

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
540	2	6+6*nac	Aerosol cumulative depositions by component
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		6*nac	aerosol cumulative deposited masses by component. (The six values for each component correspond to: total, roofs, walls, and floors, overflow bin, and underflow bin.)
550	1	4	Total aerosol cumulative deposition
	#1	2	character flag, character blank
		1	cell number
		1	cumulative aerosol mass in all deposition locations in cell, summed over all components.
560	1	nhtm*2+6	Aerosol cumulative depositions by surface
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	nhtm*2+2	cumulative mass on each structure and in pool; includes two sides for each location
570	1	nhtm*2+6	Aerosol mass deposited over timestep by surface
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	nhtm*2+2	mass added to each structure and to pool includes two sides for each location
580	1	4	Total aerosol mass deposited over timestep
	#1	2	character flag, character blank
		1	cell number
		1	aerosol mass added to all deposition locations in cell, summed over all components in timestep.

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
590	1	8	Aerosol waste location information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	total aerosol mass added to waste over timestep
		1	cumulative aerosol mass in waste location
600	2	8	Structures control information
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		1	number of heat structures ("nhtm")
		1	maximum number of nodes in any structure ("mxslab")
601	2	6+nhtm	Number of nodes per structure
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nhtm	number of nodes in each structure
602	2	6+nhtm	Structure names
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nhtm	character names of each structure
603	2	6+n	Structure node materials
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		n	name of material making up each node of structure ("n" = "nhtm"*"mxslab")

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
604	2	6+m	Structural node interface positions
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		m	position of each node interface of each structure ("m" = "nhtm"*("mxslab" + 1))
605	2	6+n	Structural node masses
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		n	mass of material in each node of each structure
606	2	6+m	Structural node interface areas
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		m	area of each node interface of each structure.
610	2	6+mxslab	Structural node temperatures
	#1	2	character flag, character blank
		1	cell number
		1	structure number
	#2	2	two character blanks
		mxslab	temperature of each node in structure
700	2	10+ncells	Fission product control information #1
	#1	2	character flag, character blank
		2	two zeros
	#2	2	two character blanks
		1	number of fission product names ("nnuc")
		1	number of fission chain elements ("nfce")
		1	number of fission product chains ("nchain")
		1	total number of fission product hosts according to the old host numbering scheme ("nhmo"). (See note on next page.)
		ncells	number of extra material hosts in each cell

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description

Note: "nhmo" is computed to be the total number of hosts in all cells that would have been available under the old pre-1.10 hosting scheme. These correspond in each cell to 1 + "nac" + 3 + "nhc" hosts represented by the GAS, each aerosol component, roofs, walls, floors, and the "nhc" extra material hosts. The lower cell and DUMMY host inventories are reported under the first extra material host, if present.

705	2	6+nf	Fission product control information #2
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		1	total number of actual fission product hosts ("nhm")
		ncells	number of actual hosts by cell ("nhost(i)")
		ncells	number of structure hosts in each cell
		ncells	number of lower cell layer hosts in each cell
		nchain	number of elements in each fission product chain ("nf" = 1+"ncells"*3+"nchain")
710	2	6+nnuc	Fission product nuclide names
	#1	2	character flag, character blank
		2	two zeros
	#2	2	two character blanks
		nnuc	names of fission product nuclides
720	2	6+nfce	Fission chain elements
	#1	2	character flag, character blank
		2	two zeros
	#2	2	two character blanks
		nfce	nuclide name array index corresponding to each fission chain element (see flag 710)
725	3	11+3*nsp	Fission product source table information
	#1	2	character flag, character blank
		1	cell number
		1	number of fission product sources
	#2	2	two character blanks
		1	source table flag
		1	number of entries in source table ("nsp")
		1	name of material source
	#3	2	two character blanks
		3*nsp	source table, consisting of "nsp" time points, "nsp" mass source rates, and "nsp" energy or temperature values

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
730	2	6+n	Fission product masses in the old hosting scheme
	#1	2	character flag, character blank
		2	two real zeros
	#2	2	two character blanks
		n	fission product masses in all cells for each chain element and each host in the old hosting scheme. (See note after flag 700.) ("n" = "nfce"*"nhmo")
740	2	6+nh	Fission product masses in the new hosting scheme
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	2 character blanks
		nh	fission product masses for each chain element and each actual host in one cell. ("nh" = "nfce"*"nhost(i)")
750	2	6+nhost(i)	Fission product host powers
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nhost(i)	fission product power for each host in the cell
760	1	4	Lower cell makeup decay power
	#1	2	character flag, character blank
		1	cell number
		1	lower cell makeup decay power
770	2	6+nhost(i)	Fission product host temperatures
	#1	2	character flag, character blank
		1	cell number
		1	real zero
	#2	2	two character blanks
		nhost(i)	temperature of each host in the cell

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
800	1	4	Engineered safety features control information
	#1	2	character flag, character blank
		1	cell number
		1	number of engineering systems
805	2	11	Engineered safety features names and setup
	#1	2	character flag, character blank
		1	cell number
		1	system number
	#2	2	two character blanks
		1	name of system
		1	cell of origination for liquid redistribution
		1	cell of destination for liquid redistribution
		1	cell of origination for liquid overflow
		1	cell of destination for liquid overflow
810	2	17	Engineered safety features transient information
	#1	2	character flag, character blank
		1	cell number
		1	system number
	#2	2	two character blanks
		1	vapor mass to atmosphere from ESF
		1	liquid mass to pool from ESF
		1	energy associated with vapor mass
		1	energy associated with liquid mass
		1	mass of liquid overflow in past timestep
		1	mass of redistributed liquid
		1	remaining height of ice in ice condenser
		1	cumulative vapor mass to atmosphere from ESF
		1	cumulative energy associated with vapor mass
		1	cumulative liquid mass to pool from ESF
		1	cumulative energy associated with liquid mass
900-999			Reserved for user-defined output to plot file

Table E-1. Plot File Contents (continued)

Flag	Rec	No. of Words	Description
1111	1	8	Code version, run identification
	#1	2	character flag, character blank
		1	character label of code version (e.g., '1.1')
		1	character label of code revision number (e.g., '0')
		1	character label of last update set
		1	additional update character label (usually blank)
		1	character*10 label of date of run
		1	character*10 label of time of run
4444	1	2	Control block terminator
	#1	2	character flag, character blank
5555	1	4	Transient block terminator
	#1	2	character flag, character blank
		1	system timestep end point (or a real zero for the first occurrence of this flag)
		1	real zero

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11. ABSTRACT *(200 words or less)*

The CONTAIN 1.1 computer code is an integrated analysis tool for predicting the physical, chemical, and radiological conditions inside a containment building following the release of radioactive material from the primary system in a severe reactor accident. It can also predict the source term to the environment. The purpose of this User's Manual is to provide a basic understanding of the features and models in CONTAIN 1.1 so that users can prepare reasonable input and understand the output and its significance for particular applications. Besides input instructions, the User's Manual also contains brief descriptions of the basic features of the models. Both light water reactors and liquid metal reactors can be modeled with CONTAIN 1.1, although many of the sodium specific models are not documented in this report. The code includes atmospheric models for steam/air thermodynamics, intercell flows, condensation/evaporation on structures and aerosols, aerosol behavior, and gas combustion. It also includes models for reactor cavity phenomena such as core/concrete interactions and coolant pool boiling. Heat conduction in structures, fission product decay and transport, radioactive heating, and the thermal-hydraulic and fission product decontamination aspects of engineered safety features are also modeled.

12. KEY WORDS/DESCRIPTORS *(List words or phrases that will assist researchers in locating the report.)*

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