
Reference Manual for the CONTAIN 1.1 Code for Containment Severe Accident Analysis

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482

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ABSTRACT

This report describes the phenomenological equations and the numerical procedures used by the CONTAIN 1.1 code to determine the conditions within nuclear power plant containment during a severe accident. The CONTAIN detailed models provide the capability to mechanistically calculate the containment internal thermal-hydraulic conditions and the amount of radioactive matter that would be released to the environment if there were a leak from the containment. Note that the CONTAIN models can be verified by comparing the code calculations to experimental results. The models described include those to account for the flows of mass and energy between containment compartments, the exchange of energy between the atmosphere and heat structures, the thermodynamic conditions, the distributions of aerosols, the decay and transport of fission products, the deflagration of hydrogen and carbon monoxide, boiling water reactor suppression pool behavior, and engineered safety features, including a spray, fan coolers, and an ice condenser. These models are solved with implicit coupling, where appropriate, to obtain a stable and computationally efficient solution.

CONTENTS

<u>Section</u>	<u>Page</u>
Abstract	iii
Acknowledgements	xiii
Nomenclature	xv
1.0 INTRODUCTION	1-1
1.1 Guide to this Manual	1-2
1.2 Overview of CONTAIN	1-4
1.2.1 Scope of CONTAIN Modeling	1-5
1.2.2 Material Properties	1-6
1.2.3 Intercell Flow and Atmosphere Thermal-Hydraulics	1-7
1.2.4 Aerosol Behavior	1-8
1.2.5 Fission Product Behavior	1-9
1.2.6 Cavity Phenomena	1-10
1.2.7 Engineered Safety Features	1-10
1.2.8 Boiling Water Reactor Models	1-11
1.3 CONTAIN Quality Assurance	1-11
1.3.1 Code Development and Maintenance	1-11
1.3.2 Configuration Control	1-12
1.3.3 Testing	1-12
1.4 Atmosphere Thermal-Hydraulic Conservation Equations	1-13
2.0 CODE ARCHITECTURE	2-1
2.1 CONTAIN Models and Variables	2-1
2.2 Processing of Phenomenological Models	2-2
2.3 Interface Arrays	2-2
2.4 Global-Level Versus Cell-Level	2-2
2.5 Upper Cell Versus Lower Cell	2-3
2.6 Memory Management	2-3
2.7 The Reference Cell	2-4
2.8 Timestep Control	2-5
3.0 THERMODYNAMICS AND INTERCELL FLOW	3-1
3.1 Flow Path Types	3-1
3.2 Implicit Flow Option	3-5
3.2.1 Trial Pressures	3-5
3.2.2 Implicit Flow Timestep Control	3-5

CONTENTS (Continued)

<u>Section</u>	<u>Page</u>
3.3 Thermal-Hydraulics	3-7
3.3.1 Buoyancy	3-9
3.3.2 Mass and Mass Components	3-11
3.3.2.1 Inertial Flow Model	3-11
3.3.2.2 Quasi-Steady Flow Model	3-13
3.3.2.3 Choked Flow Model	3-14
3.3.2.4 Explicit Sources and Sinks	3-16
3.3.2.5 Implicit Sources (Boiling)	3-17
3.3.3 Energies	3-18
3.4 Self-Consistent Thermodynamic State	3-19
3.4.1 Temperature Iteration	3-19
3.4.2 Pressure Iteration	3-21
3.5 Boiling Water Reactor Suppression Pool Vent Thermal-Hydraulic Model	3-22
3.5.1 Vent Clearing Time	3-24
3.5.2 Suppression Pool Flow Model	3-33
3.6 Nonthermodynamic Material Flow	3-38
4.0 AEROSOL BEHAVIOR MODELS	4-1
4.1 Aerosol Size Distribution	4-2
4.2 Dynamics	4-4
4.2.1 Agglomeration	4-9
4.2.2 Condensation and Evaporation	4-11
4.2.3 Deposition	4-14
4.3 Sources	4-19
4.4 Aerosol Scrubbing Model	4-19
5.0 FISSION PRODUCT BEHAVIOR MODELS	5-1
5.1 Linear Decay Chain	5-2
5.2 Fission Product Decay Heating	5-6
5.3 Targeted Release and Acceptance of Fission Products	5-9
5.4 Liquid Transport of Fission Products	5-15

CONTENTS (Continued)

<u>Section</u>	<u>Page</u>
6.0 EXPLICIT CELL MODELS	6-1
6.1 Material Properties	6-2
6.1.1 Material Properties for Coolant	6-4
6.1.2 Bulk Thermodynamic Properties	6-4
6.1.3 Transport Property Dimensionless Parameters	6-6
6.2 Hydrogen and Carbon Monoxide Burning	6-7
6.2.1 Deflagration Ignition and Propagation Criteria	6-8
6.2.2 Flame Speed and Burn Time	6-11
6.2.3 Burn Rate	6-14
6.3 Heat and Mass Transfer	6-18
6.3.1 Convective Heat Transfer	6-20
6.3.2 Mass Transfer	6-21
6.3.3 Thermal Radiation	6-28
6.3.3.1 Net Enclosure Radiation Model	6-28
6.3.3.2 Simple Radiation Model	6-31
6.3.3.3 Radiative Properties	6-33
6.3.3.3.1 Modak Radiative Property Model	6-34
6.3.3.3.2 Cess-Lian Radiative Property Model	6-38
6.4 Heat Conduction	6-39
6.4.1 Containment Structures	6-40
6.4.2 Heat Conduction Model	6-42
6.4.2.1 Conduction Equation Initial and Boundary Conditions	6-43
6.4.2.2 Heat Conduction Solution Method	6-43
6.5 Engineered Safety Features	6-48
6.5.1 Fan Cooler Model	6-49
6.5.1.1 Fan Cooler Heat Transfer Models	6-51
6.5.1.2 Fan Cooler Aerosol Deposition Model	6-55

CONTENTS
(Concluded)

<u>Section</u>	<u>Page</u>
6.5.2 Ice Condenser	6-55
6.5.2.1 Ice Condenser Melting Models	6-58
6.5.2.2 Ice Condenser Aerosol Decon- tamination Models	6-60
6.5.3 Containment Sprays	6-71
6.5.3.1 Pump Model	6-71
6.5.3.2 Heat Exchanger Models	6-72
6.5.3.3 Valve Model	6-77
6.5.3.4 Pipe Model	6-78
6.5.3.5 Orifice	6-78
6.5.3.6 Refueling Water Storage Tank	6-79
6.5.3.7 Containment Spray Aerosol Removal Model	6-79
6.5.3.8 Engineered Systems Overflow Model	6-85
6.5.3.9 Containment Spray Thermal- Hydraulics Models	6-86
6.5.3.10 Iodine Removal Models	6-91
7.0 SUMMARY	7-1
8.0 REFERENCES	8-1
APPENDIX A - DESCRIPTION OF CONTAIN MODELS CHANGED IN VERSIONS BEYOND CONTAIN 1.1	A-1
APPENDIX B - CONTAIN CODE VALIDATION SUMMARY	B-1
APPENDIX C - EXPLICIT FLOW OPTION	C-1
APPENDIX D - IMPLICIT LOWER CELL POOL BOILING MODEL	D-1

LIST OF FIGURES AND TABLES

<u>Figure</u>	<u>Page</u>
1-1 Family of CONTAIN Code Documentation	1-4
1-2 Illustration of Feedback Mechanisms Treated in the CONTAIN Code	1-6
2-1 Problem Size-Dependent Data Structure	2-4
2-2 Overall Flow Diagram of CONTAIN	2-6
3-1 Example of Regular Flow Path Connectivity	3-3
3-2 Examples of Engineered Vent Flow (a) Parallel Flow Path Connection, (b) Rupture Disc Connection	3-3
3-3 PWR Containment Building Reduced to a Configuration of 18 Interconnected Cells	3-4
3-4 Flow Timestep Calculation Logic	3-6
3-5 Timestep Control in the Implicit Intercell Flow Option	3-8
3-6 Elevations of Cells and Flow Path Ends to Calculate Gas Gravitational Head Effects	3-10
3-7 Choked Flow Representation	3-15
3-8 Cell Pressure Iteration Scheme for Implicit Flow Option	3-23
3-9 Suppression Pool Thermal-Hydraulics	3-25
3-10 Detailed Definition of the Variables of the BWR Suppression Pool System (Mark III)	3-29
3-11 Computation of Drywell Level Depression	3-30
3-12 Computation of Wetwell Level Depression	3-31
4-1 Example of Aerosol Particle Mass Concentration Distribution for a Two-Component Aerosol	4-2
4-2 Model for Water Condensation on Aerosols	4-12
5-1 Example of FP Linear Decay Chains Derived from a Branched Decay Chain	5-3
5-2 Reactor Power and Decay Time Intervals	5-8

LIST OF FIGURES AND TABLES (Continued)

<u>Figure</u>		<u>Page</u>
5-3	Example of FP Redistribution by Targeted Release and Acceptance Model for FPs Initially Located in the LC Fuel Layer	5-13
6-1	Flame Propagation Diagram	6-11
6-2	Heat Transfer Configuration (not to scale)	6-19
6-3	Equivalent Circuit for the Heat Transfer Configuration of Figure 6-2	6-19
6-4	The Influences of Noncondensables on Interface Resistance	6-23
6-5	Nodes in a One-Dimensional System	6-44
6-6	FC System	6-49
6-7	FC Geometry Depicting One Horizontal Cooling Coil (top view)	6-50
6-8	Sectional View of an Ice Compartment and Containment Region Boundaries	6-56
6-9	Simplified Diagram of an IC	6-57
6-10	Illustration of Impaction on a Typical IC Ice Basket Horizontal Strip	6-64
6-11	CS System	6-72
6-12	CONTAIN HX Models	6-73
6-13	Simplified Schematic of Counterflow HX, Emphasizing HX Terminology	6-74
6-14	Qualitative Comparison of Aerosol Collection Efficiencies	6-81
6-15	Heat Transfer Configuration	6-88
C-1	CONTAIN 1.1 Explicit Flow Options	C-2
C-2	Time Derivative Calculations for the Runge-Kutta Integration	C-3
C-3	Flow Chart for the Reduce Option	C-4

LIST OF FIGURES AND TABLES (Concluded)

<u>Figure</u>		<u>Page</u>
C-4	Network of Cells Connected by Series and Parallel (Closed Circuit) Flow Paths	C-6
C-5	Flow Chart for Self-Consistent Thermodynamic States	C-9
D-1	Pool Boiling	D-1

<u>Table</u>		<u>Page</u>
1-1	Conservation of Momentum Equation for Flow Between Cell i and Cell j	1-15
1-2	Conservation of Mass Equation for Gas k in Cell i	1-16
1-3	Conservation of Energy Equation for Cell i	1-18
1-4	Thermodynamic State Closure Equations for Cell i	1-20
2-1	Integration and Timesteps Used Within Various CONTAIN Models	2-7
5-1	Illustrative FP Targeted Release Rates	5-14
6-1	Materials Available in CONTAIN 1.1	6-3
6-2	Default Ignition and Propagation Limits	6-10
6-3	Coefficients for the Cess-Lian Correlation	6-39
A-1	Materials Recommended for Use in CONTAIN 1.11	A-2

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NOMENCLATURE*

Regular symbols (see Subscripts for additional symbols):

<u>Symbol</u>	<u>Definition</u>	<u>Units</u> **
A	Area	m ²
AC	Aerosol coefficient	
BWR	Boiling water reactor	
C	Coefficient	None
	Molar concentration	kgmoles/m ³
	Constant	
C _{FC}	Turbulent irreversible flow loss coefficient	None
CST	Coolant storage tank	
C _m	Cunningham slip (correction) factor	None
c _p	Specific heat at constant pressure	J/kg-K
c _v	Specific heat at constant volume	J/kg-K
Col	Collision efficiency	
D	Diffusivity	m ² /s
	Diameter, usually for a drop	m
Dep	Deposition rate	s ⁻¹
DF	Decontamination factor	
d	Diameter, usually for a particle	m
E	Effectiveness	
	Efficiency	
	Spray collection efficiency	

* Units are not provided everywhere in the text because all symbol parameters follow the SI system of units and the units are given in the Nomenclature list. Units may be given in the text to provide clarity.

Note that the Nomenclature does not define an expression like A(x) used to show a functional dependence. For example, P(T) may refer to the pressure P at temperature T and m(t + Δt) may refer to the mass at the time t + Δt. In addition, not all symbols are defined here because of the extensive local symbol description given in the text.

**"None" indicates that the symbol is derived from symbols with units. A blank indicates that there are no units because it is a simple ratio, a factor, a dimensionless number, an acronym, or an abbreviation.

<u>Symbol</u>	<u>Definition</u>	<u>Units</u>
ESF	Engineered safety feature	
exp	Exponent	
Fr	Fraction	
FC	Fan cooler	
FP	Fission product	
f	Friction irreversible loss factor	None
g	Gravity, acceleration because of gravity	m/s ²
H	Height	m
	Elevation	m
HEPA	High-efficiency particulate airborne	
HX	Heat exchanger	
h	Heat transfer coefficient	W/m ² -K
	Specific enthalpy	J/kg
IC	Ice condenser	
J	Molar flux	kgmole/m ² -s
j	Mass flux	kg/m ² -s
K	Irreversible loss coefficient	None
	Aerosol removal rate constant	m ³ /s
	Mass transfer coefficient	kgmoles/s-m ² -Pa
k	Thermal conductivity	W/m-K
L	Length	m
	A/L	m ⁻¹
LC	Lower cell	
LMR	Liquid metal reactor	
LOCA	Loss-of-coolant accident	
LWR	Light water reactor	
M	Molecular weight	kg/kgmole
Mo	Moles	kgmoles
m	Mass	kg
$\dot{m}$	Mass flow rate	kg/s
max	Maximum value of a selection	
min	Minimum value of a selection	
Ntu	Number of thermal units	None
n	Number per unit volume	m ⁻³
P	Pressure	Pa
PWR	Pressurized water reactor	
p	Power	W

<u>Symbol</u>	<u>Definition</u>	<u>Units</u>
Q'	Special energy effect	
Q	Energy or energy transferred Aerosol mass per unit volume of atmosphere	W m/m ³
QA	Quality assurance	
q	Energy transfer rate Heat flux	J/s W/m ²
q'''	Volumetric energy transfer	W/m ³
$\bar{K}$	Aerosol removal (deposition) coefficient	kg/m ³ -s
R	Universal gas constant	J/kgmole-K
RCS	Reactor cooling system	
RDF	Requirements definition function	
RPS	Reactor primary system	
RWST	Refueling water storage tank	
r	Radius	m
ra	Ratio	None
rt	Rate	
S	Aerosol source Surface	kg/m ³ -s
SRV	Safety relief valve	
SSat	Supersaturation ratio of atmosphere water mass to the water mass if the atmosphere was saturated	None
T	Temperature	K
t	Time	s
t _s	Timestep	s
U	Internal energy	J
UC	Upper cell	
US	United States	
USNRC	United States Nuclear Regulatory Commission	
u	Specific internal energy	J/kg
V	Volume	m ³
v	Specific volume Velocity	m ³ /kg m/s
W	Mass flow rate	kg/s
X	Mole fraction	None
x	Coordinate or direction	m
y	Coordinate or direction	m

<u>Symbol</u>	<u>Definition</u>	<u>Units</u>
α	Absorptivity Thermal diffusivity	None m^2/s
β	Coefficient of agglomeration or coagulation A constant of proportionality Volumetric coefficient of thermal expansion Ratio of drywell vent area to wetwell pool area	m^3/s K^{-1}
γ	Specific heat ratio Agglomeration shape factor	None
Δ	Difference, change	
ϵ	Emissivity Turbulent energy dissipation density Efficiency	 m^2/s^3
λ	Decay constant Molecular mean free path	s^{-1} m
μ	Viscosity	$\text{N}\cdot\text{s}/\text{m}^2$
μ'	Specific viscosity	$\text{kg}/\text{kg}\cdot\text{m}\cdot\text{s}$
ν	Kinematic viscosity Vena contraction factor	$\text{N}\cdot\text{s}/\text{kg}\cdot\text{m}^2$
ρ	Density	kg/m^3
σ	Stefan-Boltzmann constant Boltzmann constant	$\text{J}/\text{s}\cdot\text{m}^2\cdot\text{K}^4$ J/K
χ	Dynamic shape factor	
ψ	Radiosity	
ξ	Mass condensation/evaporation rate Partial pressure ratio	kg/s
ϕ	Pentagamma function	
κ	Vapor flux multiplier	kg

Miscellaneous Conventions:

θ	Sign function, one or zero Sign factor, +1 or -1
Σ	Summation
$\propto$	Proportional to

Subscript symbols:

<u>Symbol</u>	<u>Definition</u>
ANS	American National Standard
a	Aerosol(s); Atmosphere, Atmospheric; Average
a,si	Aerosol, sink
a,so	Aerosol, source
atm	Atmosphere
BD	Brownian diffusion
BL	Boundary layer
BWR	Boiling water reactor
b	Bulk
b,i	Boiling, implicit
bn	Burn
boil	Boiling
br	Boiling rate (implicit)
CO	Carbon monoxide
COR	CORCON
Cgas	Combustible gas
CS	Containment spray
c	Cell; Choked; Cold; Condensation; Convection and/or evaporation; Critical; Cylinder
cc	Cooling coil
chbn	Characteristic burn
cool	Coolant
conv	Convection
cr	Critical; Rated coolant
ct	Containment
D	Diffusion; Diffusiophoresis
d	Depletion; Droplet; Drywell; Drop
dh	Decay heat
diff	Diffusive
df	Diffusiophoretic
dw	Drywell to wetwell
ESF	Engineered safety feature(s)

<u>Symbol</u>	<u>Definition</u>
e	Exiiplicit
eb	Explicit boiling
eff	Effective
eq	Equilibrium
err	Error tolerance
evap	Evaporation
ex	Explicit(ly)
FC	Fan cooler; Flow coefficient
FL	Flow
FP	Fission product
f	Friction loss
f	Flame; Flashing; Flow
flm	Film
g	Gravity; gas
gas	Gas or gas mixture
HX	Heat exchanger
H ₂	Hydrogen
H ₂ O	Water
h	Heat; Hot
I	Impaction and interception
IC	Ice condenser
i	Inertial; Initial; Inlet; One of several
imp	Implicit
in	Internal; Into
int	Integration; Interception; Internal
J	Mass transfer related
j	One of several
k	One of several
LWR	Light water reactor
lam	Laminar
LC	Lower cell
l	Water; Aerosol section
lg	Liquid-vapor
lw	Liquid water
ly	Layer

<u>Symbol</u>	<u>Definition</u>
m	Mass
max	Maximum
min	Minimum
nc	Noncondensable
nm	Log mean
O	Oxygen
O ₂	Oxygen
of	Overflow
o	Outlet; Reference value
op	Opening
out	Out of
p	Particle; Pool; Pressure
qs	Quasi-steady
RK	Runge-Kutta
r	Radiation; Rated; Reference
rm	Remaining
rt	Rate
SRV	Safety relief valve
SVD	Suppression vent deposition
s	Sedimentation; Settling; Source; Steam; Step; Surface; System
sat	Saturation
si	Depletion rate to a "sink"
so	Source
sp	Spray
st	Steam
str	Structure(s)
sup	Suppression pool
T	Temperature; Thermophoresis
t	Temperature; Temporary; Total
th	Thermophoretic
tot	Total
tr	Transfer; Transferred; Trial
UN	²³⁹ U and ²³⁹ Np
u	Upstream

<u>Symbol</u>	<u>Definition</u>
uc	Upper cell
ud	User-defined
usd	Upstream deposition
V	Volume
v	Water vapor; Vent
vap	Water vapor
W	Mass flow rate
WF	Weighting factor
w	Water; Wetwell; Related to flow
wd	Wetwell to drywell
Δt	Timestep

Dimensionless groups:

<u>Name</u>	<u>Dimensionless Group</u>
Grashof number	$Gr = L^3 \rho^2 g \beta_g \Delta T / \mu^2$
Knudsen number	$Kn = 2\lambda / d$
Nusselt number	$Nu = h L / k$
Peclet number	$Pe = \rho c_p v D / k$
Prandtl number	$Pr = C_p \mu / k$
Rayleigh number	$Ra = Gr(Pr)$
Reynolds number	$Re = \rho v L / \mu$
Schmidt number	$Sc = \mu / \rho D_v$
Sherwood number	$Sh = Nu(Sc/Pr)^{1/3}$
Stokes number	$St = \frac{d^2 \rho v}{9\mu D}$

1.0 INTRODUCTION

This document is a reference manual for the CONTAIN 1.1 nuclear reactor containment analysis computer code. The goal of this reference manual is to describe the phenomenological models in the CONTAIN code and their associated governing equations. It is not intended to describe the solution algorithms fully; however, some solution methods are explained when needed for adequate description of the modeling.

The CONTAIN code has been developed as part of an ongoing severe accident research program by the United States Nuclear Regulatory Commission (USNRC) to assess the safety of light water reactor (LWR) nuclear reactor power systems. A critical safety feature of all United States (US) nuclear power plants is the containment system, which serves as a final barrier to protect the public from radioactive releases in the event of a reactor accident. Clearly, the ability to assess containment functionality, temperature and pressure loading, and radiological source term releases in the event of a containment failure are critical in the assessment of the overall safety of the plant. The purpose of the CONTAIN code is to provide a tool for the analysis of nuclear reactor containment systems in the assessment of reactor plant safety under severe accident conditions.

The USNRC research program has relied upon the development and application of analytical simulation tools and scaled experimental studies to evaluate the performance of nuclear reactor systems under severe accident conditions. This reliance upon simulation tools is widely recognized as necessary in the safety assessment of reactor systems because it is neither possible nor feasible to perform prototypical full scale simulations of the complex and hazardous events associated with severe accidents. Moreover, certain mitigation and accident management strategies can only be assessed through the application of computational models and the use of simulation techniques. Finally, scale distortions and the inability to represent the complete spectrum of relevant phenomena at smaller scale prohibit the exclusive use of scaled experiments in the safety assessment of these complex systems.

The CONTAIN code is just one of several analytical tools developed in the USNRC severe accident research program. The specific goal of the CONTAIN development effort has been to provide the USNRC with a best-estimate calculational tool for performing predictions of the thermal, physical, chemical, and radiological response of the containment atmosphere and its surroundings in an accident scenario. The code is mainly intended to address a broad spectrum of postulated severe accidents; however, it can also model less energetic non-core-melt events. Because this code is used to support the resolution of severe accident safety issues, and potentially influence regulatory decisions, it is important that the models within the code be documented. The purpose of this manual is to document the governing equations that are solved in

the CONTAIN code. Note that CONTAIN is not a structural response code.

1.1 Guide to this Manual

Because of the complex physical processes that CONTAIN addresses, the CONTAIN code is a very large, highly complex computational tool, with a great number of phenomenological models. As a result, this manual is also large, and contains a great number of model descriptions and associated governing equations. Moreover, there are a number of support documents that have been written relating to the CONTAIN code, such as the CONTAIN User's Manual [Mur89] and the CONTAIN Quality Assurance Procedures Document [Rus90], and a validation and assessment summary letter report [Was90]. Appendix A presents the model assessment summaries from Reference Was90. The reader may want to refer to one or more of these supporting documents while reading this manual. This section explains the organization of this manual and discusses the relationship of this document to the other supporting documents.

Note that all references to CONTAIN, for example, to the CONTAIN User's Manual, are to the 1.1 version. Differences between the 1.1 and the 1.11 and 1.12 improved versions are discussed in Appendix B. In addition, all references to the CORCON model in CONTAIN are to the CORCON-MOD2 version described in Reference Col84.

Some of the terminology used in this manual requires elaboration to facilitate understanding. The expression "self-consistent" is used frequently, as, for example, in "the procedure was done in a self-consistent manner." This expression means, in general, that the procedure was done in an implicit manner, which means that the solution satisfies the governing equation(s) when evaluated at the end of timestep conditions. The expression "first order" is also used frequently. This expression means that a model representation only accounts for the most important terms and not higher order (for example, second derivative) terms. Note that the lumped-parameter approach used in CONTAIN forces some of the modeling to be first order, because higher order information is not available.

Section 1.2 describes the general capabilities of the CONTAIN code and provides an overview of the available models. This information can be used to assess the suitability of CONTAIN for a particular class of problem solving. This section also serves as an effective introduction to the CONTAIN code for the reader who is not familiar with the CONTAIN User's Manual [Mur89]. No governing equations nor detailed model descriptions are given in Section 1.2; however, the major modeling areas are identified and briefly discussed.

A summary of the procedures followed to ensure the quality of the CONTAIN software is given in Section 1.3. A complete description of the CONTAIN quality assurance (QA) procedures are also published in a separate NUREG document [Rus90].

Section 1.4 provides the conservation equations that are solved to model the thermal-hydraulic response of the atmosphere and material mass flow, which is the most important model in the code. In reading Section 1.4, it is important to keep in mind that the equations described apply only to the flow of gases and the calculation of atmospheric conditions. That is, numerous other phenomena are modeled in CONTAIN, such as aerosol behavior and heat conduction into structures, that are not described by these equations. The equations for the other models are provided in the later sections of this manual. The conservation equations summarized in Section 1.4 are described in greater detail in Section 3.

Section 2 describes the architecture of the code, including a description of the overall code flow logic, input structure, data storage, and timestep control. Readers interested only in the governing equations and modeling capabilities of the code may want to skip this section. Note, however, that certain terms defined in Section 2 are referred to throughout the remainder of this document, such as "cell timestep."

Section 3 is the first and perhaps the most important section that describes a phenomenological model in detail. Section 3 gives the governing equations and mathematical treatments used in the code to describe containment atmosphere thermodynamics and material flow. Nearly every other model in CONTAIN affects or is affected by the models described in Section 3.

Section 4 describes the aerosol dynamics model, including the treatment of aerosol containment sources, particle agglomeration, deposition onto structures, and steam condensation and evaporation to and from aerosol particles. Section 5 describes the treatment of radionuclide decay, heating, and transport. The remaining models are described in Section 6. These include models for heat transfer to and from containment structures, the hydrogen combustion model, and the engineered safety features (ESF) modeling. All models described in Section 6 share the common characteristic of being explicitly, instead of implicitly, coupled to the main flow model described in Section 3.

A few lower cell (LC) models available in CONTAIN are not described in this manual. Of these models, the most important model is the one for corium-concrete interactions and corium pool chemistry. These processes are modeled in CONTAIN using an integrated implementation of the CORCON-MOD2 [Col84] and VANESA [Pow86] codes, which are documented in the references noted. There is a LC simple heat transfer model that is available for problems where concrete ablation is not anticipated. This model is also not fully described; however, the conduction algorithm that is used is described in Section 6. Other less important, and seldom used, models in CONTAIN that are not documented are noted in Section 6.

In addition to this report, several other potentially useful documents regarding CONTAIN have been published. Most importantly, the CONTAIN User's Manual [Mur89] describes the user input instructions

for performing CONTAIN calculations. The User's Manual also gives an overview of the models and provides CONTAIN user's with several helpful hints and offers a number of sample problems. The relationship of this Reference Manual to the User's Manual and other publications in the family of CONTAIN code documentation is illustrated in Figure 1-1.

1.2 Overview of CONTAIN

CONTAIN is a detailed mechanistic computer code for the integrated analysis of LWR severe accident containment phenomena. CONTAIN includes mechanistic models for a wide spectrum of thermal, physical, chemical, and radiological processes that may occur within the containment of a nuclear reactor in the event of a severe accident. Therefore, CONTAIN is capable of predicting pressures, temperatures, and material distributions within the containment for assessing containment loads and associated threats to containment integrity under accident conditions. Because the code also has fully integrated models for aerosol and fission product (FP) behavior and transport, it can be used to predict radiological releases to the environment in the event of containment failure.

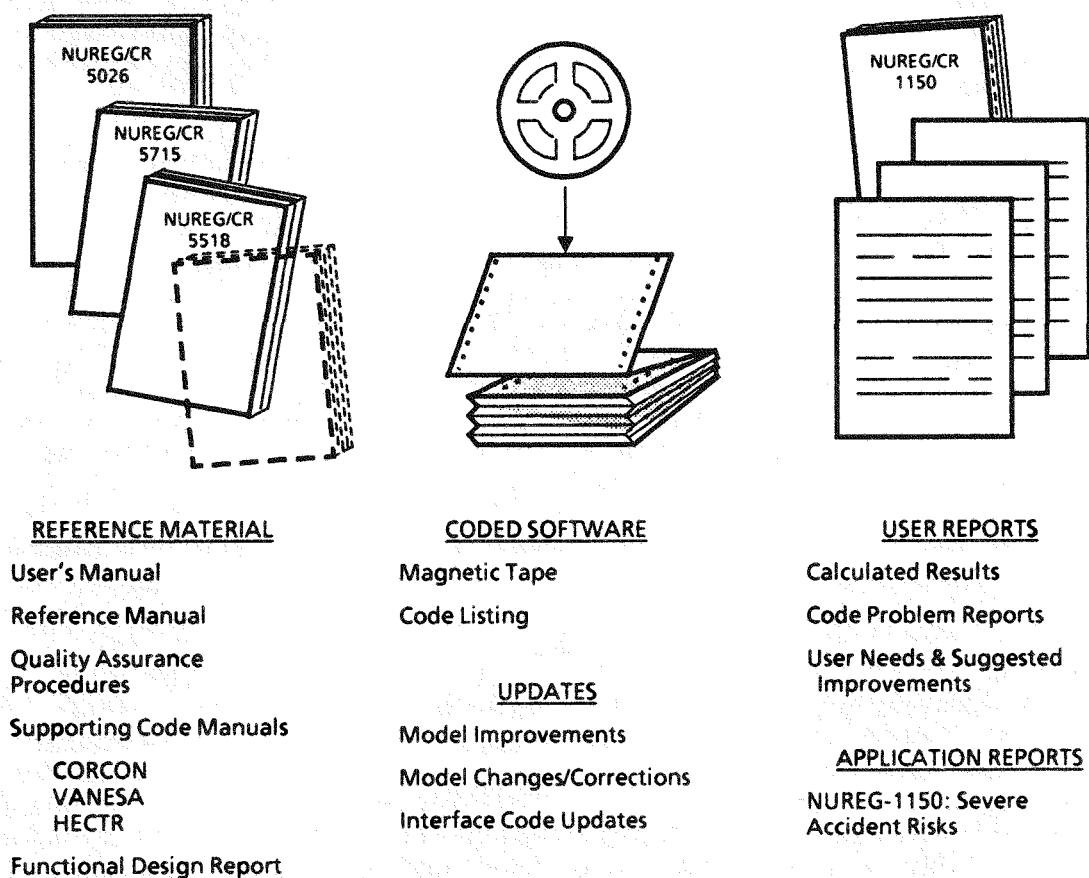


Figure 1-1. Family of CONTAIN Code Documentation

1.2.1 Scope of CONTAIN Modeling

CONTAIN employs best-estimate models where possible with an emphasis placed on mechanistic detail and numerical robustness. Although the individual models in CONTAIN are in general mechanistic, overall the code has reasonable computational efficiency because of the highly efficient control volume framework of the code. The control volume approach has proven to be useful technique for modeling a wide variety of containment configurations as well as providing a suitable framework for modeling the many different containment subsystems.

The CONTAIN modeling applies strictly to processes that occur within the containment building. Therefore, 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. Previously, several separate codes were used to examine containment phenomena. Under such an approach, one code analyzes the thermal-hydraulic phenomena, another handles the FP processes, another is used to model aerosol behavior, and so on. By contrast, CONTAIN simultaneously treats these phenomena and others as well. The benefit of this approach is illustrated in Figure 1-2, where the ability of one process to affect another through phenomenological feedback mechanisms is shown. Note that today there are several other modern codes that also use this integral approach to accident analysis, where this was relatively uncommon when CONTAIN 1.0 [Ber85] was first released in 1985.

Because the CONTAIN code does not treat in-vessel processes, it must rely upon separate analyses performed, for example, with a primary system code to provide sources of mass and energy to the containment in an accident scenario. Although CONTAIN can calculate radionuclide sources to the environment in the event of containment failure, it does not calculate doses or model processes beyond the containment boundary. Such modeling can be performed, however, using the results of a CONTAIN calculation with a separate consequence analysis code. By limiting itself to the containment, the CONTAIN code is able to maintain reasonable computational efficiency while still incorporating detailed mechanistic models.

The major processes that are modeled in CONTAIN include: intercell flow, hydrogen combustion phenomena, heat and mass transfer processes (radiation, convection, conduction, etc), aerosol behavior (agglomeration, deposition, condensation), FP behavior (decay, heating, transport), ESFs (for example, containment spray (CS), fan cooler (FC), ice condenser (IC)), a few processes specific to boiling water reactors (BWR) (for example, the suppression pool and safety release valve (SRV) discharge), and corium-concrete interactions. These global modeling categories can be further divided into numerous separate phenomenological models, a few of which are noted parenthetically above. Taken collectively, these models provide the CONTAIN code with the capability to analyze a wide variety of LWR plants and accident scenarios. Through proper user

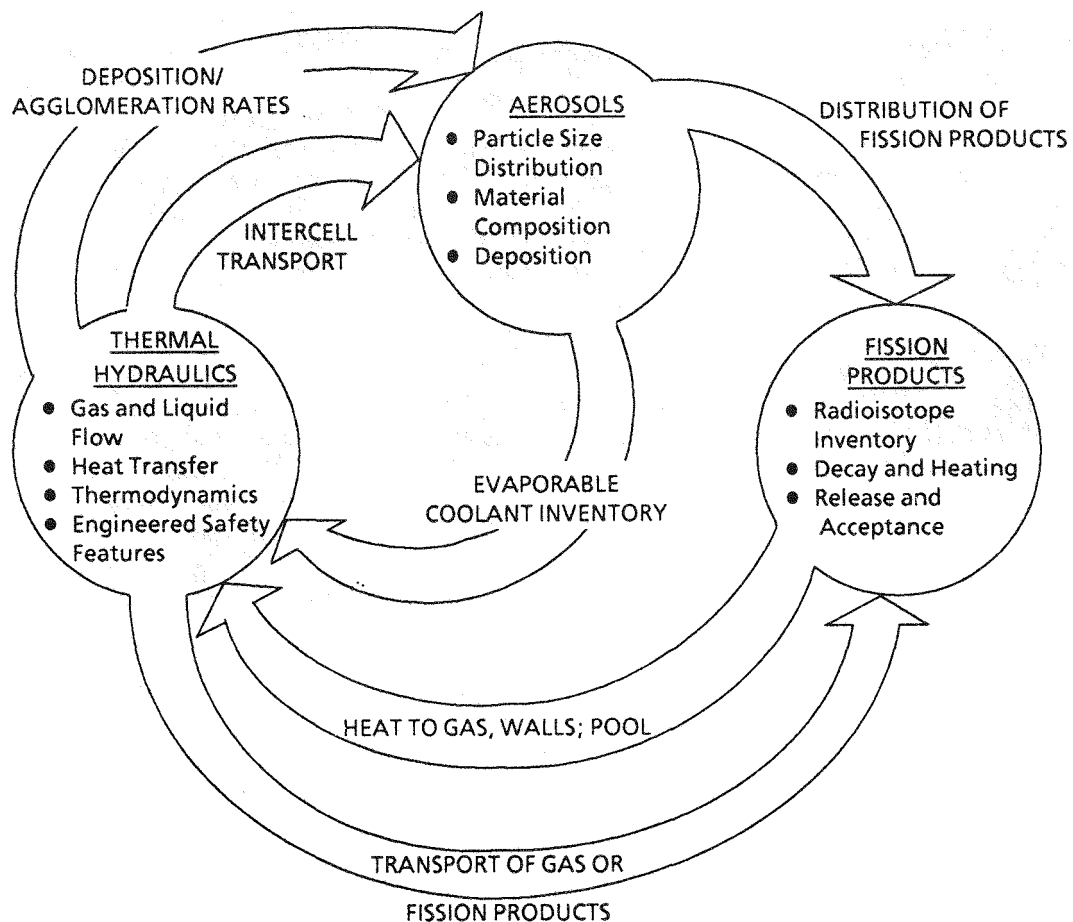


Figure 1-2. Illustration of Feedback Mechanisms Treated in the CONTAIN Code

input, large-dry, sub-atmospheric, and IC pressurized water reactor (PWR) containments, and BWR suppression pool containments can be modeled with CONTAIN. The input flexibility also allows for the representation of experimental facilities and other nonstandard configurations. This has proven to be important for performing code validation calculations. Sections 1.2.2 through 1.2.6 summarize the major modeling areas in CONTAIN. More detailed descriptions are given in Sections 3 through 6.

1.2.2 Material Properties

An important aspect of all modeling in CONTAIN is the code's ability to evaluate thermodynamic and transport properties for materials typically found in LWR plant systems. For materials commonly found in LWR systems, CONTAIN provides a self-consistent material property library of correlations for the three thermodynamical states: gas, liquid, and solid. Self-consistent property functions are provided for heat capacity, enthalpy, thermal

conductivity, viscosity, diffusivity, and density (except for gases, which use the ideal gas law). Appropriate mixture relationships are also included for these properties when more than one constituent is involved.

Less common materials, such as refractory alloys, that are not represented in the CONTAIN material library can be treated using the CONTAIN user-defined material property table capability. With this capability, material properties for essentially any gas, liquid, or solid material can be specified in user-defined tables.

The ideal gas law is assumed for the equation of state for all gases in the atmosphere, including steam. It should be noted that steam primarily behaves as an ideal gas for nearly any conceivable severe accident containment condition. Only at the high pressures seen in the primary system does steam begin to behave as a real gas. Given this fact, it is acceptable that CONTAIN treat steam as an ideal gas. Moreover, by assuming the ideal gas law in CONTAIN, the equation of state is implicitly coded into the gas flow model, thereby providing an additional degree of implicitness to the flow solver.

1.2.3 Intercell Flow and Atmosphere Thermal-Hydraulics

The backbone of all modeling in CONTAIN is the intercell flow and atmosphere thermal-hydraulics models. This modeling, which is actually a collection of several tightly integrated ones, calculates the major phenomena expected to affect atmosphere and coolant pool behavior during reactor accidents. These major phenomena include: gas flow, atmosphere temperature and pressure response, coolant pool thermal response and boiling, primary system sources, condensation and evaporation, convection heat transfer, structure heat conduction, radiation heat transport, and hydrogen burning. Some of these processes are handled implicitly, and others explicitly. The implicitly coupled models are described in Section 3, and the explicitly coupled ones are discussed in Section 6.

CONTAIN is a control-volume/flow path code that allows for an arbitrary arrangement of control volumes and flow path connections. Like all control-volume codes, CONTAIN is limited by the inherent restrictions of a lumped parameter (that is, control volume) treatment in that momentum is not stored in the control volumes. Within the control volume framework, however, the flow model is quite sophisticated. For example, the CONTAIN flow model can represent choked flow and the flashing of a coolant pool. Pool boiling, suppression pool thermal equilibrium, bubble condensation and evaporation, and pressure-dependent flow areas are also treated in the CONTAIN flow solution. The conservation equations solved in the flow solver are given in Section 1.4.

Numerous atmosphere mass and energy (heat) transfers are modeled by CONTAIN. These include mass and heat transfer with structures, heat transfer from the decay of gaseous or aerosol-borne FPs, mass and heat transfer from hydrogen deflagrations, mass and energy

transfer from chemical interactions in the cavity, mass and energy transfer from intercell flow, and user-defined mass and energy sources or sinks.

CONTAIN models condensation onto or evaporation from structure surfaces. Because spatial orientation of structures can influence the rate of condensation or evaporation, the user specifies the orientation in the input. The presence of noncondensable gases is also accounted for because their presence inhibits the condensable vapor diffusion to the surface.

CONTAIN has two radiation models, which mechanistically model the thermal radiation of the gas, steam, and aerosol cloud in the atmosphere. In the simpler formulation, the atmosphere radiates to each surface in a cell in series. For problems requiring a more detailed analysis, a net enclosure radiation model is available. The simultaneous radiative exchange between surfaces and the cell atmosphere cloud is treated mechanistically in the net enclosure model.

CONTAIN can also calculate hydrogen and/or carbon monoxide deflagrations. Whenever the combustible gas concentration exceeds the deflagration limit and the atmosphere is not inerted by either a shortage of oxygen or an excess of steam or carbon dioxide diluents, combustion is assumed to occur. An existing burn can also propagate to other volumes, if certain criteria are satisfied. The deflagration and propagation models are from the HECTR 1.5 code [Din86], except that CONTAIN does not model continuous burning. However, the user has considerable flexibility and can override the default values. Note that these models (a) do not model detonation or deflagration to detonation phenomena, and (b) are based on experiments performed at relatively low temperatures and, therefore, do not account for the effects of high temperature or burn initiation, etc.

1.2.4 Aerosol Behavior

A number of mechanistic models are available in CONTAIN for representing the behavior of aerosols. Aerosol behavior is important in containment analysis because of the role aerosols play in FP transport. The aerosol model in CONTAIN is based on the MAEROS [Gel82] code, which allows for a multisectional, multicomponent treatment of aerosols. In a multisectional treatment, the particle size distribution is discrete and can, therefore, have an arbitrary shape. In a multicomponent treatment, particles of different composition can be modeled.

The CONTAIN aerosol model also includes treatment of aerosol-vapor condensation and evaporation. The CONTAIN aerosol treatment includes models of three agglomeration processes: Brownian, gravitational, and turbulent. Also, four deposition processes are considered in the aerosol model: gravitational settling, diffusio-phoresis, thermophoresis, and particle diffusion. When aerosols

with condensate deposit onto structures, the water on the aerosol is added to the water film on the structure.

1.2.5 Fission Product Behavior

CONTAIN models the decay and transport of FPs in the containment and the heating of the containment atmosphere and surrounding structures by radionuclide decay heating. A few models are also included for the chemical interaction of certain radionuclide species (for example, elemental iodine and methyl iodide); however, comprehensive mechanistic modeling of chemical radionuclide behavior is not available.

To determine the location of the radionuclides being studied, CONTAIN tracks them as if they were physically combined with other materials or "hosts", such as, the gas molecules, aerosol particles, or structure walls. The reason for this FP host system is that the masses of FP involved are often very small compared to the masses of the aerosol hosts. Thus, the predicted transport of airborne FPs is based on the mechanistic thermal-hydraulic modeling of the movement of the airborne host materials.

In addition to these models, each FP can also be transferred from one host to another at user-specified rates, which can depend upon host temperatures. This flexible system, denoted as "targeted release-and-acceptance," for FP transport is necessary because of the high degree of uncertainty involving the physical and chemical forms of FPs and their affinities for the various materials. In the past, the experimental and modeling data base for the chemical changes in radionuclides has been insufficient to provide reliable mechanistic models for a code like CONTAIN; however, the availability of new data and new modeling techniques offers hope for improvements in this area. Until such improvements are made, however, the targeted release and acceptance formalism is provided to allow the analyst to evaluate the consequences of different assumptions.

The decay of FPs and the heating of the host materials are modeled in CONTAIN according to the half-lives and power coefficients of fission chain elements. These chains may be comprised of either (a) individual parent-daughter radionuclides with power related to the decay constant, or (b) FP groups with a given time-dependent power curve. Because the decay heat of each radionuclide (or FP group) is deposited into its respective host material, the FP heating couples back to the thermal-hydraulics (see Figure 1-2).

Despite the flexibility in being able to specify either individual radionuclides or FP groups, it is usually difficult to specify in detail all of the radionuclides or groups 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 individually specified radionuclides and the FP groups 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.

1.2.6 Cavity Phenomena

In a core-melt accident involving a breach of the primary vessel, a bed or pool of core debris and coolant may develop in the bottom of the reactor cavity. As heat is transferred from the core debris bed or pool to the concrete, the temperature of the concrete increases and the concrete can undergo thermal ablation. Ablation of the concrete floor presents the threat of basemat penetration while simultaneously producing water vapor, noncondensable gases (including combustible hydrogen and carbon monoxide), and aerosol ablation products. Further chemical reactions may take place in the core debris, generating hydrogen, carbon monoxide, and other products. These products can carry FPs, heat, and reaction products through the coolant pool into the upper containment atmosphere. The CORCON-MOD2 [Col84] and VANESA [Pow86] phenomenological codes have been integrated into CONTAIN to deal with these phenomena. A detailed description of the modeling in these two codes is not duplicated here.

The CORCON-MOD2 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 (UC) system can interact with this upper surface. The VANESA code models aerosol production and FP evolution from the core debris as a result of the gas from the core-concrete interactions sparging through the molten materials.

Aerosols generated in the cavity are scrubbed if they pass through a coolant pool on their way to the atmosphere. The pool in this case will also scrub any FPs in aerosol form. Gaseous materials introduced into the pool will be equilibrated at the pool temperature before being passed to the cell atmosphere. The scrubbing model is also described in Reference Pow86 and is thus not duplicated in this manual.

For situations where ablation is not expected to occur, a more efficient transient one-dimensional heat conduction model is provided. This model calculates only the transient thermal response of the cavity using the CONTAIN conduction model. The conduction model is described in Section 6.

1.2.7 Engineered Safety Features

CONTAIN provides models for internal CSSs, FCs, and IC ESFs. The decontamination of aerosols by all three of these ESFs is modeled. The FC model uses either a mechanistic condensation model or a

simpler plant-specific correlational approach. CONTAIN also has a first order depletion rate model for elemental iodine (I_2) and methyl iodide (CH_3I) removal by sprays. Simple models for coolant pool water movement through pipes, valves, and by overflow are also included. These models are described in Section 6.5.

1.2.8 Boiling Water Reactor Models

The CONTAIN code includes models to accommodate suppression pool containment configurations. These models include SRV modeling, suppression pool flow modeling, a vent clearing model, and scrubbing models in the suppression pool. Because both vertical and horizontal vents can be modeled, the CONTAIN code can accommodate the Mark I, II, and III containment designs. The suppression pool models are implicitly coupled to the flow modeling and are described in Section 3.5.

1.3 CONTAIN Quality Assurance

The CONTAIN code has been developed with an established set of procedures for QA. These procedures are designed to ensure the quality of the CONTAIN models and to control the configuration of the software. This is accomplished through the systematic evaluation and control of changes to the CONTAIN code so as to prevent modeling inadequacies and error introduction or propagation. A complete description of these procedures is given in Reference Rus90. The three major features of the CONTAIN QA procedures are: code development and maintenance, configuration control, and testing. These features are briefly described below.

1.3.1 Code Development and Maintenance

The CONTAIN code development and maintenance system is implemented through the following major functions: requirements definition, code development, change tracking, testing, and user support. These functions are discussed in this section. Note that the testing described here is one element of the overall testing program, denoted developmental testing.

The requirements definition function (RDF) provides a number of mechanisms for controlling requirements specification errors. The RDF conducts an independent review of the requirements formulated during the user interface. This step is a direct check on the support person's decision that the change stimulus actually merits a requirements change. The RDF determines the priority of the recommended change with respect to the other planned changes and determines when it should be acted upon. Finally, the RDF determines the functional relationship between the requirement and those requirements already being implemented, and assigns the change to a code developer.

The code development process begins when a change has been defined and the model/code developers have been assigned. These assignments are made by the project leader for the code version.

The developers are responsible for designing, coding, documenting, and performing developmental testing for their own modification.

The change tracking function provides a means for judging the completeness of the modification process relative to the quality measures exerted in the other development and maintenance system functions. Change tracking is accomplished by using identifiers that cross-reference problem reports and code change documents to the update that corrects the problem. Also, all CONTAIN updates are required to contain two special lines that ensure the proper order in the linking of all updates. As a result of these required lines and the UPDATE utility itself, it is impossible (without generating UPDATE and compiler errors) to assemble the updates out of order. This function ensures that the code is internally consistent, functionally complete, and coherent relative to its documentation.

Developmental testing is conducted by the developer during code development. This testing primarily verifies that the models perform as intended in the requirements phase of the development. The content and extent of this testing is left to the discretion of the developer; however, the developer is held accountable for correcting any errors found during the more rigorous independent and integral testing phases.

The user support function includes all communication with the user community, including code documentation. The primary purpose of this function is to provide technical assistance to analysts who are using the CONTAIN code to address their particular severe accident issue.

1.3.2 Configuration Control

The CONTAIN QA procedures include a configuration control system. The objective of the configuration control QA component is to ensure that users or analysts accessing the CONTAIN code are presented with a complete, consistent version of the fully tested CONTAIN code. The configuration control system governs two forms of CONTAIN: the operational baseline and the developmental baseline. The operational baseline is the software version of CONTAIN that is released for formal use in addressing severe accident issues. The developmental baseline is the controlled software under development, testing, and use by the CONTAIN staff. This control system ensures that the released version of CONTAIN has successfully fulfilled all of the checks and balances employed in the CONTAIN QA procedures.

1.3.3 Testing

The testing function has the following primary objectives: verification, integration, regression prevention, and validation. Verification is accomplished primarily through the developmental testing discussed above. The objective of verification is to test each individual update set to determine that test input data are

properly translated to yield the correct results according to the design. The objective of integration is to exercise aspects of an update set that interact with other parts of the code to ensure that in context transformations are performed correctly. The objective of regression prevention is to ensure that the addition of an update set does not change any CONTAIN results other than those the update set is intended to change.

Developmental testing is conducted by the developer during code development. Independent testing is conducted by a person different from the developer to provide objectivity in uncovering any errors that the developer may have missed. Once all of the updates have been independently tested and accepted, they are integrated and tested as a whole. This successive set of testing ensures that the updates are as error-free as possible.

Validation is done to test each individual update set to determine that the results produced are correct relative to the mathematical model implemented by the update set. A minimal amount of validation is also pursued at the discretion of the developmental and independent tester. Formal model validation is a process performed external to the formal QA testing function. A summary of CONTAIN validation efforts is provided in Appendix A.

1.4 Atmosphere Thermal-Hydraulic Conservation Equations

The basic equations that govern the thermal-hydraulic behavior in CONTAIN are the conservation equations of momentum, mass, and energy. In addition, CONTAIN uses the ideal gas law equation of state, which specifies the relationships between pressure, temperature, and mass within a control volume. These four equations are solved simultaneously in CONTAIN as explained in Section 3. A multitude of other support or closure equations are also solved to provide mass and energy sources and sinks to the conservation equations. The support equations are solved separately (explicitly) from the conservation equations.

The conservation equations are discussed in detail in Section 3 of this manual. The purpose of this section is to summarize the application of these equations to the modeling of the hydrodynamic gases, including coolant and noncondensable, in the atmosphere. Tables 1-1 through 1-4, grouped at the end of this section, present the equations as ordinary differential equations for the control-volume formulation. This section also gives a brief review of terms in these equations.

An inherent restriction of CONTAIN is that the flow equation used is relatively simple. This flow equation is based on solution of the one-dimensional momentum and continuity equations for the flow path with the assumption of constant flow density during the timestep. Note that as a result of this and other assumptions inherent to a control volume treatment, the code does not account for momentum convection differences between the flow path inlet and flow path outlet. Table 1-1 gives the momentum conservation

equation solved in CONTAIN in terms of the mass flow rate W_{ij} between cells i and j . As presented in this table, the driving force is the total pressure differential between the cells at the ends of the flow path. This differential includes gravitational forces for all flow paths except for vents between the drywell and the wetwell for bypass flow in a BWR. The irreversible flow losses in the momentum equation depend upon a user-specified irreversible loss coefficient. For the suppression pool by-pass flow, this coefficient is internally forced to be unity. Section 3.3.2.1 gives a detailed description of the flow loss coefficient.

The mass conservation equation for a control volume (cell) is given in Table 1-2. The equation given in this table is a simple balance expression on the flow of gases into a control volume from other cells and out of the control volume to other cells. Mass source and sink rates resulting from phenomenological processes modeled explicitly outside of the atmosphere conservation equations are also accounted for in this balance. This includes the addition of a user-defined "source" of mass into the containment resulting from flow from the reactor primary system (RPS), that is, blowdown. The equations that describe these explicit rates are given in Section 6. Table 1-2 also shows the mass contribution from pool boiling, which is calculated within the flow solver (see Section 3.3.2.6 for more details). A mass balance equation is not provided for the LC because the LC models used in CONTAIN are described elsewhere [Col84, Pow86].

The energy conservation equation for a control volume is given in Table 1-3. The equation in this table shows how the calculational results depend on the work due to flow, work against gravity or dissipation because of gravity, and the energy source and sinks within the control volume. Note that the kinetic energy term is neglected in the energy equation. For containment analyses, the gas flow is often at a low velocity and not directed; therefore, the kinetic energy term becomes unimportant [Ber85]. Many of the energy sources and sinks in Table 1-3 are calculated separately from the atmosphere conservation equations. The governing equations for these processes are given throughout the remaining sections of this manual. Note that the addition to the containment of energy resulting from flow from the RPS is modeled as a user-defined "source."

The last conservation equation is the equation of state for gases that is given in Table 1-4. The equation in this table provides a relationship between density, pressure, and temperature. An iterative procedure is performed in CONTAIN to calculate the self-consistent thermodynamic state of temperature given the internal energy and masses of a control volume. Note that once the temperature is obtained from the internal energy, a pressure iteration is done using this temperature.

Table 1-1
Conservation of Momentum Equation for Flow
Between Cell i and Cell j

$$\frac{dW_{ij}}{dt} = \left[\Delta P_{ij} - C_{FC} \frac{|W_{ij}| W_{ij}}{\rho_{ij} A_{ij}^2} \right] \frac{A_{ij}}{L_{ij}}$$

where for regular flow paths or engineered vents

$$\Delta P_{ij} = P_i - P_j + \Delta P_{ij,g}$$

with

$$\Delta P_{ij,g} = g[\rho_i(H_i - H_1) + \rho_a(H_1 - H_2) - \rho_j(H_j - H_2)]$$

and for suppression pool bypass flow paths

$$\Delta P_{ij} = P_w - P_d$$

where

- W_{ij} = mass flow rate through flow path between cells i and j;
- t = time;
- ΔP_{ij} = pressure difference between cells i and j;
- C_{FC} = irreversible flow loss coefficient, which is defined in Section 3, and
- ρ_{ij} = 1 for suppression pool bypass flow;
- ρ_{ij} = the gas flow density in flow path ij depends on the flow option used with $\rho_{ij} = \rho_i$ for the implicit flow option, which is the recommended flow option, and $\rho_{ij} = \rho_a$ used for the explicit flow option;
- A_{ij} = area of flow path ij;
- L_{ij} = inertial length of flow path ij;
- P_i = pressure in cell i;
- P_j = pressure in cell j;
- $\Delta P_{ij,g}$ = pressure effects because of gravity;
- g = acceleration because of gravity;
- ρ_i = gas density in cell i;
- H_i = elevation of cell center in cell i;
- H_1 = elevation of flow path opening in cell i;
- ρ_a = arithmetic average density = $(\rho_i + \rho_j)/2$;
- H_2 = elevation of flow path opening in cell j;
- ρ_j = gas density in cell j;
- H_j = elevation of cell center in cell j;
- P_w = BWR wetwell pressure; and
- P_d = BWR drywell pressure.

Table 1-2
Conservation of Mass Equation for Gas k in Cell i

$$\frac{dm_{i,k}}{dt} = \dot{m}_{in} - \dot{m}_{out} + \dot{m}_{ex,so} - \dot{m}_{ex,si} + \dot{m}_{br}$$

where

$$\begin{aligned}
 m_{i,k} &= \text{mass of gas component k in cell i;} \\
 &\text{Note that many of the term definitions have an implied value for k. For example, water vapor terms are only for the k corresponding to water vapor.} \\
 t &= \text{time;} \\
 \dot{m}_{in} &= \text{mass flow rate of gas k into cell i;} \\
 &= \sum_j \frac{W_{ji} \theta_{ji} m_{j,k}}{m_j} \\
 W_{ji} &= \text{mass flow rate of all gases through flow path ji (from cell j to cell i);} \\
 \theta_{ji} &= \begin{cases} 1 & \text{if } W_{ji} > 0 \\ 0 & \text{if } W_{ji} \leq 0 \end{cases} \begin{matrix} \text{(flow is into cell i)} \\ \text{(flow is out of cell i)} \end{matrix} \\
 m_{j,k} &= \text{mass of gas component k in cell j;} \\
 m_j &= \text{total atmospheric gas mass in cell j;} \\
 \dot{m}_{out} &= \text{mass flow rate of gas k out of cell i;} \\
 &= \sum_j \frac{W_{ij} \theta_{ij} m_{i,k}}{m_i} \\
 W_{ij} &= \text{mass flow rate of all gases through flow path ij (from cell i to cell j);} \\
 \theta_{ij} &= \begin{cases} 1 & \text{if } W_{ij} > 0 \\ 0 & \text{if } W_{ij} \leq 0 \end{cases} \begin{matrix} \text{(flow is into cell i)} \\ \text{(flow is out of cell i)} \end{matrix} \\
 m_{i,k} &= \text{mass of gas component k in cell i;} \\
 m_i &= \text{total atmospheric gas mass in cell i;} \\
 \dot{m}_{ex,so} &= \text{source rate from explicit cell models,} \\
 &= \dot{m}_{bn,so} + \dot{m}_{CS,so} + \dot{m}_{a,so} + \dot{m}_{ud,so} + \dot{m}_{eb} + \dot{m}_{LC,so} + \dot{m}_{c,so} + \dot{m}_{SRV,so} \\
 \dot{m}_{bn,so} &= \text{source rate of water vapor and/or CO}_2 \text{ as a result of burning, see Section 6.3;} \\
 \dot{m}_{CS,so} &= \text{evaporation rate of water droplets in CS, see Section 6.5.3.9;} \\
 \dot{m}_{a,so} &= \text{evaporation rate of water from aerosols, see Section 4;} \\
 \dot{m}_{SRV,so} &= \text{BWR-SRV mass transfer source rate;}
 \end{aligned}$$

Table 1-2 (concluded)
Conservation of Mass Equation for Gas k in Cell i

$\dot{m}_{ud,so}$	=	user-defined source rate for gas component k;
$\dot{m}_{eb}$	=	evaporation rate of liquid because of LC explicit pool boiling, see Section 3.3.2.4;
$\dot{m}_{LC,so}$	=	source rate of gas component k from the LC models;
$\dot{m}_{c,so}$	=	evaporation rate of liquid from the liquid film on the heat structures, see Section 6;
$\dot{m}_{ex,si}$	=	depletion rate from explicit cell models,
	=	$\dot{m}_{bn,si} + \dot{m}_{CS,si} + \dot{m}_{a,si} + \dot{m}_{FC} + \dot{m}_{IC} + \dot{m}_{ud,si} + \dot{m}_{LC,si} + \dot{m}_{c,si} + \dot{m}_{SRV,si}$
$\dot{m}_{bn,si}$	=	depletion rate of CO, O ₂ , and/or H ₂ as a result of burning, see Section 6.2.3;
$\dot{m}_{CS,si}$	=	condensation rate of vapor onto the water droplets in CS, See Section 6.5.3;
$\dot{m}_{a,si}$	=	condensation rate of water onto aerosols, see Section 4;
$\dot{m}_{FC}$	=	condensation rate of vapor onto the FC, see Section 6.5.1;
$\dot{m}_{IC}$	=	condensation rate of vapor in the IC, see Section 6.5.2;
$\dot{m}_{SRV,si}$	=	BWR-SRV mass transfer sink rate;
$\dot{m}_{ud,si}$	=	user-defined depletion rate of gas component k;
$\dot{m}_{LC,si}$	=	condensation rate of vapor onto the LC layer; and
$\dot{m}_{c,si}$	=	condensation rate of vapor onto the heat structures, see Section 6; and
$\dot{m}_{br}$	=	implicit flow boiling source rate, see Section 3.3.2.5.

Table 1-3
Conservation of Energy Equation for Cell i

$$\frac{dU_i}{dt} = q_w + q_e + q_{sup} + q_{boil} + q_g + q_{LC}$$

where

$$\begin{aligned} \frac{dU_i}{dt} &= \text{rate of change of the total internal energy in cell i;} \\ q_w &= \text{rate of energy transferred into cell i because of flow, and} \\ &= \sum_j W_{ji} \theta_{ji} h_j - \sum_j W_{ij} \theta_{ij} h_i \\ W_{ji} &= \text{mass flow rate of gases through flow path ji (from cell j to cell i);} \\ h &= \text{specific enthalpy in cell j, and} \\ &= \frac{U + PV}{m}, \\ U &= \text{internal energy in cell j;} \\ P &= \text{pressure of cell j;} \\ V &= \text{volume of cell j; and} \\ m &= \text{total gas mass in cell j;} \\ W_{ij} &= \text{mass flow rate of gases through flow path ij (from cell i to cell j);} \\ q_e &= \text{rate of energy transferred into cell i because of the explicit cell models contribution, and} \\ &= q_{bn} + q_{eb} + q_r + q_c + q_{FP} + q_{ESF} + q_a + q_{SRV} + q_{ud} \\ q_{bn} &= \text{burn source, see Section 6;} \\ q_{eb} &= \text{explicit pool boiling energy, see Section 3.3.2.4;} \\ q_r &= \text{thermal radiation source, see Section 6;} \\ q_c &= \text{convection/evaporation/condensation source, see Section 6;} \\ q_{FP} &= \text{FP decay heat, see Section 5;} \end{aligned}$$

Table 1-3 (concluded)
Conservation of Energy Equation for Cell i

$$\begin{aligned}
 & q_{\text{ESF}} = \text{ESF energy transfer rate, see Section 6;} \\
 & q_{\text{a}} = \text{aerosol energy transfer rate;} \\
 & q_{\text{SRV}} = \text{BWR-SRV energy transfer rate; and} \\
 & q_{\text{ud}} = \text{user-defined energy transfer rate;} \\
 q_{\text{sup}} &= \text{energy transfer rate because of the suppression pool} \\
 & \text{vent flow, and} \\
 &= \dot{m}_{\text{vap,v}} h_{\ell g} + \text{CPG } \Delta T_{\text{vap}} / \Delta t_f \\
 & \dot{m}_{\text{vap,v}} = \text{vapor mass rate through vent carried by} \\
 & \text{the passing noncondensable gases;} \\
 & h_{\ell g} = \text{latent heat of evaporation;} \\
 & \text{CPG} = \text{specific heat of noncondensable gases} \\
 & \text{multiplied by the total noncondensable} \\
 & \text{gases in the bubbles;} \\
 & \Delta T_{\text{vap}} = \text{amount of temperature change in the} \\
 & \text{suppression pool surface because of the} \\
 & \text{passing noncondensable gases; and} \\
 & \Delta t_f = \text{flow timestep;} \\
 q_{\text{boil}} &= \text{energy transfer rate because of the implicit pool} \\
 & \text{boiling, and} \\
 &= \left[\frac{Q_p - m_p h_{\ell}}{\Delta t_f} \right] \frac{h_{\text{vap}}}{h_{\ell g}}, \text{ see Section 3.3.2.5;} \\
 & Q_p = \text{pool energy;} \\
 & m_p = \text{pool mass;} \\
 & h_{\ell} = \text{specific enthalpy of coolant liquid; and} \\
 & h_{\text{vap}} = \text{specific enthalpy of vapor;} \\
 q_g &= \text{energy transfer rate because of the work against} \\
 & \text{gravity, and} \\
 &= -W_{ij} \theta_{ij} g (H_j - H_i) \\
 & g = \text{acceleration of gravity;} \\
 & H_i = \text{elevation of cell center for cell i;} \\
 & H_j = \text{elevation of cell center for cell j; and} \\
 q_{\text{LC}} &= \text{energy transfer rate because of the LC models} \\
 & \text{contribution (not documented here).}
 \end{aligned}$$

Table 1-4
Thermodynamic State Closure Equations for Cell i

Internal Energy:

$$U_i = \sum_k^N (h_k m_k - R M_{o_k} T_i) + m_\ell h_\ell$$

where

$$U_i = \text{internal energy of gases, water vapor and liquid water in cell i;}$$

$$N = \text{number of gases (including water vapor) in cell i that are treated as ideal gases;}$$

$$k = \text{gas component k;}$$

$$h_k = \text{specific enthalpy of gas component k, and}$$

$$= \frac{U_k + P_k V_i}{m_k}$$

$$U_k = \text{internal energy of gas in cell k, and}$$

$$P_k = \text{partial pressure of gas component k;}$$

$$m_k = \text{mass of gas (including water vapor) component k in cell i;}$$

$$R = \text{universal gas constant;}$$

$$M_{o_k} = \text{number of moles of gas component k;}$$

$$T_i = \text{gas temperature in cell i;}$$

$$m_\ell = \text{mass of liquid water in the atmosphere, and}$$

$$= m_{H_2O} - \frac{P_{sat} M_{vap} V_i}{R T_i}$$

$$m_{H_2O} = \text{total water (vapor + liquid) mass in atmosphere,}$$

$$P_{sat} = \text{saturation pressure,}$$

$$M_{vap} = \text{molecular weight of water; and}$$

$$h_\ell = \text{specific enthalpy of liquid water.}$$

Pressure:

$$P_i = \sum_k^N \frac{R M_{o_k} T_i}{V_i} + \frac{R M_{vap} T_i}{V_i}$$

$$P_i = \text{pressure in cell i, and}$$

$$V_i = \text{volume of cell i, which is adjusted to account for changes in the pool volume.}$$

2.0 CODE ARCHITECTURE

CONTAIN uses a modular design whereby each of its phenomenological models is calculated by a set of distinct subroutines. Conceptually, the processing of a single model is a relatively straightforward process. However, it is the interfacing between models that makes CONTAIN the powerful computational tool that it is. And it is this interfacing that is the focus of this chapter.

2.1 CONTAIN Models and Variables

Each phenomenological model in CONTAIN can be viewed simplistically as a function that advances a set of fundamental variables, which describe the state of the model system, forward in time by some timestep. These fundamental variables are then used to determine all other state variables for the (model) system. In other words, each fundamental variable represents a degree of freedom in the CONTAIN modeling, so the set of fundamental variables uniquely defines the system with no redundancies. Variables that can be derived from the fundamental variables are called state variables. As an example, the masses and energies of materials in the cell atmosphere are fundamental variables, whereas the temperature and pressure of the atmosphere are state variables that can be derived from the fundamental variables.

Every fundamental variable is "owned" by a particular model. This ownership means that, for each fundamental variable, only one model is allowed to modify that variable. For example, the condensation model "owns" the fundamental variable for the mass of the condensate film on a structure. While a model can only modify fundamental variables that it owns, it is allowed to read fundamental variables owned by other models.

In some cases, a fundamental variable might need to be modified by several different models. This is the case, for example, with the atmosphere mass arrays. Atmosphere masses are affected by numerous processes such as condensation, pool boiling, hydrogen burns, and intercell flow, to name just a few. However, ownership of the atmosphere mass arrays can be given to only one of these models. In CONTAIN, the intercell flow model owns the atmosphere mass arrays. Therefore, the other models are required to communicate with the intercell flow model through the use of interface arrays to change the atmosphere masses.

Interface arrays are not owned by any particular model. Instead, they can be read or modified by any or all of the CONTAIN models. These arrays are described in more detail in Section 2.3.

In addition to the fundamental variables and interface arrays, each model has a collection of internal variables used to perform its calculations. These are variables that are unique to the model and are not referenced by other models. Finally, the CONTAIN models need access to a rather extensive library of chemical and physical

data. This library is stored in property variables that can be referenced by any of the models, but are never modified.

2.2 Processing of Phenomenological Models

The phenomenological models in CONTAIN are processed so that each model (or group of models) is integrated forward in time over the current timestep. The fundamental variables that are not owned by the model (or model group) are held fixed at the values existing at the beginning of the timestep while the fundamental variables that belong to the model may be updated by the model within the timestep. As a result, the values of the fundamental variables used by each model depend on which models have been processed for the timestep. Thus, a fundamental variable that could be changed by more than one model may not have the same value for all the models that use it within a timestep. Inconsistencies that could arise are checked, and appropriate adjustments are made.

2.3 Interface Arrays

As mentioned earlier, interface arrays provide a means of telling the owning model of a fundamental variable about changes to the variable calculated by another model. Interface arrays are, in general, directly tied to a fundamental variable. For example, there is an interface array that represents changes to atmosphere masses calculated by all models in the timestep. The intercell flow model, which owns the atmosphere mass array fundamental variable, uses the interface array to update the atmosphere masses.

The interface arrays provide a powerful tool for modeling interactions between various models. As might be inferred from the discussion above, the basic computational cycle of CONTAIN can result in discrete changes to fundamental variables. These discrete changes are often inappropriate for handling interactions between models, even with very small timesteps. For example, discrete changes in the atmosphere masses could wreak havoc on the intercell flow calculations.

To avoid such problems, the interface arrays are converted into rates of change. In this way, changes calculated by one model are smoothly integrated into the calculations performed by another model without taking excessively small timesteps.

Finally, it is worth pointing out that source tables specified in the input deck are handled by interface arrays. The tables are translated into rates of change and these rates are added to the interface arrays, which the CONTAIN models are programmed to utilize.

2.4 Global-Level versus Cell-Level.

CONTAIN divides the phenomenological models into two basic types, global-level models and cell-level models. The distinction between

the two types 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 in the input are used by a model in the time-dependent calculations.

The global-level is used for models that are strongly coupled between cells. The principal global model is the intercell gas flow model, which requires simultaneous access to the temperatures, pressures, and atmosphere compositions of all the cells.

In contrast, the cell-level is typically used for models where feedback between cells is not important. CONTAIN uses the "reference cell" concept for processing the cell-level models. 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. Thus, strong coupling to processes outside the cell cannot be accommodated efficiently. However, relatively strong coupling between the processes within a cell may be accommodated because the cell-level 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.)

There is, in some cases, a degree of arbitrariness determining whether a model should be at the cell-level or at the global-level. Such is the case if the model is not strongly coupled either to other cells or to other physical models within the cell. An example is the FP decay model. Such models may be placed in the global-level for efficiency reasons, or may be placed in the cell-level to use cell-level fundamental variables easily. In the case of FP decay, this model is at the global-level; however, there are FP transport models, such as spray washout, that are at the cell-level.

2.5 Upper Cell versus Lower Cell

The cell-level models are further organized into UC and LC models. While this does not have a significant impact on the calculations, it does affect the organization of the CONTAIN input file. The UC includes atmosphere thermodynamics, surface heat transfer, surface condensation, radiative heat transfer, hydrogen and carbon monoxide combustion, and ESFs. The LC includes models for heat transfer in the cavity, and core-concrete interactions. The CORCON (core-concrete interaction) and VANESA (radionuclide and aerosol release) models are part of the LC processing.

2.6 Memory Management

CONTAIN employs a dynamic memory allocation scheme whereby most of the information required for the calculations is stored in four large arrays, known as the H, IH, OH, and LH arrays. The H array contains real data, the IH array holds integer data, the OH array

holds character data, and the LH array holds logical data. Together they can be referred to as the H arrays.

To access the data stored within the arrays, CONTAIN uses a two-level pointer scheme consisting of global and cell-level pointers. The organization of the pointers corresponds to the physics and engineering models in CONTAIN. Figure 2-1 illustrates a typical layout of the H array. As shown in this figure, CONTAIN first assigns the storage space for the global models. These models include the default or user-defined atmosphere materials, flow information, FP element information, and aerosol global parameters. After the permanent space is allocated for the global models, CONTAIN assigns permanent data space for each cell within the problem. Typically, each permanent cell space contains a number of spaces for each of the cell-level models. For example, as illustrated in Figure 2-1, the spaces for the cell models include FP hosts, atmospheric properties, lower cell model parameters, external source tables, and heat structure information.

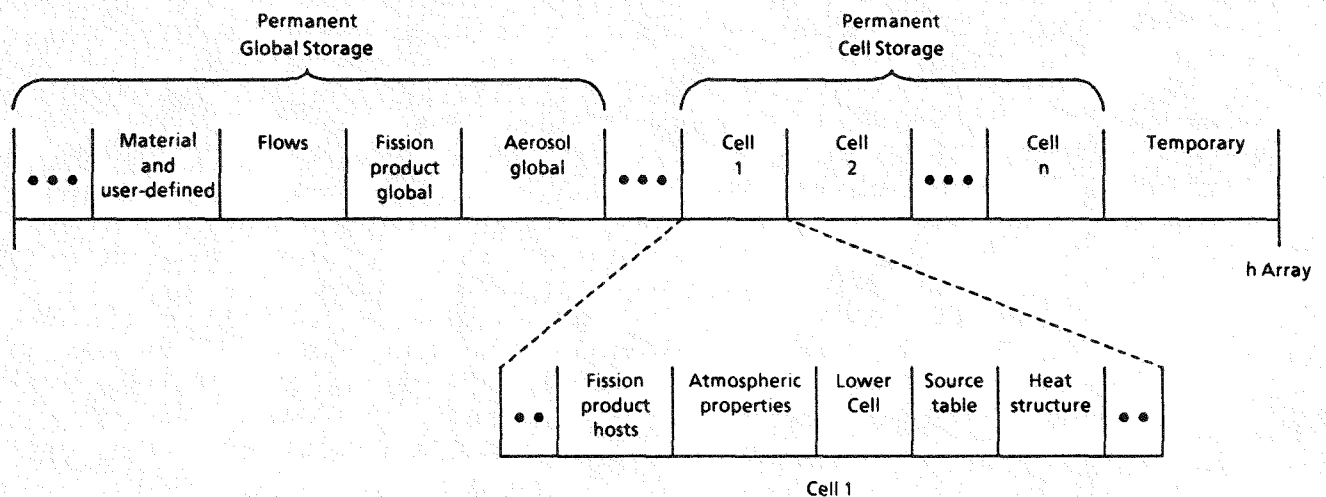


Figure 2-1. Problem Size-Dependent Data Structure

Beyond the permanent space required by the problem, the remainder of the space in the H arrays is designated as temporary space for global and cell models. Temporary space is allocated as needed by a model, and then returned at the completion of the model. Typical temporary variables include storage matrices for the flow model, LC to UC interface arrays, and working space for the built-in Runge Kutta integrator.

2.7 The Reference Cell

As mentioned earlier, CONTAIN makes use of the reference cell concept for cell-level processing. This has implications in memory management. At the beginning of cell-level processing, data from the H arrays are loaded into a collection of "reference cell" variables. These variables consist both of pointers to cell-level

arrays and of scalar state variables such as cell volume and pressure. Because properly addressing the H arrays is a somewhat cumbersome task, the reference cell variables make cell-level processing easier. When calculations for the reference cell are completed, the variables are unloaded by copying them back to the H arrays.

One consequence of the "reference cell" memory management is that cell-level information for only one cell at a time needs to be in central memory. This feature, together with the dynamic memory allocation scheme, greatly reduces memory requirements, allowing small memory computers to run realistic problems that would otherwise not fit into 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 quite feasible.

2.8 Timestep Control

CONTAIN has four different types of calculational timesteps. Two of these, the system (or global) timestep and the cell timestep, are primarily under user control. The third type, the integration 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 maximum system and cell timesteps are specified through input. 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 that CORCON has advanced.

Figure 2-2 presents the overall calculational flow diagram of CONTAIN. The cell timestep Δt_c controls how far each model is advanced with each pass through the cell loop. Likewise, the system timestep Δt_s controls how far each model is advanced with each pass through the global loop. Note that both Δt_c and Δt_s can be modified at the beginning of each pass through their respective loops. Furthermore, the cell timestep can be controlled by the user to be different for different cells.

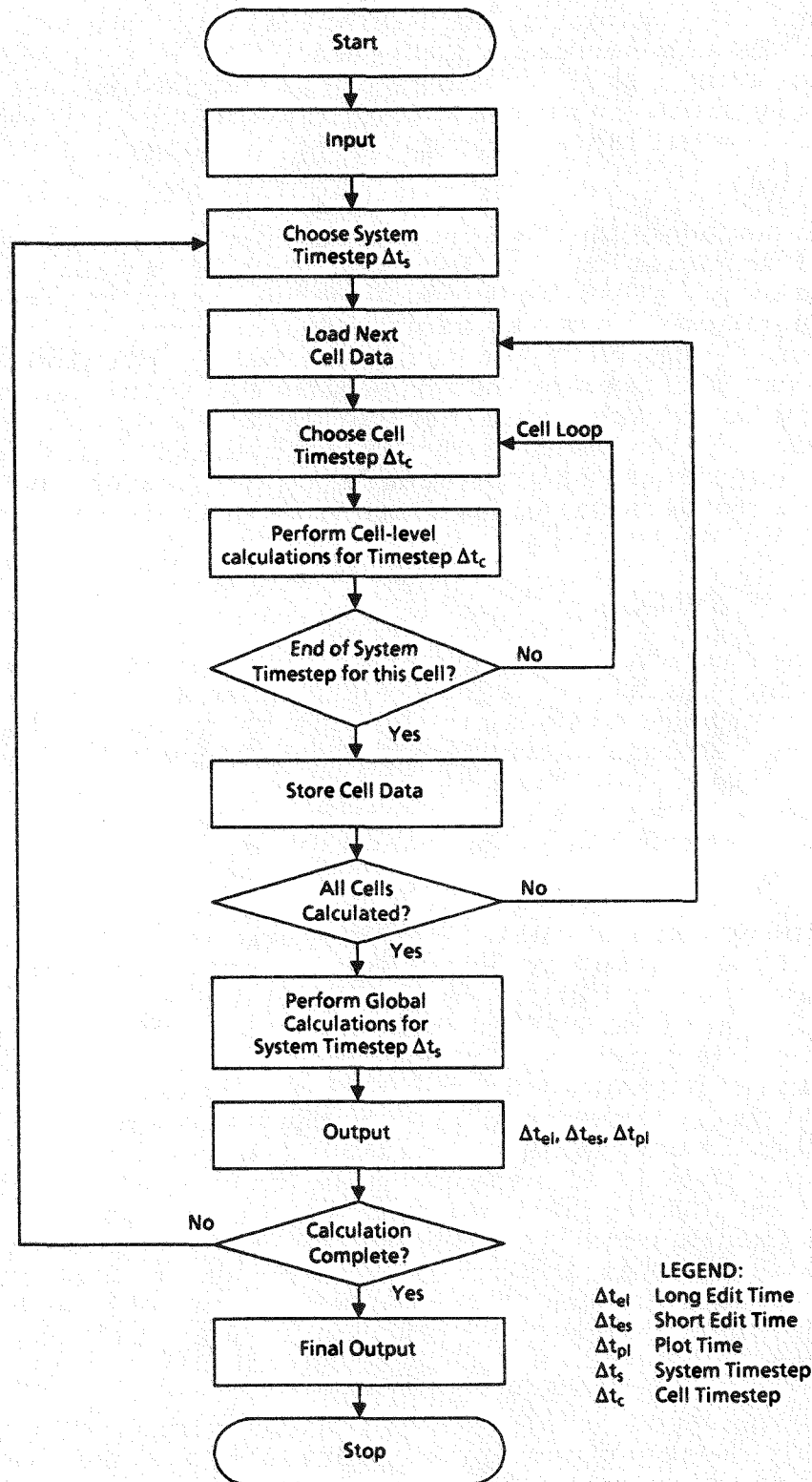


Figure 2-2. Overall Flow Diagram of CONTAIN

Not shown in Figure 2-2 are the timesteps controlling the individual models. Each model has its own internal timestep Δt_{in} , which controls the frequency at which fundamental variables owned by the model are updated for internal use. Many cell-level models simply use the cell timestep for Δt_{in} , and some of the global-level models use the system timestep for Δt_{in} . However, other models use an integration timestep, such as a Runge-Kutta timestep, which is calculated automatically depending on the error tolerances specified or the stability requirements for the model.

Table 2-1 shows the types of timesteps used by each of the major models in CONTAIN. The internal timestep Δt_{in} is the timestep used by the model for internal calculations. 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, as shown in this table, determines the frequency with which the variables and interface arrays are updated for use outside the model.

Table 2-1
Integration and Timesteps Used Within Various CONTAIN Models

<u>Model</u>	<u>Internal Timestep</u>	<u>Integration Method</u>	<u>Interface Timestep</u>
Flow/Thermodynamics	Convection	Implicit	System
	Runge-Kutta	Explicit	System
Aerosol Processes	Runge-Kutta	Explicit/ Closed Form	System
FP Decay	System	Closed Form	System
LC Conduction	Cell	Implicit	Cell
Heat Structures	Cell	Implicit	Cell
ESFs	Cell	Explicit	Cell

In addition to the calculational timesteps described above, CONTAIN makes use of other timesteps that control the frequencies of various types of outputs. These are the long edit timestep Δt_{el} , the short edit timestep Δt_{es} , and the plot timestep Δt_{pl} . The guidelines and input requirements of these timesteps are described in the CONTAIN User's Manual [Mur89].

3.0 THERMODYNAMICS AND INTERCELL FLOW

The flow between cells in CONTAIN is handled by the atmospheric intercell flow model. All movement of hydrodynamic gases and other materials that do not participate in the atmosphere thermodynamics (such as aerosols, gaseous FPs, and condensed phase atmospheric materials other than water) is done at the global level of the calculations. (See Section 2 for the levels of calculations in CONTAIN.) CONTAIN currently has two types of flow paths, the regular flow path and the engineered vent. The engineered vent allows the user to model more than one flow path between cells and provides additional flexibilities in modeling the flow through a flow path. The suppression pool vent in BWRs is a special flow path defined independently of engineering vents.

The flow between cells is handled by one of two flow options: implicit or explicit. The implicit flow option is preferred because of its calculation efficiency. The use of the implicit flow option will be described in this section and that of the explicit flow option in Appendix C. Either option may use one or more of three flow models in CONTAIN: inertial, quasi-steady, and critical flow. The inertial and quasi-steady flow models are used in calculating the convection of hydrodynamic gases between cells. Critical flow is used to ensure that the flow does not exceed the physical limit of certain geometries (such as an orifice).

An additional feature of CONTAIN is a generic model of the BWR suppression pool thermal-hydraulics. Vent clearing, gas venting and liquid overflow are handled by this feature.

The implicit flow option calculates the thermodynamic pressure within a cell simultaneously with flow. Implicit pool boiling is calculated within the implicit flow option. An exception occurs when it is determined that the pool will boil dry in the next timestep at which time the pool boiling is treated explicitly. Of course, the pool boiling is treated explicitly when the explicit flow option (Appendix C) is used.

Section 3.1 describes the CONTAIN flow path types and Section 3.2 discusses the implicit flow option. The thermal-hydraulics and flow models are described in Section 3.3. Section 3.4 presents the method of calculating the self-consistent thermodynamic state for the implicit flow option. Section 3.5 discusses the suppression pool vent thermal-hydraulics, and the intercell flow of nonhydrodynamic gases in the atmosphere. Section 3.6 describes the intercell flow as a function of the mass flow rate calculated by the flow models for the nongas components such as aerosols, gaseous FPs and user-defined materials.

3.1 Flow Path Types

In CONTAIN, two types of flow path options exist, regular and engineered vent. The regular flow path is set up so only a single flow path can be specified between two cells; multiple flow paths

between two cells are not possible. The engineered vent has all the attributes of the regular flow path and allows greater flexibility in designating multiple flow paths. Thus, the engineered vent is the preferred flow path option for most problems.

Figure 3-1 illustrates some aspects of the regular flow path connection options used in CONTAIN. Flow can occur between two physically adjacent cells through their common areas, as between cells 1 and 2 and cells 3 and 4. Flow paths can run between separated areas through connectors (such as a pipe, a duct, or possibly a cable room) as is shown between cells 1 and 4 and cells 2 and 3. Thus, flow paths can connect nonconsecutively numbered cells. In addition, for regular flow paths, the flow area as a function of pressure may be specified through tables. Also, constant slow rates can be specified in the user-specified slow rate options.

Figure 3-2 illustrates two aspects of the engineered vent flow option. In contrast to the regular flow path, the engineered vent can model two or more parallel flow paths (Figure 3-2a), as would occur between containment rooms having multiple connecting vertical cable riser ducts or horizontal cable conduits. As shown in Figure 3-2b, the engineered vent, like the regular flow path, can be tailored to user-specified conditions, such as, a time-dependent opening of an orifice in a pipe connecting two cells. By employing the different flow paths available, a detailed flow configuration can be modeled. Figure 3-3 illustrates an 18-cell CONTAIN model for a PWR containment.

The engineered vent model provides more alternatives for modeling flow than does a regular flow path. For example, even though the engineered vent model is available only with the implicit option, its vent flow area as a function of pressure difference ΔP can be calculated (a) explicitly, with the ΔP -dependent area based on the ΔP at the beginning of the timestep, or (b) implicitly, with the ΔP -dependent area based on the ΔP at the end of the timestep. However, the implicit representation requires more central processing unit time. This option allows the modeling of one-way doors and liquid heads in the flow path. As another example, the user can specify either the mass or volumetric flow rate as a function of time.

User-input specifications and UC geometry information are required when vents are employed. The user-supplied irreversible flow loss coefficient along with other user-supplied information, such as opening and closing times, is used to calculate mass flow rates between cells through the vent. The gas flow calculated by the engineered vent interacts with UC models, such as the atmospheric mass and energy balance model, and couples with the implicit flow option.

The BWR drywell to wetwell suppression pool vent is a special type of flow path, used to limit the BWR containment pressures under

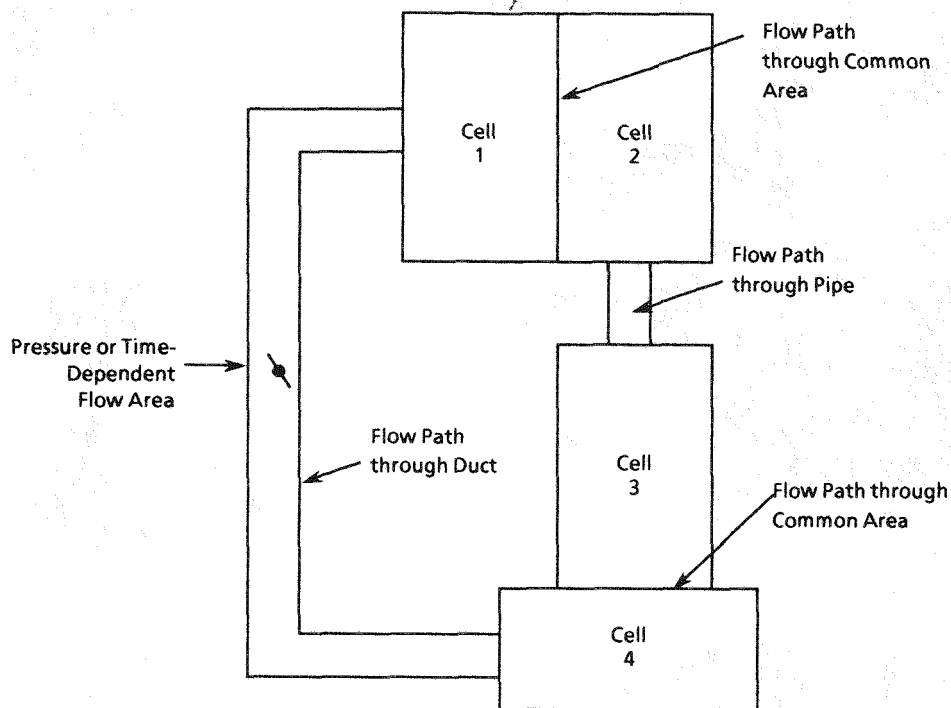


Figure 3-1. Example of Regular Flow Path Connectivity

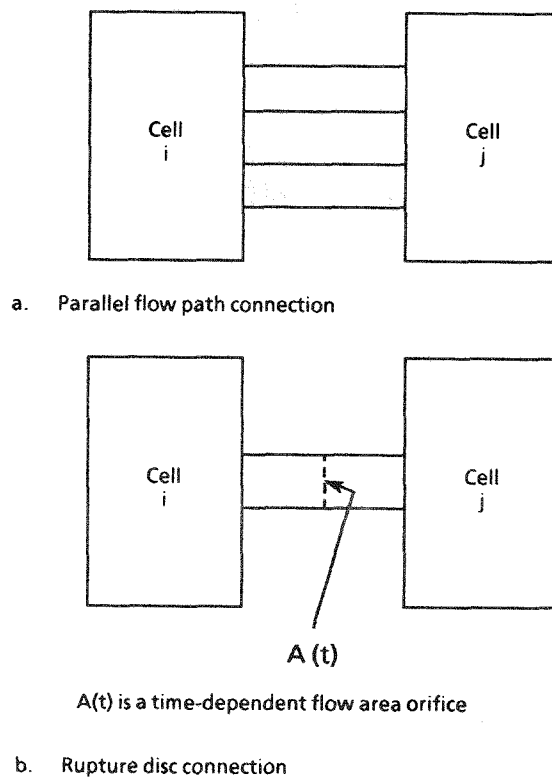


Figure 3-2. Examples of Engineered Vent Flow (a) Parallel Flow Path Connection, (b) Rupture Disc Connection

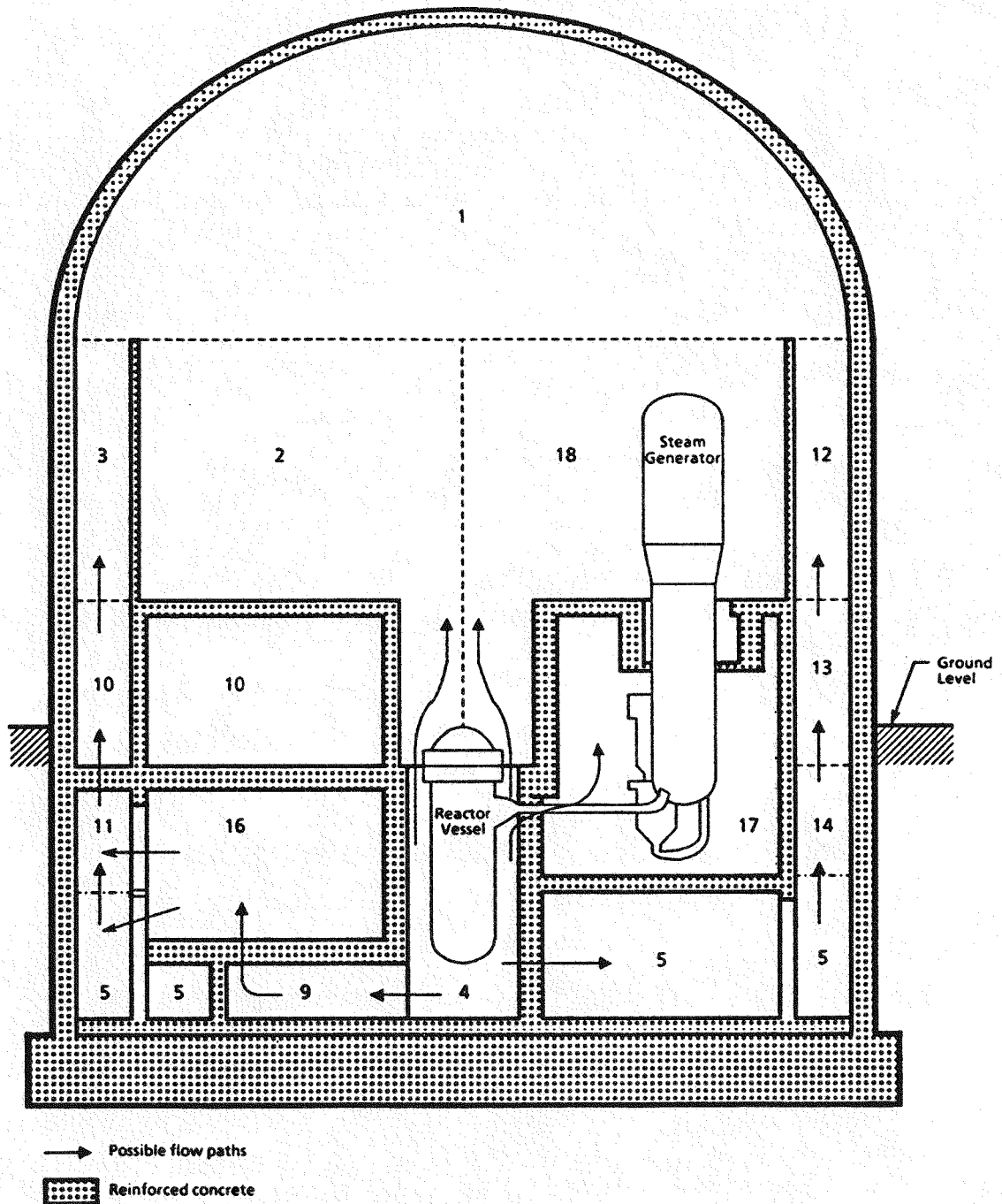


Figure 3-3. PWR Containment Building Reduced to a Configuration of 18 Interconnected Cells

accident conditions. Note that 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. The engineered vents and suppression pool vent may be used only with the implicit flow option.

The flow equations in Section 3.3 that are applicable for both regular flow paths and engineered vents will be discussed in terms of the mass flow between cell i and cell j , W_{ij} . W_{ij} is the total noncondensable gas and condensable material mass flow rate from i to j . (For the flow in the suppression pool vent, W_{ij} should be interpreted as the flow entering the pool.)

3.2 Implicit Flow Option

3.2.1 Trial Pressures

The implicit flow option solves for the pressures P_i in cell i at the end of each flow timestep in a self-consistent manner for all cells designated by the user as implicit. (These cells are the first N_{imp} cells in the problem. In practice, only environment cells of volumes greater than 10^8 m^3 should be excluded from the implicit solution scheme.) These implicit, self-consistent pressures, rather than the explicit, or beginning of timestep, pressures are used to calculate the flow rates between cells for the timestep. The implicit pressures are also used to calculate the boiling rates of pools and the rate of saturation of gas in suppression pool vent flow when the implicit flow option is invoked. When the implicit solver is used, the pressures P_i for the first N_{imp} cells i should be taken to be trial pressures in the discussions to follow.

The implicit pressures are calculated in a self-consistent manner. In the self-consistent solution scheme, a set of trial pressures for cell i , sometimes referred to in the following as $P_{tr,i}$, is used to evaluate the flow, boiling, and saturation rates. The latter rates determine the mass and energy present in each of the cell atmospheres at the end of the flow timestep and thus determine the endpoint thermodynamic state in each of the cells, as discussed in Section 3.4.1. The trial pressures are compared to the thermodynamic state pressures in each of the cells. As discussed in Section 3.4.2, the trial pressures are iterated until the pressure difference, or residual, given in Equation (3-25) becomes less than the error tolerance P_{err} specifiable by the user. In the discussion that follows, P_i should be taken to be the trial pressure for the first N_{imp} cells.

3.2.2 Implicit Flow Timestep Control

The accounting for intercell flow is based on an integration that incrementally advances the timestep to the system timestep Δt_g . To do this integration, an integration timestep, or the flow timestep, Δt_f is selected automatically to span Δt_g . Figure 3-4 illustrates the logic of this calculation.

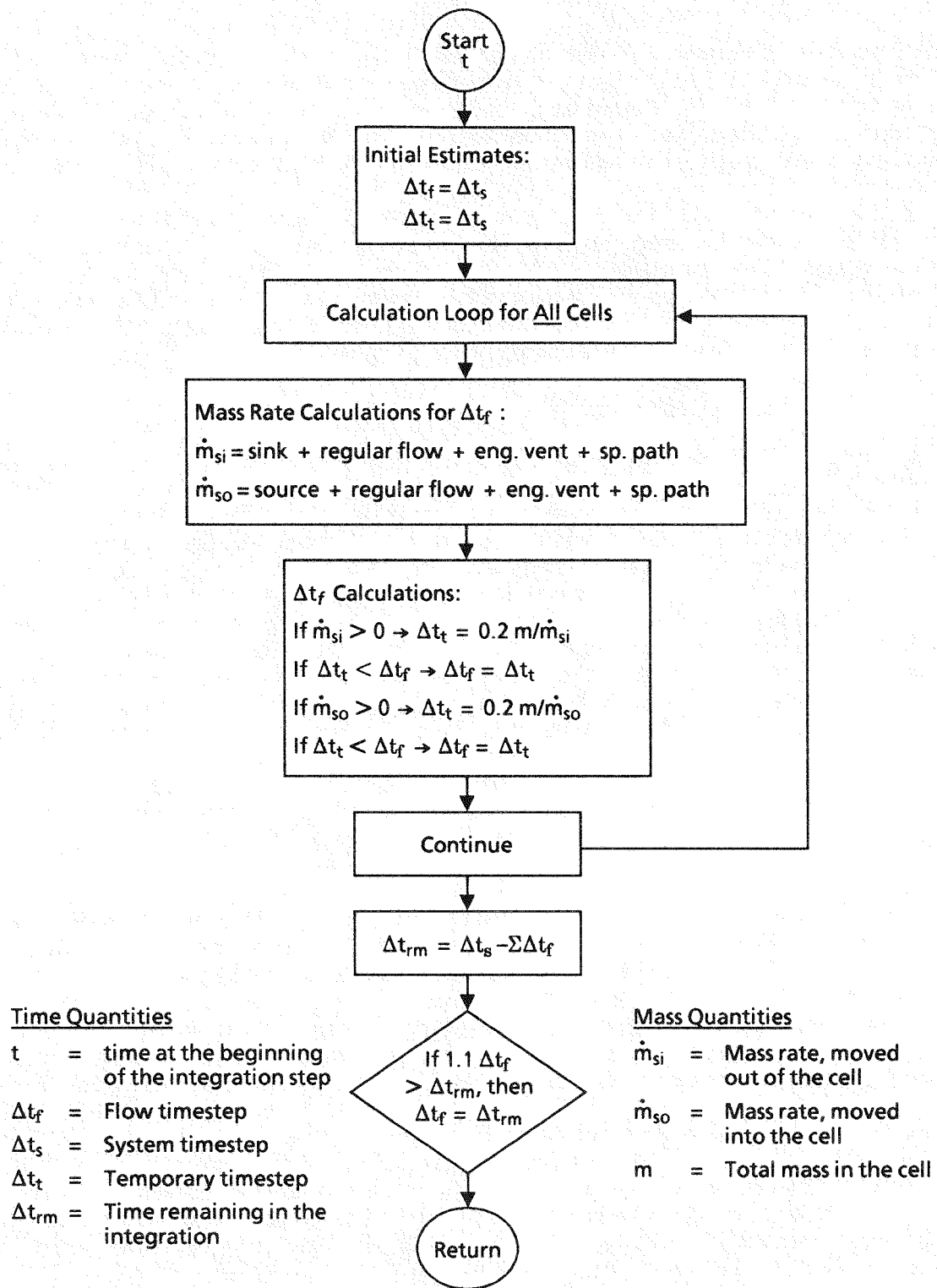


Figure 3-4. Flow Timestep Calculation Logic

For the implicit flow option, the determination of Δt_f is done internally. Figure 3-4 shows a flow diagram for this determination. The calculation of Δt_f is based on both inflow and outflow as well as on both initial and extrapolated flow conditions. Basically, both the flow rates of the hydrodynamic mass going into ($\dot{m}_{so}$) and moving out ($\dot{m}_{si}$) of a given cell are used to determine the size of Δt_f . Δt_f is selected to ensure that the inventory in a cell does not change (through flows or sources) by more than 20% in total mass during a Δt_f . Both the initial condition (at the beginning of the integration) and the extrapolated condition (during integration) are used. The final check ensures that the Δt_f calculated does not exceed the integration time interval. Once this check is satisfied, a Δt_f value is passed back to the flow calculation.

The actual integration for the implicit flow option is performed, once the Δt_f determination is done, see Figure 3-5. If the abort call in the implicit flow option is initiated, the existing Δt_f will be reduced by half. Then the calling sequence to the implicit flow option is repeated. After Δt_f has been reduced by a factor of eight, the implicit flow option is simply aborted. If this option is not aborted, the integration continues until Δt_s is achieved. Then the processes for the next Δt_s will be performed.

3.3 Thermal-Hydraulics

The CONTAIN computer code uses a multicompartment configuration that allows an arbitrary arrangement of control volumes (cells) and flow path connections. CONTAIN is limited by the inherent restrictions of a lumped parameter treatment in that momentum is not stored in control volumes and the complete Navier-Stokes equation is not represented. In CONTAIN, the flow of gases is derived from the acceleration flow with the option of being quasi-steady. A critical flow limit is used. The flow in a flow path can be calculated in three different ways in CONTAIN:

- The flow can 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 method, known as the inertial flow model, is available with either the implicit or explicit (Runge-Kutta) integration method. The flow is modeled as turbulent with critical flow limits on the flow rate when used with the implicit method. The flow is modeled as turbulent and noncritical when used with the Runge-Kutta method.
- The flow can 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 method 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

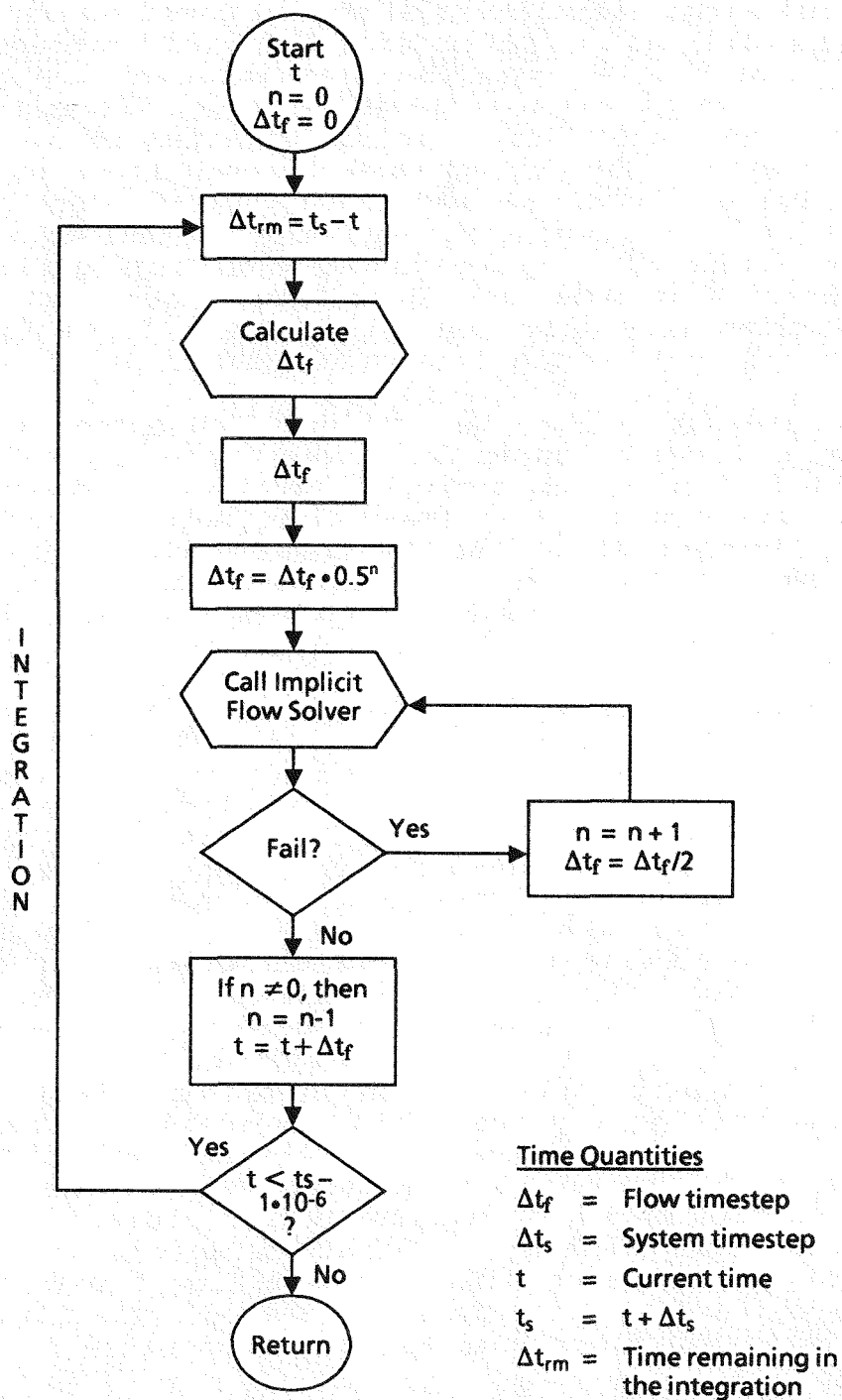


Figure 3-5. Timestep Control in the Implicit Intercell Flow Option

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 flow option. However, for some special flow paths, the implicit flow option may use a quasi-steady flow model.

- Finally, the flow can be set to a user-specified mass flow rate or a volumetric flow rate independent of the pressure difference.

Section 3.3.1 describes the buoyancy modeling and limitation within the flow models. Section 3.3.2 discusses the mass flow models, including the types of mass sources/sinks. Section 3.3.3 presents the calculations of energy due to flows and gravitational effects and sources/sinks.

3.3.1 Buoyancy

Mass buoyancy because of the gravitational or density effect only pertains to the flow equations used with the implicit flow option. The effect of gravitational head within each cell and the acceleration due to gravity in a flow path can be described as follows.

If one considers two cells, i and j , connected by a flow path (see Figure 3-6), the gravitational head $g \rho_i (H_i - H_1)$, for the difference in elevation between the center of cell i and the end of the flow path attached to i , is based on the cell gas 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 of the flow path attached to j , is based on the gas density ρ_j in cell j . The gravitational head developed within the flow path $g \rho_a (H_1 - H_2)$ is based on the average of the densities of the two cells $\rho_a = (\rho_i + \rho_j)/2$.

The pressure effect resulting from the gravitational head within each cell and the acceleration because of gravity in the flow path is

$$\Delta P_{ij,g} = g \rho_i (H_i - H_1) + g \rho_a (H_1 - H_2) - g \rho_j (H_j - H_2) \quad (3-1)$$

Note that the use of the average, rather than donor, density precludes the modeling of certain effects, such as siphoning, that may not be obvious. These effects, important for liquid flow, are believed to be minor effects for gas flow. The user is allowed some flexibility in modeling the effect of gravity (that is, with H_1 , H_2 , H_i , and H_j). It should be noted that Equation (3-1) is a simplistic first-order approximation. Second-order (and higher-order) effects resulting from the variation in density within a cell because of gravity are, in general, not accurately treated by Equation (3-1).

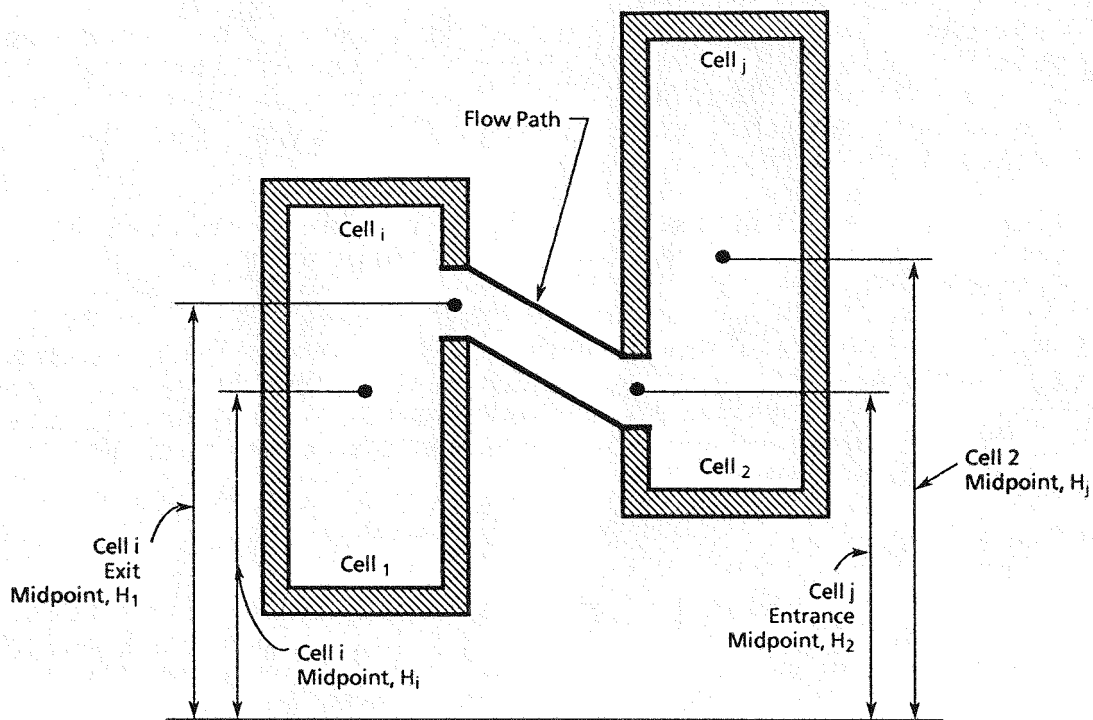


Figure 3-6. Elevations of Cells and Flow Path Ends to Calculate Gas Gravitational Head Effects

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 available with a lumped-parameter code. The first-order effect is 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 generally 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 caused by conditions such as hot spots within one cell.)

If the density ρ is assumed to vary as $\rho \approx \rho_0 (1 - C H)$, where C is a constant, then it can be shown that the additional term

$$\Delta G_{ij} = - \frac{1}{2} C \rho_0 g \left[(H_i - H_1) (H_i - H_2) - (H_j - H_1) (H_j - H_2) \right] \quad (3-2)$$

should appear on the right of Equation (3-1), when second-order effects in H are correctly treated. Note that C in Equation (3-2) is $M g / R T$ for isothermal flow or is $M g / \gamma R T$ for adiabatic flow, assuming an ideal gas. (M is gas molecular weight, R is the universal gas constant, T is the temperature, γ is the ratio of specific heats, and g is the acceleration of gravity.) In Equation (3-2), ρ_0 is the gas density corresponding to zero height. Note that this additional term, given by Equation (3-2), vanishes if the flow path ends are specified to be at the cell center elevations ($H_1 = H_i$, $H_2 = H_j$).

3.3.2 Mass and Mass Components

This section describes the models used to determine the total gas flow rates of the hydrodynamic gases, which also transport aerosols and gaseous FP. The intercell flow models described include the inertial, quasi-steady state, and choked flow models. The use of the total mass flow rate of the gases W_{ij} is shown in Table 1-2.

The subsections that follow describe the flow models available in CONTAIN and the mass sources and sinks that contribute to intercell flow. Although the descriptions focus on the implicit flow option, the majority of the flow models and concepts may also be applied to the explicit flow option described in Appendix C. Note that the user may specify flow rates directly for both regular flow paths and engineered vents. User-specified constant mass flow rates or volumetric flow rates are allowed for regular flow paths, whereas time-dependent rates are allowed for engineered vents.

3.3.2.1 Inertial Flow Model. In the majority of flow situations, the inertial flow model is used. This model takes into account the inertia of the gas in the flow path, as well as the irreversible flow losses. If a flow path is opened suddenly at a fixed pressure difference, the fluid inertia delays the buildup of the flow rate to the steady-state value. When 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.

The inertial flow model used in CONTAIN is a simple one-dimensional momentum (acceleration) equation for turbulent flow as follows (see also Table 1-1):

$$\frac{dW_{ij}}{dt} = \left[\Delta P_{ij} - \frac{C_{FC} |W_{ij}| W_{ij}}{\rho_{ij} A_{ij}^2} \right] \frac{A_{ij}}{L_{ij}} \quad (3-3)$$

where

ΔP_{ij} = driving pressure difference (Pa),
 C_{FC} = irreversible flow loss coefficient (dimensionless),
 ρ_{ij} = gas flow density (kg/m^3),
 A_{ij} = flow path area (m^2), and
 L_{ij} = inertial length (m) of the path.

The quantities A_{ij} and L_{ij} are specified by the user in the input.

ΔP_{ij} in Equation (3-3) is defined as

$$\Delta P_{ij} = P_i - P_j + \Delta P_{ij,g} \quad (3-4)$$

where

P_i and P_j = the trial pressures of cell i and j to be determined by the flow solver, respectively (Pa),
 and
 $\Delta P_{ij,g}$ = pressure difference due to gravitational effect, defined by Equation (3-1).

The irreversible flow loss coefficient C_{FC} is also input by the user on an order of unity that is typically determined empirically. C_{FC} , as used here, relates to discharge coefficients (C_D) and flow loss coefficients (K_{FL}). Specifically, Reference Flo79 has

$$C_{FC} = \frac{1}{2C_D^2} \quad (3-5)$$

and Bir60 and Kay64 have

$$C_{FC} = \frac{K_{FL}}{2}$$

Equation (3-3) was derived by considering a cylindrical cell slug of uniform density gas, being accelerated by a pressure differential (ΔP). The equation accounts for inertia effects and the effects of irreversible frictional flow losses.

The first-order nonlinear differential equation described in Equation (3-3) is solved by using the finite difference numerical method in the form:

$$\frac{W_{ij}(t + \Delta t_f) - W_{ij}(t)}{\Delta t_f} = L \Delta P_{ij} - \frac{L C_{FC} [W_{ij}(t + \Delta t_f)]^2}{\rho_{ij} A_{ij}^2} \quad (3-6)$$

where

$$L = A_{ij}/L_{ij}, \text{ and} \\ \Delta t_f = \text{flow timestep(s)}.$$

To solve for $W_{ij}(t + \Delta t_f)$ for a given $W_{ij}(t)$, Equation (3-6) can be rewritten and rearranged as

$$W_{ij}(t + \Delta t_f) + \frac{L \Delta t_f C_{FC} [W_{ij}(t + \Delta t_f)]^2}{\rho_{ij} A_{ij}^2} = L \Delta t_f \Delta P_{ij} + W_{ij}(t) \quad (3-7)$$

Then, $W_{ij}(t + \Delta t_f)$ can be determined from

$$W_{ij}(t + \Delta t_f) = \frac{\left[-1.0 \pm \sqrt{1 + 4 C_{FC} L \Delta t_f [W_{ij}(t) + L \Delta t_f \Delta P_{ij}] / (\rho_{ij} A_{ij}^2)} \right]}{2 C_{FC} L \Delta t_f / (\rho_{ij} A_{ij}^2)} \quad (3-8)$$

ρ_{ij} in Equation (3-8) for the explicit flow option, described in Appendix C, is taken as $(\rho_i + \rho_j)/2$. In the implicit flow option, ρ_{ij} is taken as the donor cell density (ρ_i or ρ_j). To determine the donor cell, the sum $L \Delta t_f \Delta P_{ij} + W_{ij}(t)$ is used. If this sum is > 0 , cell i is the donor cell. The definition of the pressure difference ΔP_{ij} depends on the user options. (See Equation (3-1) and Equation (3-4) for the user-specified variables.) For the explicit flow option, ΔP_{ij} is simply the difference in the cell pressure $P_i - P_j$. (The cell pressure is interpreted as the mean pressure in the cell or the pressure at its center of mass.) For the implicit flow option, ΔP_{ij} as shown in Equation (3-4) is the cell pressure difference and the gravitational head associated with the flow path opening (see Section 3.3.1).

3.3.2.2 Quasi-Steady Flow Model. The quasi-steady flow model is used in both the implicit and explicit flow options. However, this flow model is largely used with the explicit flow option described in Appendix C. The implicit flow option uses this model for the

engineered vent with the reversible area-pressure table option and the suppression pool gas vent flow.

The basic assumption of the quasi-steady flow model is that the flowing gas inertia is negligible. The mass flow rate is calculated by neglecting acceleration, that is, dW_{ij}/dt in Equation (3-3) is set equal to zero. Therefore, Equation (3-3) becomes

$$\Delta P_{ij} = C_{LFC} W_{ij} + C_{FC} |W_{ij}| W_{ij} / [\rho A_{ij}^2] \quad (3-9)$$

where

- ΔP_{ij} = pressure differential between cell i and cell j (Pa). ΔP_{ij} is determined as described in Section 3.3.2.1; for the implicit flow option, see Equation (3-4).
- W_{ij} = mass flow rate (kg/s) through flow path ij,
- ρ = upstream cell density for implicit flow option or average density for explicit flow option (kg/m^3),
- A_{ij} = cross-sectional flow area (m^2),
- C_{FC} = user-defined turbulent flow coefficient, and
- C_{LFC} = a quasi-laminar flow coefficient specified by the user as discussed in Appendix C as well as in the CONTAIN User's Manual [Mur89].

The first term on the right-hand side of Equation (3-9) is used for the explicit solver to prevent numerical problems. For the implicit flow option, this term is assumed to be zero. Therefore, Equation (3-9) can be used to solve for the mass flow rate in terms of ΔP_{ij} :

$$W_{ij} = \theta_{ij} \sqrt{|\Delta P_{ij}| \rho_{ij} A_{ij}^2 / C_{FC}} \quad (3-10)$$

where

- θ_{ij} = 1 and -1 for $\Delta P_{ij} > 0$ and $\Delta P_{ij} < 0$, respectively, and
- ρ_{ij} = gas density of the upstream cell (kg/m^3).

Note that Appendix C contains a discussion on the flow controls for handling of the quasi-steady flow in the explicit flow option. Also note that Section 3.5 gives a discussion on the modeling of flow using the quasi-steady flow model for the suppression pool vents.

3.3.2.3 Choked Flow Model. Choked or critical gaseous flow through flow paths or orifices occurs when the mass flow rate reaches a fixed value independent of the pressure ratio across the orifice or intercell connection.

The flow rate is choked at the flow exit to a fixed W_{ij} and is constrained to flow at the speed of sound. The critical flow rate $W_{ij,c}$ is given by

$$W_{ij,c} = \theta_{ij} A_{ij} \nu_{ij} [\gamma_u P_u \rho_u f_u]^{1/2} \quad (3-11)$$

where

- θ_{ij} = 1 and -1 for $P_i > P_j$, and $P_j > P_i$, respectively;
- P_i = cell pressure (Pa) in cell i;
- P_j = cell pressure (Pa) in cell j;
- ν_{ij} = vena contracta factor;
- γ_u = ratio of specific heat is c_p/c_v in the upstream cell u;
- P_u = cell pressure (Pa) in upstream cell u; and
- ρ_u = gas density (kg/m^3) in upstream cell u).

$$f_u = \left[\frac{2}{1 + \gamma_u} \right] (\gamma_u + 1) / (\gamma_u - 1) \quad (\text{dimensionless}) \quad (3-12)$$

Note that ν_{ij} is generally less than unity and is defined as the ratio of the minimum area intersected by the flow streamlines to the geometric cross-sectional area A_{ij} of the flow path [Lam45], that is, $\nu_{ij} = A_{\text{contract}}/A_{ij}$ (see Figure 3-7). The upstream cell in Equation (3-11) is determined to be cell i if θ_{ij} is 1, and cell j, if θ_{ij} is -1.

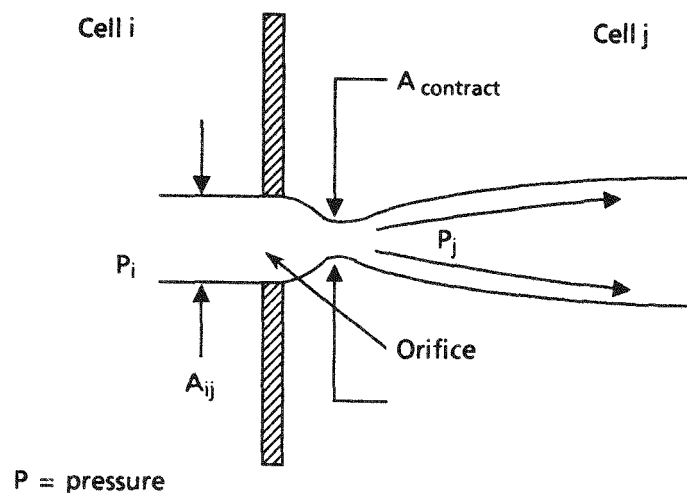


Figure 3-7. Choked Flow Representation

At any time, W_{ij} is given by the minimum of Equation (3-8), and Equation (3-11) or Equation (3-10) and Equation (3-11) for flow paths in which flow is calculated from cell pressure differences and flow area as shown below. Note that choked flow is not modeled for suppression pool gas vent flow.

$$W_{ij} = \left\{ \begin{array}{l} \min(W_{ij,i}, W_{ij,c}) \\ \text{or} \\ \min(W_{ij,qs}, W_{ij,c}) \end{array} \right\} \quad (3-13)$$

where

$W_{ij,i}$ = inertial flow calculated by Equation (3-8),
 $W_{ij,qs}$ = quasi-steady flow calculated by Equation (3-10), and
 $W_{ij,c}$ = choked flow calculated by Equation (3-11).

3.3.2.4 Explicit Sources and Sinks. There are a number of ways that the UC atmosphere of a cell receives or is depleted of masses. Many of the sources and sinks for mass in the cell are explicitly coupled to the cell and are part of the cell models. These sources and sinks $\dot{m}_{ex}$ include

$$\dot{m}_{ex} = (\dot{m}_{bn} + \dot{m}_{esf} + \dot{m}_c + \dot{m}_a + \dot{m}_{ud} + \dot{m}_{eb} + \dot{m}_{LC})/\Delta t_f \quad (3-14)$$

where

$\dot{m}_{bn}$ = the amount of combustible gases consumed, and the amount of product mass gain during a burn (see Section 6.2);
 $\dot{m}_{esf}$ = the amount of mass removed or added by an ESF system (see Section 6.5);
 $\dot{m}_c$ = the amount of mass condensed on or evaporated from structures (see Section 6.3);
 $\dot{m}_a$ = the amount of mass removed or added in the aerosol field (see Section 4);
 $\dot{m}_{ud}$ = user-defined sources/sinks;
 $\dot{m}_{eb}$ = the amount of mass evaporated at the explicit LC pool boiling, and
 $\dot{m}_{LC}$ = the amount of mass added or removed by the LC models.

$\dot{m}_{esf}$ in Equation (3-15) can be defined as a sum of the three major ESF systems (ICs, FCs, and CSs).

$$\dot{m}_{esf} = \dot{m}_{ic} + \dot{m}_{fc} + \dot{m}_{cs} \quad (3-15)$$

where

m_{ic} = vapor mass removed by the IC (see Section 6.5.2),
 m_{fc} = vapor mass condensed onto the FC (see Section 6.5.1),
 and
 m_{cs} = vapor mass removed/added by the CS (see Section 6.5.3).

Each term in Equation (3-14) is a cell model and, therefore, no intercell source/sink is considered in this equation. The mass source/sink terms in Equation (3-14) are handled by the interface models. The ESF models are described in Section 6.5.

The explicit pool mass evaporation only occurs when the implicit boiling source model determines that the remaining pool water will be boiled in the current timestep. The implicit pool boiling source is set to zero.

3.3.2.5 Implicit Sources (Boiling). The pool boiling in CONTAIN is calculated within the implicit flow solver (see Section 3.2), even though pool boiling is a part of the LC model. This is accomplished by calculating the amount of energy conducted to the pool to heat it beyond its saturation temperature at the cell pressure and transmitting it to the implicit solver. Appendix D presents a brief discussion of the implicit LC pool boiling model, and the detailed CORCON-MOD2 heat transfer correlations used in this model.

The amount of energy available for boiling in a single system timestep Δt_s is assumed to be transferred at a constant rate throughout this timestep. This is done with a factor calculated to estimate the mass and energy fraction associated with each flow timestep Δt_f :

$$F_{\Delta t} = \frac{\Delta t_f}{\Delta t_s} \quad (3-16)$$

The pool mass m_p is given by

$$m_p = m_{pi} + m_s(\Delta t_s) F_{\Delta t} - m_{b,i} \quad (3-17)$$

where

m_{pi} = initial pool mass (kg) at the beginning of Δt_s ,
 $m_s(\Delta t_s)$ = mass source from the explicit cell models during Δt_s (kg), [assuming $F_{\Delta t}$ is applied to $m_s(\Delta t_s)$], and
 $m_{b,i}$ = mass boiled from the pool as determined by the implicit flow solver (kg).

If zero pool mass is calculated, no pool energy calculation is performed. Otherwise, the pool energy is given by

$$Q_p = Q_{pi} + Q_s(\Delta t_s)F_{\Delta t} - Q_{b,i} \quad (3-18)$$

where

Q_{pi} = initial pool energy (J) at the beginning of Δt_s ;
 Q_s = energy (J) corresponding to m_s from the explicit cell models during Δt_s ; and
 $Q_{b,i}$ = energy (J) removed corresponding to $m_{b,i}$ and the specific enthalpy (J/kg) for saturated vapor.

To calculate the amount of mass boiling correctly during Δt_f , a saturation temperature T_{sat} corresponding to the trial pressure P_{tr} is calculated. The resulting T_{sat} is used for calculating the saturation enthalpy values used in the boiling mass calculations.

The total pool internal energy calculated by Equation (3-18) includes an accounting for the energy transferred from the LC pool boiling model. If the total pool internal energy exceeds the corresponding saturated condition based on the trial pressure, the excess energy will result in boiling of pool mass. In the equation form, the amount of pool mass boiled m_{br} in a given timestep is expressed by

$$m_{br} = \frac{Q_p - m_p h_\ell}{h_{vap} - h_\ell} \quad (3-19)$$

where

h_ℓ and h_{vap} = specific enthalpy (J/kg) of liquid and vapor, respectively, evaluated at the saturation condition corresponding to P_{tr} .

The corresponding energy going to the atmosphere because of boiling is given in Section 3.3.3.

3.3.3 Energies

In any thermal-hydraulic code, like CONTAIN, the conservation of energy in a cell must be satisfied. The amount of energy entering a cell from intercell flow and/or intracell sources (such as burn and decay heating) or user-defined source minus the amount of energy exiting the cell because of intercell flow and/or intracell sinks (such as condensation of coolant, ESFs) must be equal to the change of total internal energy for a given flow timestep Δt_f . The conservation of energy equation for a cell is given in Table 1-3. This conservation of energy equation is used to determine the thermodynamic state within the cell as described in Section 3.4.

In addition to intercell flow energy gain and loss, the internal energy balance for a cell requires knowing the energy sources and sinks within a cell as a result of intracell effect. The explicit cell models classified in this category are described in Table 1-3.

In addition to the explicit effects, the internal energy of cell i is affected by implicit boiling and defined as

$$Q_{i,boil} = m_{br} \cdot h_v \quad (3-20)$$

where

- m_{br} = the amount of boiled pool mass (kg) (calculation shown in Section 3.3.2.5), and
- h_v = specific enthalpy of vapor at saturation at the trial pressure (J/kg).

Many of the heating rate terms in the conservation of energy equation are described in other sections throughout this manual. For example, Section 5 describes the FP decay heat, whereas Section 6 describes the energy transfer rates of explicit cell models. The energy transfer associated with the BWR suppression pool vent is discussed in Section 3.5.

3.4 Self-Consistent Thermodynamic State

This section describes the iterations on cell temperature and pressure to estimate the thermodynamic state at $t + \Delta t_f$. The temperature iteration is done in the intercell flow model for each pressure iteration point. And the pressure iteration is done in the implicit flow model. A similar iteration scheme is described for the explicit flow option in Appendix C.

3.4.1 Temperature Iteration

Based on the amount of mass and energy in cell i as calculated in Section 3.3.2 and Section 3.3.3, a cell temperature is iterated implicitly. A 3-point secant iteration method is used to determine the temperature. This method requires three input pairs of temperature and the corresponding cell internal energy. One pair must correspond to a positive energy; one pair must correspond to a negative energy; and the last pair must be at an intermediate point. The internal energy function for this iteration is given by

$$f(T_i) = U_i(T_i) - U_i \quad (3-21)$$

where

- $U_i(T_i)$ = total internal energy (J) calculated based on cell temperature T_i ,

U_i = actual internal energy (J) for cell i, and
 T_i = an initial estimate of cell temperature used in the iteration (K).

T_i in Equation (3-21), in practice, is chosen to be close to the last known cell temperature (at the beginning of the timestep). U_i in Equation (3-21) is calculated as described in Table 1-3.

On the other hand, $U_i(T_i)$ in Equation (3-21) is calculated from

$$U_i(T_i) = \sum_k^{N_g} h_k m_k + (h_\ell - h_{\text{vap}}) m_\ell - R M_{o_g} T_i \quad (3-22)$$

where

h_k and m_k = specific enthalpy (J/kg) and mass (kg) of gas k in the atmosphere,
 N_g = number of gases in the cell i atmosphere, including the water vapor,
 h_ℓ and h_{vap} = specific enthalpy of water liquid and of vapor (J/kg),
 m_ℓ = mass of liquid water in the atmosphere (kg),
 R = universal gas constant (N-m/mole-K), and
 M_{o_g} = total moles of gases and water vapor (moles).

m_ℓ in Equation (3-23) is given by

$$m_\ell = m_{\text{wt}} - m_{\text{vap}} \quad (3-23)$$

where

m_{wt} = total water mass (kg) in the cell, and
 m_{vap} = actual vapor mass (kg) existing in the atmosphere at saturation conditions.

m_{vap} is calculated according to the ideal gas law as

$$m_{\text{vap}} = \frac{P_{\text{sat}} M_{o_{\text{vap}}} V_i}{R T_i} \quad (3-24)$$

where

P_{sat} = saturation vapor pressure at T_i (Pa),
 $M_{o_{\text{vap}}}$ = molecular weight of vapor (kg/mole), and
 V_i = volume (m^3) for cell i.

The objective of this temperature iteration is to find a cell temperature at which $f(T_i)$ in Equation (3-21) approaches zero.

3.4.2 Pressure Iteration

After the temperature iteration is completed as discussed above, a new value of cell temperature T_n is returned to the implicit flow solver to calculate a similar function for the pressure iteration in the implicit flow option:

$$f(P_{tr,i}) = P_{tr,i} - R M_o g T_i / V_i \quad (3-25)$$

where $P_{tr,i}$ = trial pressure (Pa) of cell i .

Using this equation, a pressure iteration scheme to solve for implicit (end-of-timestep) pressures was developed specifically for CONTAIN. It recognizes that pressure dependence in the problem is inherently nonlinear, and thus no attempt is made to use linear equation methods to solve Equation (3-25). Because the algebraically linearized form of this equation is not needed and all functional derivatives are evaluated numerically, it is a relatively simple matter to generalize the flow equations to include additional pressure-dependent processes. As a result, the original CONTAIN pressure iteration scheme was readily extended to include (a) the pool boiling and (b) the pool condensation/-evaporation effects in the flow of gas through BWR suppression pool vents. Thus, both of these processes are treated implicitly with respect to pressure.

The solution algorithm is based on a multidimensional secant method to solve the set of N_{imp} nonlinear simultaneous equations for $P_{tr,i}$ for each cell represented by Equation (3-25) [Bar65]. N_{imp} is the number of implicit cells. Because of its slow convergence, the original point relaxation method proposed for CONTAIN is not used.* The point relaxation method is used extensively for hydrocodes (as, for example, in Reference Tra84) because the number of nodes used in the application of these codes is typically much larger than the number of cells used with CONTAIN and a method such as the secant method would be prohibitively expensive. In contrast to CONTAIN, convergence is apparently not a problem with the point relaxation method for hydrocode applications, presumably because different equations are being solved. Fortunately, the CONTAIN cells are intended to be macroscopic volumes and thus relatively few are needed for a typical application.

An alternative to the secant method is the Newton-Raphson method. The latter method has the disadvantages of requiring a relatively large number ($N_{imp} + 1$ as opposed to 1) function evaluations per iteration and having the tendency to go into limit cycles. However, the secant method has the disadvantage of requiring management of the cluster of $N_{imp} + 1$ points in pressure space so

*Information supplied by W. A. Stark, Jr. and W. B. Rivard of Flow Sciences, Inc., 1984.

that they do not collapse into a singular configuration. (An example of such a configuration is a cluster in which the points are co-planar.) The possibility of a singular configuration is enhanced greatly in a typical containment problem by the fact that the pressure difference between cells with a relatively large flow area between them is typically many orders of magnitude smaller than pressure within the cells.

In the basic secant method, a cluster of $N_{imp} + 1$ points in pressure space are used to characterize the residual function surfaces. A linear approximation to the function surfaces is made to construct the surfaces from the $N_{imp} + 1$ function values. The point in pressure space corresponding to the simultaneous solution for the N_{imp} residuals within the linear approximation is then computed. This new point is used to replace the point in the original cluster with the largest norm, or root mean square, residual value. This process is repeated iteratively until sufficient accuracy with respect to the simultaneous solution is attained.

As shown in Figure 3-8, the secant method in CONTAIN has been extended to cope with a number of potential problems involving ways that the cluster can collapse to a singular configuration. Two ways CONTAIN addresses these problems are:

- (1) The first iteration is treated as a Newton-Raphson step (with numerical evaluation of function derivatives) if one is far from a solution and the first iteration corresponds to a better guess. Such a treatment prevents a large initial stepout from the original cluster.
- (2) Because of the typically large disparities of size or flow path areas between different cells, it is possible that part of the problem may be "solved" (for example, an isolated cell) before the rest. Because the cluster will become singular if the part of the problem that is "solved" is unnecessarily retained in successive iterations, the condition of a partial solution is detected by the solver.

As indicated in Figure 3-8, if a partial solution is detected, only a "reduced" problem is retained on successive iterations. As indicated also in this figure, the solver has been extended to cope with functions with a large increase in steepness near the zero of the function: if, on successive iterations, the residual for a cell increases by more than a factor of ten in magnitude and changes sign, the last step is bisected.

3.5 Boiling Water Reactor Suppression Pool Vent Thermal-Hydraulic Model

The BWR suppression pool vent thermal-hydraulic model includes a model for the clearing of water in the vents, a gas flow model, and a pool condensation/evaporation model. In the suppression pool vent clearing model, liquid levels in the wetwell, drywell, and

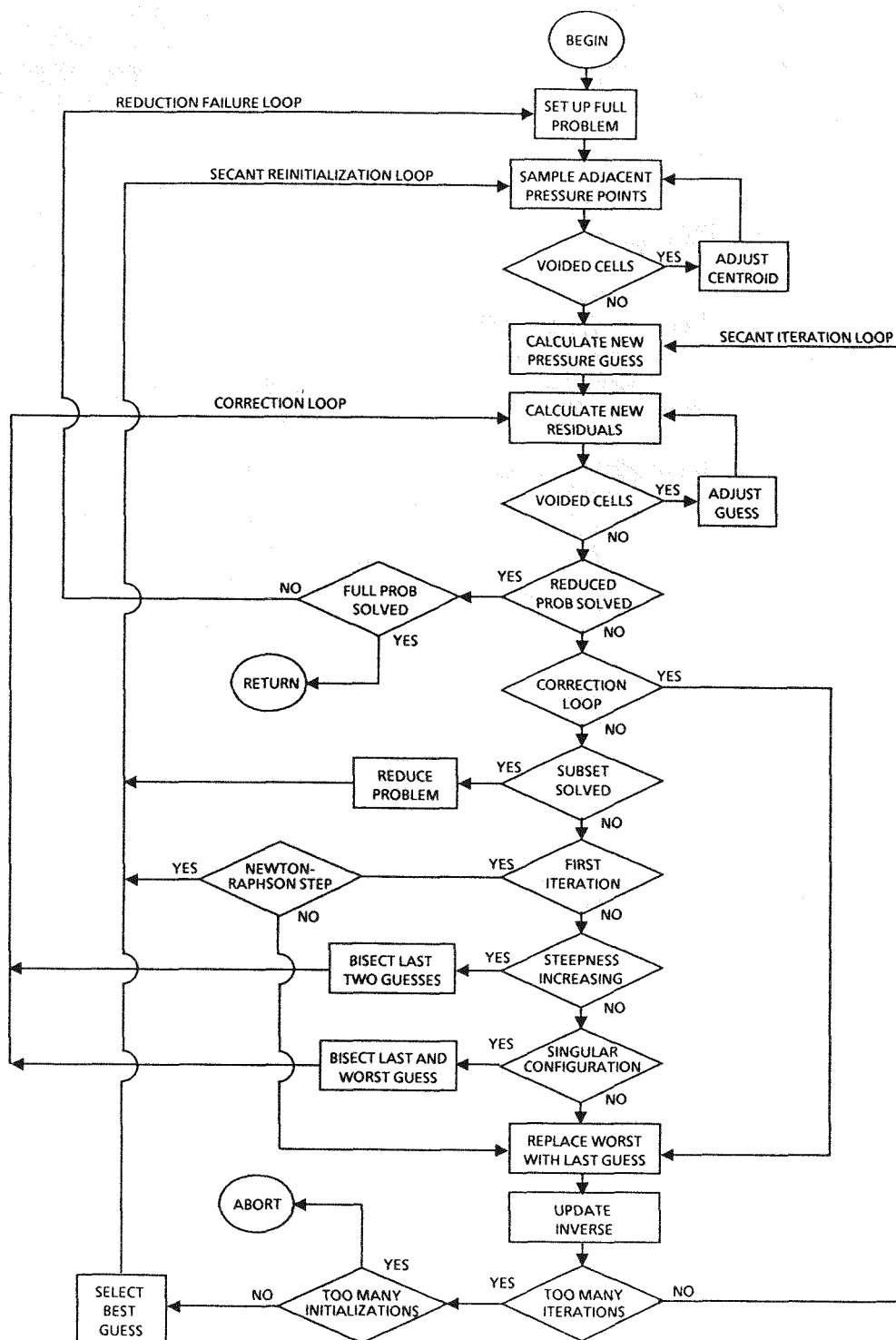


Figure 3-8. Cell Pressure Iteration Scheme for Implicit Flow Option

vent 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 level velocity calculated from gas pressure differences and liquid heads in both drywell and wetwell cells. A quasi-steady gas flow model is used to determine the suppression pool gas flow once the suppression pool vent is cleared. The energy and mass exchanges between the vented gas and the pool are calculated by assuming that the gas and pool temperatures equilibrate and the gas is 99% saturated with coolant vapor.

Note that if more than one vent is specified, 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 user-provided value of the difference in pressures required to barely open and to fully clear a single vent as the difference in pressures required to barely open the upper vent and fully clear the lower vent.

Section 3.5.1 describes the mathematical models used to calculate the suppression pool vent clearing time. Section 3.5.2 describes the mathematical models used to calculate the vent mass and energy transfer in the pool boiling model.

3.5.1 Vent Clearing Time

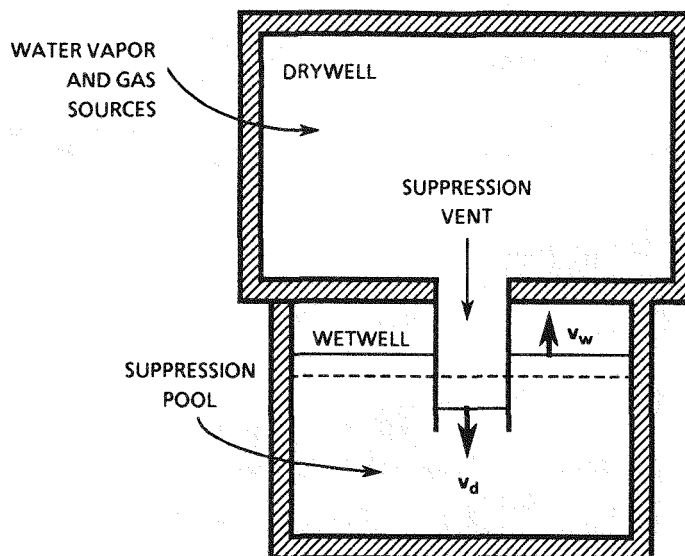
The suppression pool vent clearing time is calculated based on the time required for the liquid level on either side of the suppression pool to drop to the level at which the vent begins to clear. The equation for the liquid level velocity is based on the Bernoulli mechanical energy balance equation. (Figure 3-9 displays the liquid level velocities for the suppression pool of Mark I, Mark II, and Mark III BWR containments.)

Based on the Bernoulli equation,

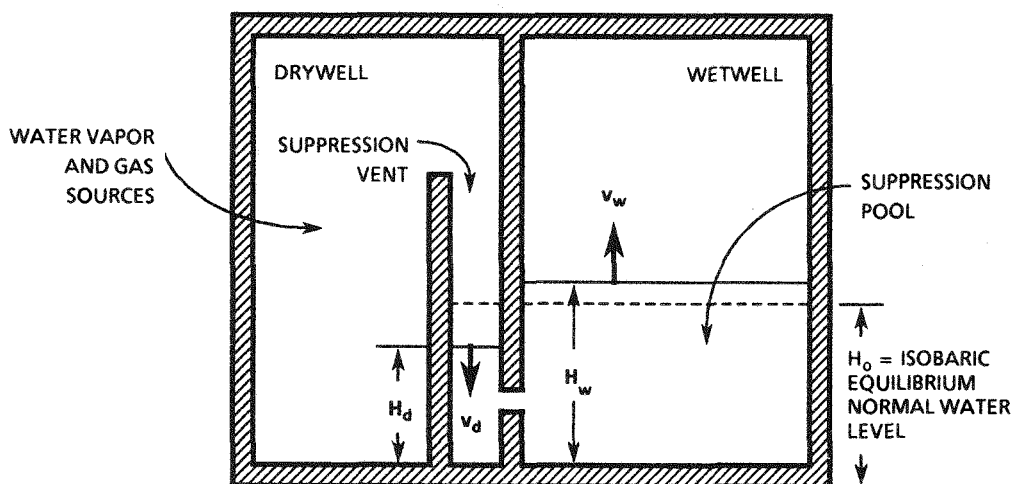
$$P_w - P_d + \rho_l g(H_w - H_d) + \frac{\rho_l (v_w^2 - v_d^2)}{2} + \sum \Delta P_L = 0 \quad (3-26)$$

where

- P_w = wetwell pressure (Pa);
- P_d = drywell pressure (Pa);
- v_w = wetwell pool rising or depressing velocity (m/s);
- v_d = drywell vent rising or depressing velocity (m/s);
- ρ_l = pool density (kg/m³);
- g = acceleration of gravity (9.8 m/s²);
- H_w = wetwell liquid level (m);



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.



Horizontal Vent System Schematic used to represent a Mark III. The dashed line represents the normal water levels; the solid line, the displaced levels.

Figure 3-9. Suppression Pool Thermal-Hydraulics. Note that only one vent is modeled and, therefore, the multiple vent Mark III can only be approximated.

H_d = drywell liquid level (m); and
 ΔP_L = irreversible loss term (N/m^2).

According to this relationship the amount of liquid depressed in the drywell vent should be equal to the amount of liquid risen in the wetwell, then $\beta v_d = v_w$, where β is the ratio of the drywell vent area to the wetwell pool area. By substituting this definition of v_w into Equation (3-27), the relation becomes

$$P_w - P_d + \rho_l g (H_w - H_d) + \rho_l (\beta^2 - 1) \frac{v_d^2}{2} + \Delta P_L = 0 \quad (3-27)$$

ΔP_L in Equation (3-27) can be rewritten as a function of flow. According to Reference Bir60, for flow from the drywell to the wetwell ΔP_L can be defined as

$$\Delta P_L = \frac{1}{2} \rho_l K v_w^2 \quad (3-28)$$

where K is the friction loss factor in the turbulent flow regime. For sudden expansion, $K = (1/\beta - 1)^2$ in respect to the downstream velocity. Therefore, by substitution, Equation (3-28) with respect to the definition of K and in terms of v_d becomes

$$\Delta P_L = \frac{1}{2} \rho_l (1 - \beta)^2 v_d^2 \quad (3-29)$$

and Equation (3-27) becomes

$$\Delta P_{dw} + g \rho_l \Delta H_{dw} + \rho_l \frac{v_d^2}{2} (\beta^2 - 1 + [1 - \beta]^2) = 0 \quad (3-30)$$

where $\Delta H_{dw} = H_w - H_d$, and
 $\Delta P_{dw} = P_w - P_d$.

For additional loss terms as identified by the user, another term should be added to Equation (3-30)

$$\Delta P_{dw} + g \rho_l \Delta H_{dw} + \rho_l \frac{v_d^2}{2} (\beta^2 - 1 + [1 - \beta]^2 + K_{dw}) = 0 \quad (3-31)$$

where

K_{dw} = user-defined additive irreversible loss coefficient for flow going from the drywell vent to wetwell.

If the flow goes from wetwell to drywell, then Equation (3-29) becomes

$$-\Delta P_{dw} - g \rho_L \Delta H_{dw} + (1 - \beta^2 + K_{wd}) \rho_L \frac{v_d^2}{2} = 0 \quad (3-32)$$

where

K_{wd} = user-defined additive irreversible loss coefficient for flow going from the wetwell to drywell.

The vent clearing time depends on the cell pressures and the initial liquid level in the drywell side of the suppression pool. It is also influenced by the overflow from the suppression pool, as can happen over the weir wall in a Mark III when the wetwell pressure is higher than the drywell pressure. Because CONTAIN tries to integrate the flow in a single pass, a very complicated logic has been built into the code to ensure that the proper mass is accounted for.

Equation (3-31) and Equation (3-32) are used to determine the level of the suppression pool in the vent (drywell side) at the end of the system timestep Δt_s . To avoid confusion and to gain simplification, let us use an $F = \beta^2 - 1 + (\beta - 1)^2 + K_{dw}$ for flow going from the drywell to wetwell, and an $F = 1 - \beta^2 + K_{wd}$ for flow going from wetwell to drywell. Note that each factor (F) represents a different flow direction.

Let us define

$$x = \hat{H}_d - H_o \quad (3-33)$$

where

H_o = the isobaric equilibrium level, is a constant over the timestep, and

$\hat{H}_d$ = the drywell level if overflow is neglected.

Therefore,

$$\frac{dx}{dt} = \frac{d\hat{H}_d}{dt} = -v_d \quad (3-34)$$

Because

$$H_o - \hat{H}_w = (\hat{H}_d - H_o)\beta, \quad (3-35)$$

where

$\hat{H}_w$ = wetwell level if overflow is neglected, then

$$\hat{H}_w = H_o - (\hat{H}_d - H_o)\beta \quad (3-36)$$

In terms of x , substituting the above definitions into Equation (3-34), and using the resulting v_d in Equation (3-31) gives

$$\frac{dx}{dt} = - \left[\frac{2[P_d - P_w + g \rho_l (1 + \beta) x]}{F \rho_l} \right]^{1/2} \quad (3-37)$$

Let us define

$$A = \frac{2(P_d - P_w)}{F \rho_l} \text{ and } B = \frac{2g(1 + \beta)}{F} \quad (3-38)$$

then, the integration of Equation (3-37) from x to x_{eq} is

$$\int_{x_o}^{x_{eq}} (A + Bx)^{-1/2} dx = - \int_t^{t+t_{eq}} dt \quad (3-39)$$

where

x_o = initial value of $\hat{H}_d - H_o$ at the beginning of the timestep,
 x_{eq} = final value at (non-isobaric) equilibrium position, and
 t_{eq} = time to attain such an equilibrium position from the initial position.

Therefore, the time to attain equilibrium t_{eq} from a nonequilibrium position x_o is

$$t_{eq} = - \left[\frac{2F[P_d - P_w + g \rho_l (1 + \beta) x_{eq}]}{\rho_l g^2 (1 + \beta)^2} \right]^{1/2} + \left[\frac{2F[P_d - P_w + g \rho_l (1 + \beta) x_o]}{\rho_l g^2 (1 + \beta)^2} \right]^{1/2} \quad (3-40)$$

Combining equations,

$$\rho_l g \hat{H}_d + P_d = \rho_l g \hat{H}_w + P_w \quad (3-41)$$

and

$$\hat{H}_d = H_o + x \text{ and } \hat{H}_w = H_o - \beta x \quad (3-42)$$

results in

$$x_{eq} = \frac{P_w - P_d}{(1 + \beta) \rho_l g} \quad (3-43)$$

By applying Equation (3-43) to the first term of Equation (3-40), we get

$$t_{eq} = \left[\frac{2F[P_d - P_w + g \rho_l (1 + \beta) x_o]}{\rho_l g^2 (1 + \beta)^2} \right]^{1/2} \quad (3-44)$$

Figure 3-10 displays various definitions to help in understanding the complicated logic behind the vent clearing calculation. At the beginning of the system timestep Δt_s , the code calculates the suppression pool area. Any pool sources added to the suppression pool are then determined. Readjustment of $\hat{H}_d$ and $\hat{H}_w$ is done so that $\hat{H}_d$ and $\hat{H}_w$ are bounded within H_v and H_{of} . H_v is defined as the vent clearing height and H_{of} is defined as the overflow height. If the isobaric equilibrium height (normal water level) $H_o < (H_v + 0.0001 \text{ m})$, then a bypass situation is assumed; the vent clearing calculation is bypassed; and the information is passed to the flow model with a flag indicating the bypass situation.

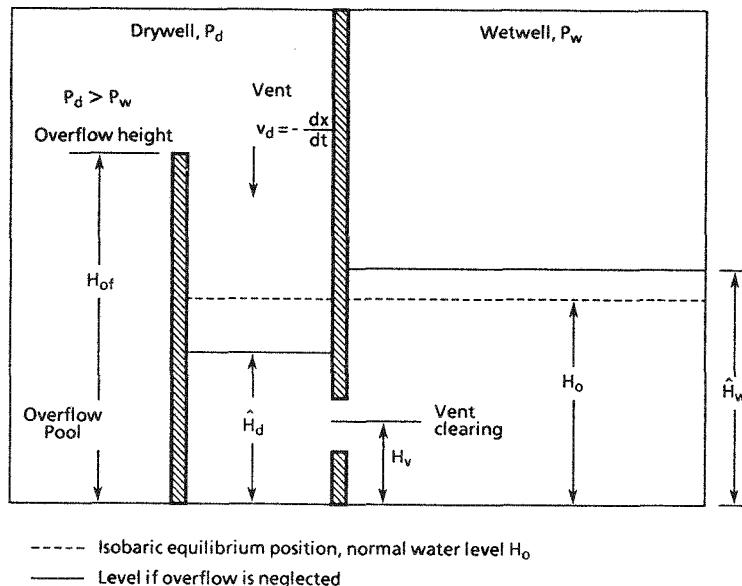


Figure 3-10. Detailed Definition of the Variables of the BWR Suppression Pool System (Mark III)

To compute the vent clearing time when $P_d > P_w$, Equation (3-44) is used. The time t_{eq} is the total time it takes to reach equilibrium from the initial water level. If this time is greater than Δt_s , that means equilibrium is not reached at the end of the timestep. However, if $H_v > x_{eq} + H_o$, the vent may clear before the end of the timestep.

To compute the duration of vent covering or vent clearing time t_{vc} , let us examine Figure 3-11 as an example. If $\hat{H}_d$ is above H_v , and $H_o < H_v$, then

$$t_{vc} = t_{eq} - t_{op} \quad (3-45)$$

where

t_{op} = time to achieve equilibrium starting at the vent opening height, and calculated by Equation (3-44), but with $x_o = H_v - H_o$.

Note that t_{op} is really fictitious because liquid flow between the drywell and wetwell stops after the level drops below H_v .

When the wetwell level decreases because $P_w > P_d$, two sets of equations are used to compute the vent clearing time. These two sets of equations are needed to address the possible overflow situations at the drywell side should the flow overrun the overflow wall. The first set describes the calculations up to the point of overflow and the second set describes the calculations with overflow. The calculations t_{eq} , t_{op} , and t_{vc} for the case of a decreasing wetwell level are similar to those used for a depressed drywell level.

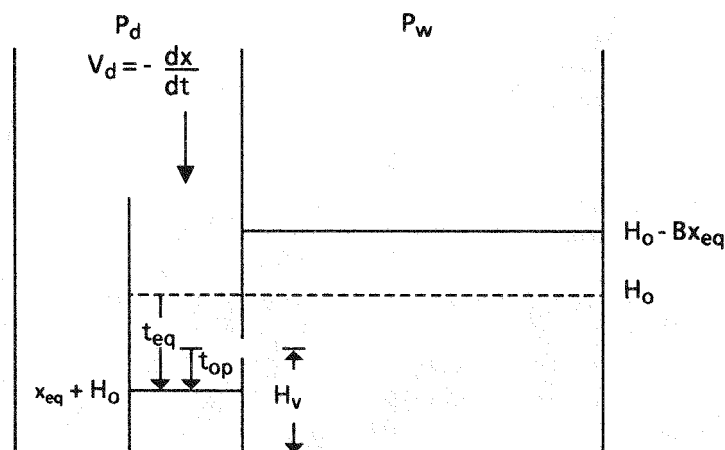


Figure 3-11. Computation of Drywell Level Depression

For decreasing wetwell level, an equation similar to Equation (3-44) is obtained from Equation (3-32), assuming overflow does not occur, with $F = 1 - \beta^2 + K_{dw}$:

$$t_{eq} = \left[\frac{2F[P_w - P_d - \rho_l g(1 + \beta)x_o]}{\rho_l g^2(1 + \beta)^2} \right]^{1/2} \quad (3-46)$$

where

$$x_o = (H_o - \hat{H}_{w,o}) / \beta \quad (3-47)$$

where

$\hat{H}_{w,o}$ = the initial value of $\hat{H}_w$ at the beginning of the timestep.

As illustrated in Figure 3-12, the time to overflow t_{of} is computed as $t_{of} = t_{eq} - t_{tr}$, where t_{tr} is the time from overflow to equilibrium when the gravitational head of the overflow is considered. It is calculated by Equation (3-46) with $x_o = H_{of} - H_o$. If vent clearing occurs prior to overflow, the vent clearing time t_{vc} is calculated in a manner similar to that for flow from the drywell to the wetwell.

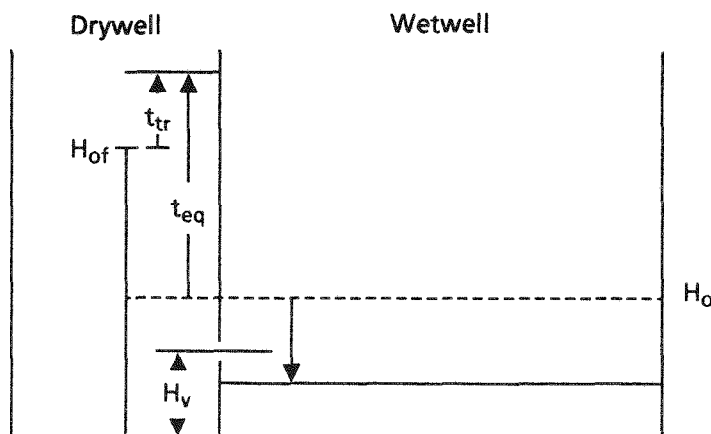


Figure 3-12. Computation of Wetwell Level Depression

The second equation set is more complicated because it tries to compute the effects of the overflow on the gravitational head correctly, by using an equation similar to Equation (3-37), but with the following definitions:

$$g \rho_l \Delta H_{dw} = g \rho_l (H_{of} - \hat{H}_w) \quad \text{for } \hat{H}_d > H_{of} \quad (3-48)$$

By using Equation (3-43), Equation (3-48) becomes

$$g \rho_l \Delta H_{dw} = g \rho_l (H_{of} - H_o + \beta x) \quad (3-49)$$

Thus a new equation can be integrated:

$$\frac{dx}{dt} = - \left[\frac{2[P_w - P_d - g \rho_l (H_{of} - H_o + \beta x)]}{F \rho_l} \right]^{1/2} \quad (3-50)$$

The integration of Equation (3-50) yields

$$t_{eq} = \left[\frac{2F[P_w - P_d - g \rho_l (H_{of} - H_o + \beta x_o)]}{g^2 \beta^2 \rho_l} \right]^{1/2} \quad \text{if } H_d = H_{of} \quad (3-51)$$

For $x_o = H_{of} - H_o$, we get

$$t_{of,eq} = \left[\frac{2F[P_w - P_d - g \rho_l (H_{of} - H_o)(1 + \beta)]}{g^2 \beta^2 \rho_l} \right]^{1/2} \quad (3-52)$$

where $t_{of,eq}$ = time to equilibrium under overflow conditions.

There are two cases to consider:

1. If $H_{d,o} < H_{of}$, where $H_{d,o}$ is the initial value of H_d , then the vent covering time is:

$$t_{vc} = t_{of} + t_{of,eq} - t_{op} \quad (3-53)$$

where

t_{op} = time from vent opening to equilibrium, which is given by Equation (3-51) with $x_o = (H_{w,o} - H_v)/\beta$, where $H_{w,o}$ is the initial value of H_w .

2. If $H_{d,o} \geq H_{of}$, liquid is removed from the drywell side of the pool until $H_{d,o} = H_{of}$; then the vent covering time is calculated as

$$t_{vc} = t_{of,eq} - t_{op} \quad (3-54)$$

3.5.2 Suppression Pool Flow Model

The suppression pool gas flow is calculated as a quasi-steady flow using the following equation (see Section 3.3.2.2):

$$W_{sup} = \left(|P_w - P_d| \rho_g A_{eff}^2 \right)^{1/2} \quad (3-55)$$

where

P_w = wetwell pressure (Pa),
 P_d = drywell pressure (Pa),
 ρ_g = atmospheric gas density (kg/m^3), and
 A_{eff} = effective gas flow area (m^2) from Equation (3-56a).

As discussed below, A_{eff} is taken to open linearly with pressure, beginning at the gas pressure difference sufficient to support the liquid level. To prevent surging, once the vent has cleared, it is assumed to remain so until the gas flow rate is calculated to be zero for a timestep. After this, the vent clearing calculation is reinitiated.

A_{eff} in Equation (3-55) is calculated as a function of user-defined pressure drops:

$$A_{eff} = (\Delta P - \Delta P_{min}) A_v / (\Delta P_{max} - \Delta P_{min}) \quad \text{for } \Delta P > \Delta P_{min} \quad (3-56a)$$

$$A_{eff} = 0 \quad \text{for } \Delta P \leq \Delta P_{min} \quad (3-56b)$$

where

A_v = flow area with an accounting for flow losses,
 ΔP = $P_d - P_w$ for flow from drywell to wetwell,
 ΔP = $P_w - P_d$ for flow from wetwell to drywell,
 ΔP_{min} = minimum pressure difference to support the liquid head at opening, based on the current pool inventory, and

$\Delta P_{\max}$ = the maximum pressure difference, defined as:

$$\Delta P_{\max} = \Delta P_{\min} + (\Delta P_d \text{ or } \Delta P_w, \text{ depending on flow direction}) \quad (3-57)$$

where

ΔP_d and ΔP_w = user-specified pressure differences between drywell and wetwell (Pa).

Detailed descriptions of ΔP_d and ΔP_w are presented in the CONTAIN User's Manual [Mur89].

To account for vent covering or uncovering, W_{sup} in Equation (3-55) is reduced as follows:

$$W = W_{\text{sup}}(1 - F_{\text{vc}}) \quad (3-58)$$

where

W = the reduced flow,

F_{vc} = a factor used to adjust suppression pool vent flow according to the time the vent is open, defined as:

$$F_{\text{vc}} = t_{\text{vc}} / \Delta t_s \quad (3-59)$$

where t_{vc} is previously defined in Section 3.5.1, and Δt_s = system timestep(s).

The flow Equation (3-3), with ij subscripts interpreted to refer to the vent flow, is used to calculate the suppression pool vent flow W_{sup} , for vents in the bypass (uncovered) state. C_{FC} in Equation (3-3) is taken to be unity. Both A_{ij} and L_{ij} are interpreted as user-defined vent area and vent inertial length. Finally, ΔP_{ij} is taken as the pressure difference between drywell and wetwell, and no choked flow and gas gravitational head corrections (Equation 3-1) are modeled.

As soon as W_{sup} is calculated, thereby accounting for the time of vent covering, the amount of noncondensable gas and vapor entering the suppression pool is determined.

To account correctly for the mass and energy transferred during vent flow, it is important to understand the three main stages of mass and energy transfer for the suppression pool.

The condition of the suppression pool prior to vent flow is governed by Q_p calculated in Equation (3-18) in Section 3.3.2.5. Stage 1 accounts for the enthalpies added to the pool because of

the flow of noncondensable gas and condensation of vapor. The noncondensable gas passed through the pool is first assumed to acquire the temperature of the pool T_p :

$$\Delta Q_p = Q_{sup,v} - Q_{sup,nc} \quad (3-60)$$

where

$$\begin{aligned} \Delta Q_p &= \text{pool energy (J) change,} \\ Q_{sup,v} &= \text{the energy (J) associated with the atmosphere that enters the suppression pool during venting, and} \\ Q_{sup,nc} &= \text{the energy (J) associated with the noncondensable gas escaping because of suppression pool venting.} \end{aligned}$$

$Q_{sup,v}$ in Equation (3-60) is given by:

$$Q_{sup,v} = \frac{|W_{sup}\Delta t_f|(U_u(t) + P_{u,tr}V_u)}{m_{t,u}} \quad (3-61)$$

where

$$\begin{aligned} U_u &= \text{internal energy (J) of the upstream cell u,} \\ P_{u,tr} &= \text{trial pressure (Pa) of the upstream cell u,} \\ V_u &= \text{volume (m}^3\text{) of the upstream cell u, and} \\ m_{t,u} &= \text{total atmospheric mass (kg) in the upstream cell u.} \end{aligned}$$

$Q_{sup,nc}$ in Equation (3-60) is given by

$$Q_{sup,nc} = |W_{sup}\Delta t_f|h_{nc}\frac{m_{nc,u}}{m_{t,u}} \quad (3-62)$$

where

$$\begin{aligned} h_{nc} &= \text{specific enthalpy (J/kg) of the noncondensable gas evaluated at } T_p, \text{ and} \\ m_{nc,u} &= \text{noncondensable gas mass (kg) in the upstream cell u.} \end{aligned}$$

Because the noncondensable gas will not condense in the pool, the only pool mass increase comes from vapor condensation. The change of pool mass, Δm_p is given by:

$$\Delta m_p = |W_{sup}\Delta t_f|\frac{m_{v,u}}{m_{t,u}} \quad (3-63)$$

where $m_{v,u}$ is the vapor mass (kg) in the upstream cell u.

Stage 2 accounts for the flashing because of vent flow. Based on the trial pressure given in Section 3.3 for evaluating the enthalpies, the amount of pool mass flashing m_f is given by:

$$m_f = \frac{Q_p + \Delta Q_p - (m_p + \Delta m_p)h_\ell}{h_v - h_\ell} \quad (3-64)$$

where Q_p and m_p are the pool energy and mass, respectively, and h_ℓ and h_v are the liquid and vapor saturation enthalpy for the pool and vapor, respectively.

Stage 3 accounts for the vapor taken up by the noncondensable gas of the vent flow. It is assumed that the noncondensable gases carry the vapor at a pressure that is 0.99 of the saturation pressure.

The pressure in bubbles containing the noncondensable gases at the pool surface is assumed to be the same as that in the atmosphere:

$$0.99 P_{\text{sat}}(T') + P_{\text{nc}}(T') = P_{\text{tr}} \quad (3-65)$$

where

P_{tr} = trial pressure of the downstream cell,
 $P_{\text{nc}}(T')$ = noncondensable gas pressure in the bubble at the new self-consistent pool temperature T' , and
 $P_{\text{sat}}(T')$ = saturation vapor pressure at T' .

And it is assumed that the noncondensable gas passing through the pool is 99% saturated at the pool surface. Note that T' is the new self-consistent equilibrium temperature of the pool, correctly adjusted for the vapor energy removed by the bubbles.

Equation (3-65) may be written, according to an ideal gas assumption, as

$$m_{\text{vap},v} = \frac{M_{\text{vap}} 0.99 P_{\text{sat}}(T') M_{\text{Onc}}}{P_{\text{tr}} - 0.99 P_{\text{sat}}(T')} \quad (3-66)$$

where

M_{vap} = molecular weight of water vapor (kgmole), and
 M_{Onc} = noncondensable gas passing through the vent in a flow timestep (kgmoles).

The energy balance for the suppression pool, taking into account the fact that vaporization into the bubbles cools the pool and the gas passing through, is given by:

$$m_{\text{vap},v} h_{\text{fg}} = \Delta Q'_p - (\text{CVP} + \text{CPG}) \Delta T_{\text{vap}} \quad (3-67)$$

where

- $\Delta Q'_p$ = changes in the pool energy because of processes considered in Stage 1 and Stage 2 (J),
- h_{fg} = latent heat (J/kg), of evaporation ($h_v - h_l$) evaluated at T_p ,
- CVP = specific heat of pool multiplied by the sum of total pool mass plus any additional mass of vapor condensed on the pool minus any flashed (J),
- CPG = specific heat of noncondensable gases multiplied by the total noncondensable gases in the bubbles (J), and
- ΔT_{vap} = amount of temperature change or $T' - T_p$ (K).

In terms of ΔT_{vap} , $m_{\text{vap},v}$ in Equation (3-66) can be redefined as

$$m_{\text{vap},v} = \frac{0.99K \left[P_s + \frac{dP_s}{dT} \Delta T_{\text{vap}} \right]}{\Delta P - 0.99 \frac{dP_s}{dT} \Delta T_{\text{vap}}} \quad (3-68)$$

where

- P_s = pool saturation pressure (Pa),
- ΔP = $P_{\text{tr}} - 0.99 P_s$ (Pa),
- K = $M_{\text{vap}} M_{\text{nc}}$, the vapor flux multiplier (kg), and
- dP_s/dT = temperature derivative of the saturation pressure (Pa/K).

ΔT_{vap} in Equation (3-67) is therefore

$$\Delta T_{\text{vap}} = \frac{1}{2C_A} \left(C_B - \sqrt{C_B^2 + 4C_A C_C} \right) \quad (3-69)$$

C_A , C_B , and C_C in Equation (3-68) are coefficients given by:

$$C_A = 0.99 (\text{CVP} + \text{CPG}) \frac{dP_s}{dT} \quad (3-70)$$

$$C_B = \Delta P (CVP + CPG) + 0.99 \frac{dP_s}{dt} (\Delta Q_p + h_{fg} - K) \quad (3-71)$$

and

$$C_C = 0.99 h_{fg} K P_p - \Delta Q_p \Delta P \quad (3-72)$$

After ΔT_{vap} is determined, T' is obtained as $\Delta T_{vap} + T_p$.

The corresponding energy transferred to the gas in the vaporization step $Q_{vap,v}$ is given by

$$Q_{vap,v} = m_{vap,v} h_v + CPG \Delta T_{vap}. \quad (J) \quad (3-73)$$

These energy and mass calculations are used in determining the thermal state of the drywell and wetwell cells.

3.6 Nonthermodynamic Material Flow

This section describes how airborne nonthermodynamic materials are transported between cells. In CONTAIN, these components include suspended aerosols, gaseous FPs, liquids (other than the coolant), and suspended solids. The scrubbing of aerosol materials by the suppression pool is described in Section 4.4.

For a nonaerosol nonthermodynamic material (k), the general mass equation with respect to intercell flow is

$$\frac{dm_{i,k}}{dt} = - \sum_j^{N_c} \theta_{ij} W_{ij} \frac{m_{u,k}}{m_{u,t}} \quad (3-74)$$

where

θ_{ij} = sign function as defined in Table 1-3,
 $m_{u,k}$ = k component mass (kg) in donor cell u, and
 $m_{u,t}$ = total (thermodynamic) atmospheric mass (kg) of donor cell u.

Equation (3-74) is also used in engineered vent and suppression pool vent calculations. To account for flow effects, the airborne materials are redistributed once per system timestep. Note that suspended liquids and solids are considered massless by the flow solver.

In the implicit flow option, aerosols are considered to flow at the sum of the hydrodynamic gas convective velocity and the component of the aerosol settling velocity along the flow path axis. The

angle of inclination of flow paths used to calculate the settling velocity is user-specified. Deposition within such flow paths is not modeled. In the explicit flow option, aerosol slip is not considered.

The effects of aerosol agglomeration, deposition, and condensation within a cell are calculated separately in a model that disregards flow during a given timestep. Likewise, the mass of suspended aerosol does not affect the flow rate.

The implicit flow or explicit flow option can be used to calculate aerosol mass transport from one cell to another cell. The implicit flow option is described in Section 3.2 and the explicit flow option in Appendix C.

For aerosols within the implicit flow option, the aerosol sectional mass flow rate including the slip is calculated as

$$\frac{dm_{i,k,l}}{dt} = - \sum_j^{N_c} \left[\theta_{ij} v_{ij} A_{ij} \frac{m_{u,k,l}}{V_u} \right] \quad (3-75)$$

where

$$\begin{aligned} m_{i,k,l} &= \text{aerosol component } k \text{ mass (kg) of aerosol section } l \\ &\quad \text{in cell } i, \\ \theta_{ij} &= \text{theta function similar to that in Table 1-3 by} \\ &\quad \text{substituting } W_{ij} \text{ with } v_{ij}, \\ V_u &= \text{cell volume (m}^3\text{) of donor cell } u, \text{ and} \\ v_{ij} &= \text{the sum of the atmospheric gas velocity and the} \\ &\quad \text{aerosol gravitational slip velocity, and it is given} \\ &\quad \text{by:} \\ &= v_{\text{gas}} + v_g \end{aligned} \quad (3-76)$$

where

$$\begin{aligned} v_{\text{gas}} &= \text{thermodynamic gas velocity through flow} \\ &\quad \text{path } ij, \text{ given by } W_{ij}/(\rho_{ij} A_{ij}), \text{ and} \\ v_g &= \text{gravitational slip velocity for the} \\ &\quad \text{aerosols.} \end{aligned}$$

A downward slip velocity is given by

$$\begin{aligned} v_{gd} &= (1 - F_T) \left[(1 - F_P) C_{T1,P1} + F_P C_{T1,P2} \right] \\ &\quad + F_T \left[(1 - F_P) C_{T2,P1} + F_P C_{T2,P2} \right] \end{aligned} \quad (3-77)$$

where $C_{T1,P1}$, $C_{T1,P2}$, $C_{T2,P1}$, and $C_{T2,P2}$ are terminal velocity coefficients of aerosols at the interpolation end points. Subscripts T1, T2, P1 and P2 are the user-defined end points of the

lowest temperature T_1 ; highest temperature T_2 ; lowest pressure P_1 ; and highest pressure P_2 , respectively. A table of these coefficients as functions of temperatures and pressures should be available from user-defined inputs or by default (see Section 4).

F_T and F_P in Equation (3-78) are defined as

$$F_T = (T_u - T_1)/(T_2 - T_1), \text{ and} \quad (3-78)$$

$$F_P = (P_u - P_1)/(P_2 - P_1) \quad (3-79)$$

where

T_u = temperature of upstream cell in (K), and

P_u = pressure of upstream cell (Pa).

Because v_{gd} in Equation (3-78) only accounts for the downward direction, any change from this position in the flow path such as inclination should be accounted for

$$v_g = v_{gd} \cdot F_{\cos} \quad (3-80)$$

where $F_{\cos}$ is the user-defined cosine of angle of the flow path axis with respect to the vertical position.

4.0 AEROSOL BEHAVIOR MODELS

This section describes the models used in CONTAIN to simulate the behavior of aerosols in containment following an accident in a LWR. Events occurring early in a LWR accident may aerosolize FPs and core materials that may be expelled from the reactor coolant system. Other events occurring late in the accident may also generate aerosols by core-concrete interaction, pool boiling, and resuspension processes.

The principal aerosol quantities of interest are the mass and chemical composition distributions of aerosol particles throughout containment. The aerosol models used in CONTAIN to determine these distributions are based on the MAEROS code [Gel82].

Several enhancements to the MAEROS models have been added for use in CONTAIN. These enhancements apply to aerosol processes that occur in LWR accidents. Sodium aerosol and the processes that occur during accidents in liquid metal reactors (LMR) are treated in CONTAIN-LMR [Mur90].

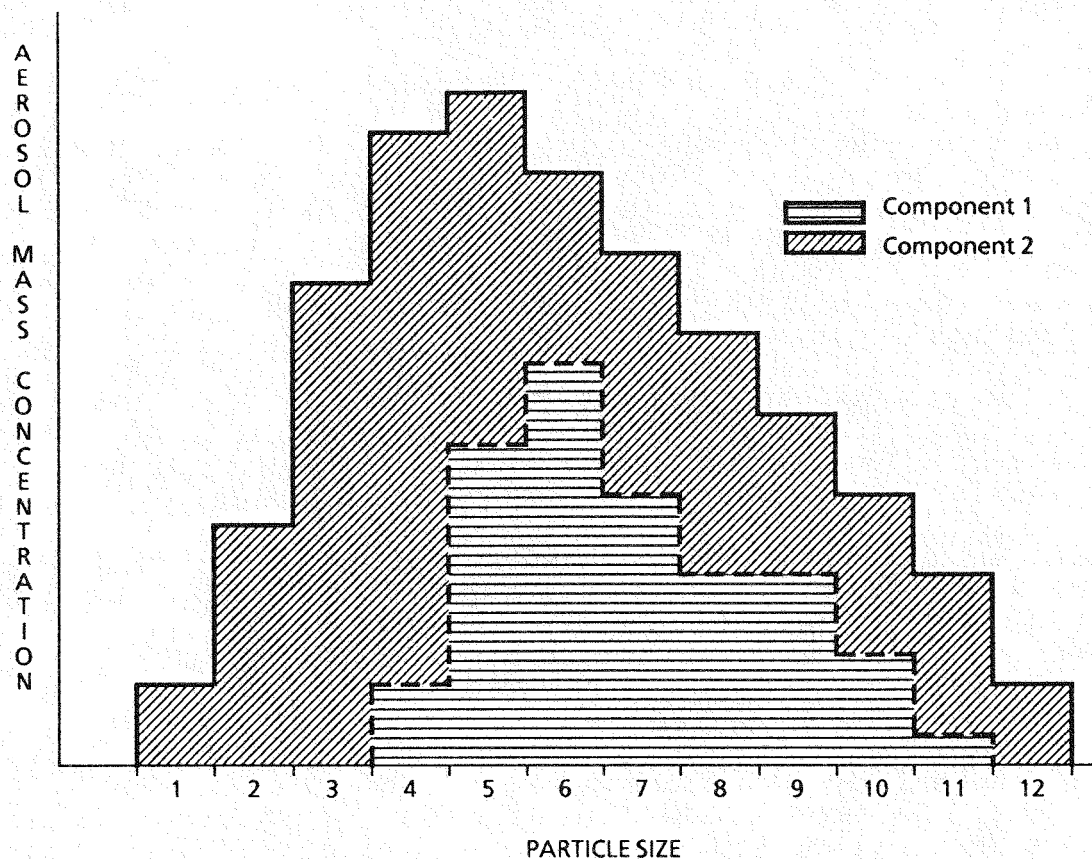
The aerosol modeling approach used in CONTAIN allows for multisectional and multicomponent treatment of aerosols. This means that the aerosol-size distribution is divided into particle size classes called sections, each of which can have a different chemical composition. Thus, a section is an aerosol-size grouping and a component is a particular type of material.

Figure 4-1 illustrates the sectional representation of a two-component aerosol with 12 sections. The mass concentrations of component 1 in each section are given by the stair-stepped broken line above the horizontally shaded region. The total aerosol mass concentrations in each section are given by the uppermost stair-stepped solid line. Therefore, the mass concentrations of component 2 in each section are given by the slanted-shaded region.

One powerful feature of CONTAIN is that water condensation on and evaporation from aerosols is modeled in a manner consistent with the atmosphere-thermo-hydraulic calculation for heat transfer to structures. That is, the latent heat associated with the coolant mass transfer between the atmosphere and aerosol surfaces is incorporated in the total internal energy transfer to and from the atmosphere. (See Section 6.4 for the heat and mass transfer models for the heat structures.) In addition, evaporation/condensation of coolant processes for the aerosols and heat structures can occur simultaneously with condensation or evaporation from heat sinks, agglomeration of aerosols, and deposition of aerosols on surfaces.

The calculation of the aerosol particle size distribution proceeds under the influence of four general processes:

- agglomeration (or coagulation), whereby two particles collide and form one larger particle;



Section boundaries are spaced such that adjacent particle mass boundaries increase by at least a factor of 2.

Figure 4-1. Example of Aerosol Particle Mass Concentration Distribution for a Two-Component Aerosol

- particle size change by condensation or evaporation of water onto or from the particle;
- aerosol sources (user-specified and LC source terms); and
- particle deposition onto surfaces.

The aerosol behavior models used in CONTAIN 1.1 include models for aerosol agglomeration, evaporation/condensation, deposition, and intercell flow of aerosol. Section 4.1 describes how the particle size distribution is represented in CONTAIN. The agglomeration, condensation/evaporation, and deposition models describe changes in aerosol mass and composition in each cell, and are discussed in Section 4.2. The other independent models are discussed in Subsections 4.2.1 through 4.2.3. A discussion of aerosol sources is given in Section 4.3. Section 3 describes the atmospheric flow model that governs the aerosol flow between cells. The specific model for intercell flow of aerosols and other nongas components of the atmosphere is discussed in Section 3.6.

4.1 Aerosol Size Distribution

In CONTAIN, the aerosol particle size distribution is discretized into particle size classes called sections. The distribution of

aerosol within a section is approximately constant with respect to the logarithm of particle mass. The values of this constant will generally differ among sections and will be time-dependent.

Although the particle size distribution is generally unrestricted in CONTAIN, the initial and source particle size distributions are taken to be lognormal. Normally, the three lognormal size distribution parameters are constants that are independent of time. However, the user may specify these parameters as time-dependent for aerosol sources. A different size distribution may be specified for each aerosol component. CONTAIN currently limits the number of aerosol components to eight.

The lognormal aerosol mass distribution $m(d_p)$ with a spherical equivalent diameter d_p is given by

$$m(d_p) \propto \exp \left\{ - \frac{1}{2} \left[\frac{\ln^2(d_p/d_{vm})}{d_{dv}^2} \right] \right\} / d_p \quad (4-1)$$

where

- α = proportional to,
- d_{vm} = the volume-equivalent mass median diameter (the diameter of a spherical particle with the same density and mass as the mass median particle), and
- d_{dv} = the natural logarithm of the geometric standard deviation with respect to diameter [Yos79].

In CONTAIN, Equation (4-1) is integrated over each section to determine the aerosol mass concentrations within each section. Particle mass outside the computational domain is redistributed within the computational domain by renormalizing the section mass concentrations. For computational purposes, ten to twenty is the ideal number of sections (size classes). The section boundaries are determined by partitioning the particle size domain geometrically. CONTAIN currently assumes the particles are spherical, having the same masses as the irregularly shaped particles.

Lower and upper sections have been added to keep track of aerosol mass that may become undersized and oversized, respectively. Aerosol particles can become undersized by evaporation of water. Particles can become oversized by condensation of water vapor or agglomeration. The cell OVERFLOW model in CONTAIN controls the disposition of mass that leaves the computational domain, or "mesh." By default, the mass in the lowest section 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 floor structures. If more than one floor structure is in the cell, the aerosol mass is

divided proportionally 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 available. Finally, if a pool has not been defined, the mass will be lost from the "mesh" and placed into a waste holding location. Additional input requirements for the overflow of undersized and oversized aerosols are described in the CONTAIN User's Manual [Mur89]. Note that deposition onto a floor structure is assumed not to be affected by the pool, if a pool is modeled.

4.2 Dynamics

The aerosol dynamics (size and composition) model is used to calculate the changing aerosol size distributions as dynamic processes affect the aerosol in each cell at each timestep. Particle agglomeration, deposition, and condensation/evaporation processes are included in the aerosol dynamics calculation. The model accepts information from

- user-specified sources, including sources from in-vessel processes calculated with such codes as MARCH, TRAC and SCDAP/RELAP; and
- other CONTAIN models:
 - aerosols from LC core-concrete interactions;
 - water vapor from pool boiling;
 - aerosol sources from adjacent cells; and
 - atmosphere temperature and pressure.

The aerosol dynamics model calculates the new aerosol mass and composition information that is used by the aerosol intercell flow model.

The modeling of the aerosol size distribution is governed by a complex integro-differential equation. Gelbard and Seinfeld (1980) have developed a method of discretizing this equation into a form that can be solved numerically. In their method, the full range of aerosol masses is divided into m contiguous arbitrarily sized sections, and Q_ℓ is defined as the total mass of aerosol per unit volume of fluid in section ℓ at time t . Thus,

$$Q_\ell(t) = \sum_{k=1}^s Q_{\ell,k}(t) \quad (4-2)$$

where $Q_{\ell,k}(t)$ is the mass of component k in section ℓ , and s is the total number of components. The upper bound of section $\ell - 1$ is

equal to the lower bound of section ℓ for $\ell = 2, 3, \dots m$. These equations can be written:

$$\begin{aligned} \frac{dQ_{\ell,k}}{dt} = & \frac{1}{2} \sum_{i=1}^{\ell-1} \sum_{j=1}^{\ell-1} \left[{}^1a\bar{\beta}_{i,j,\ell} Q_{j,k} Q_i + {}^1b\bar{\beta}_{i,j,\ell} Q_{i,k} Q_j \right] \\ & - \sum_{i=1}^{\ell-1} \left[{}^2a\bar{\beta}_{i,\ell} Q_i Q_{\ell,k} - {}^2b\bar{\beta}_{i,\ell} Q_{\ell} Q_{i,k} \right] \\ & - \frac{1}{2} {}^3\bar{\beta}_{\ell,\ell} Q_{\ell} Q_{\ell,k} - Q_{\ell,k} \sum_{i=\ell+1}^m {}^4\bar{\beta}_{i,\ell} Q_i + {}^1\bar{G}_{\ell,k} Q_{\ell} \\ & - \sum_{i=1}^{N_a} \left[{}^2\bar{G}_{\ell,i} Q_{\ell,k} - {}^2\bar{G}_{\ell-1,i} Q_{\ell-1,k} \right] + {}^3\bar{G}_{\ell-1,k} Q_{\ell-1} + \bar{S}_{\ell,k} - \bar{R}_{\ell,k} \end{aligned} \quad (4-3)$$

where

$dQ_{\ell,k}(t)/dt$ = time rate of change of aerosol mass of component k (per unit volume) in section ℓ at time t ;
 k = aerosol component (for example, water or a specific FP) = 1, 2, ... N_a ; and
 ℓ = discretized section (or physical size range) of the aerosol = 1, 2, 3, ... m .

This set of equations describes the evolution of the aerosol size and composition distributions within each computational cell. Each cell has its own particle size and chemical composition distributions, and the aerosols are carried from one cell to the next by gas flow.

To integrate Equation (4-2) forward in time, the kernel for agglomeration and the rate constants for aerosol deposition and condensation on aerosols need to be known on a sectional basis. For example, the kernel β_{m_i, m_j} is for agglomeration of particles of size m_i with those of size section m_j . When defined on a sectional basis, the integrated agglomeration kernel and the rate constants are referred to collectively as sectional coefficients. The sectional coagulation coefficients require two-dimensional integration over particle sizes. The sectional deposition coefficients require only one-dimensional integration.

Simplifications in the coefficients and in Equation (4-3) occur if the geometric constraint

$$m_{i+1}/m_i > 2 \quad (4-4)$$

is satisfied, where m_i is the particle mass at the lower boundary of section i . The geometric constraint ensures that the agglomeration of two particles results in a new particle that will fit into either the section that contains the larger of the two original particles or the section just above it. This constraint thus reduces the number of sectional agglomeration coefficients.

The calculation of the coefficients is somewhat costly; a full calculation for 20 sections requires about 10 s processing time on a CRAY 1S computer. Therefore, the coefficients are either read in from a file 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 3752 storage locations for an aerosol with 20 sections.

The following constraints pertain to the current coefficient set:

- The aerosol material density is assumed to be the same for all components.
- The aerosol shape, as modeled by the dynamic and agglomeration shape factors, is independent of aerosol 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.
- 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 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 ($T_{\min}$ and $T_{\max}$) and two pressures ($P_{\min}$ and $P_{\max}$). Changing thermal-hydraulic conditions during the problem are accommodated by interpolating between these sets of coefficients. The $T_{\min}$, $T_{\max}$, $P_{\min}$, and $P_{\max}$ parameters are chosen to bound the temperatures and pressures expected. (See Section 4.2.3 for an example of using this interpolation.) 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 embedded.

Each term in Equation (4-3) represents a distinct mechanism for changes in mass concentration of component k in a particular section.

The coefficients used in each term correspond to these mechanisms:

<u>Coefficient</u>	<u>Represents</u>
$\bar{\beta}$	Agglomeration (or coagulation), $m^{-3}-s^{-1}-kg^{-1}$,
$\bar{G}$	Gas-particle conversion (condensation/ evaporation), $m^{-3}-s^{-1}$,
$\bar{S}$	Sources, kg/m^3-s ,
$\bar{R}$	Removal (deposition) kg/m^3-s .

The first two terms and the fourth term in Equation (4-3) represent the addition of component k into section ℓ through agglomeration. The third, fifth and sixth terms account for removal of component k from Section ℓ by agglomeration.

The $\bar{\beta}$'s are called sectional coagulation coefficients, and they can be evaluated by using a variety of formulas that incorporate the effects of the different physical processes. These processes include gravitational agglomeration (a larger particle overtakes a smaller one as they both fall) and agglomeration through diffusion (either Brownian or turbulent).

The six agglomeration terms in the Gelbard-Seinfeld approach use sectional coefficients ($\bar{\beta}$) that refer respectively to the following processes:

- $1^a \bar{\beta}_{i,j,\ell}$ addition of component k in section ℓ , by removal of component k in section j when a particle in section j coagulates with a particle in section i to form a particle in section ℓ .
- $1^b \bar{\beta}_{i,j,\ell}$ addition of component k in section ℓ , by removal of component k in section i when a particle in section i coagulates with a particle in section j to form a particle in section ℓ .
- $2^a \bar{\beta}_{i,\ell}$ removal of component k in section ℓ , resulting from a particle in section i coagulating with a particle in section ℓ .
- $2^b \bar{\beta}_{i,\ell}$ addition of component k in section ℓ , resulting from a particle in section i coagulating with a particle in section ℓ , with the resulting particle remaining in section ℓ .
- $3 \bar{\beta}_{\ell,\ell}$ removal of component k in section ℓ , by two particles in section ℓ coagulating and the resulting particle is in a section higher than ℓ .

${}^4\overline{\beta}_{i,\ell}$ removal of component k in section ℓ , by a particle in section ℓ coagulating with a particle in section i, where $i > \ell$.

Intraparticle chemical reactions can occur between constituents of the aerosol, for example, Cs (cesium) + I (iodine) = CsI. The modeling of aerosol size/composition changes resulting from chemical reactions is not currently implemented in CONTAIN, but the inclusion of this phenomenon into the sectional model can be readily implemented.

The four condensation terms used in CONTAIN include $\overline{G}$ coefficients. The model for aerosol mass change resulting from condensation/evaporation processes is taken from Reference Bye65. Both condensation and evaporation may take place on aerosols, and either process can occur simultaneously with condensation or evaporation from heat sink surfaces. The four condensation/evaporation coefficients used in Equation (4-3) refer to the following process:

Gas-to-Particle Condensation/Evaporation Coefficients

- ${}^1\overline{G}_{\ell,k}$ addition of component k to section ℓ by condensation/evaporation of component k onto particles in section ℓ ;
- ${}^2\overline{G}_{\ell,i}$ removal of component k from section ℓ by condensation/evaporation of component i onto particles in section $\ell+1$;
- ${}^2\overline{G}_{\ell-1,i}$ removal of component k from section $\ell-1$ by condensation/evaporation of component i onto particles in section ℓ ; and
- ${}^3\overline{G}_{\ell-1,k}$ addition of component k in section ℓ due to the mass of condensation/evaporation vapor of component k onto particles in section $\ell-1$.

Condensation on and evaporation from aerosol particles are the principal couplings between thermal-hydraulics and aerosol behavior. Section 4.2.2 describes the condensation model and the development of the $\overline{G}$ coefficients in Equation (4-3).

In Equation (4-3), particle removal (or deposition) is addressed by the $\overline{R}$ term. Deposition occurs through a number of processes, including gravitational settling, diffusion to surfaces, thermophoresis (a Brownian process causing migration of particles toward lower temperatures), and diffusiophoresis (deposition induced by condensation of water vapor onto structural surfaces).

For some ESF decontamination calculations, two additional processes, interception and inertial impaction, are included. Again, these processes are accounted for in CONTAIN through formulas for $\overline{R}$, in terms of various state variables. Section 4.2.3 describes the deposition model that develops these $\overline{R}$ terms.

Mass of any component may be added to any section at various times by user input or from other CONTAIN models. Section 4.3 describes the source model for the S term in Equation (4-3).

4.2.1 Agglomeration

When two aerosol particles collide, they can combine to form a larger particle. This process is known as agglomeration or coagulation. The sectional method used in MAEROS and CONTAIN treats four agglomeration processes: Brownian diffusion, differential gravitational settling, turbulent shear agglomeration, and turbulent inertial agglomeration. A basic assumption about these processes is that only two particles can combine at a time.

According to the discussion in Reference Wil87, the dependence of the agglomeration coefficients β (m^3/S) upon the aerosol properties is implemented in CONTAIN as follows:

(4-5)

$$\begin{aligned} \text{Brownian:} \quad \beta_B &\propto \gamma \chi^{-1} f(d_i, d_j); \\ \text{Gravitational:} \quad \beta_{\text{grav}} &\propto \text{Col}_g \gamma^2 \chi^{-1} (d_i + d_j)^2 (d_i^2 - d_j^2); \\ \text{Turbulent, Shear:} \quad \beta_{T1} &\propto \text{Col}_{T1} \gamma^3 \epsilon^{1/2} (d_i + d_j)^3; \text{ and} \\ \text{Turbulent, Inertial:} \quad \beta_{T2} &\propto \text{Col}_{T2} \gamma^2 \chi^{-1} \epsilon^{3/4} (d_i + d_j)^2 (d_i^2 - d_j^2). \end{aligned}$$

In Equation (4-5) above, γ and χ are the agglomeration and dynamic shape factors, respectively; ϵ is the turbulent energy dissipation density; and d_i and d_j are the diameters of the two interacting particles, with $d_i > d_j$. The collision efficiencies for the gravitational, turbulent shear, and turbulent inertial processes are represented by Col_g , Col_{T1} , and Col_{T2} , respectively, and specific values (discussed below) are normally assigned in the code. The magnitude of the Brownian kernel increases with increasing values of the size ratio d_i/d_j . The role of the various parameters appearing in the kernels is also discussed below.

The agglomeration kernels also have dependencies on containment atmosphere properties (pressure, temperature, viscosity), which are not displayed in the proportionalities in Equation (4-5); these dependencies may not be major sources of uncertainty in aerosol calculations and will not be considered further here.

Except when they include significant amounts of liquid, aerosol particles are not usually assumed to be spherical, and the effective aerosol densities may be significantly less than the bulk density of the materials of which the aerosols are composed. In aerosol codes, these effects may be taken into account by using a formalism based on fully dense spherical aerosols modified through the use of the agglomeration shape factor γ and the dynamic shape factor χ . The shape factors γ and χ are inputted by the user to represent the effect of nonspherical shape upon aerosol collision

cross sections and aerosol-atmosphere drag forces, respectively. Unit values of the shape factors correspond to dense aerosol of spherical shape, while porous spherical agglomerates lead, in theory, to values somewhat greater than unity. Highly irregular aerosols and agglomerates can have shape factors substantially greater than unity, often with γ and χ being quite unequal.

Given a description of the aerosol shapes and densities, shape factors could, in principle, be derived theoretically. However, this is not practical, so empirical values are obtained by fitting code calculations to the results of aerosol experiments. The values obtained may be sensitive to aerosol composition and to atmospheric conditions, especially the relative humidity. Humid conditions tend to produce more nearly spherical aerosols. Only limited information is available concerning the dependence of shape factors upon the relevant parameters (for example, particle characteristics and atmospheric conditions), and these parameters are themselves quite uncertain under accident conditions.

Agglomeration rates can be enhanced by turbulence in the containment atmosphere. In the past, very little attention has been given to estimating values of turbulent energy dissipation density ϵ appropriate for accident conditions, and uncertainty in its value may contribute to uncertainty in the aerosol agglomeration rates. In CONTAIN, the user can input the value of ϵ or use the default value of $0.001 \text{ m}^2/\text{s}^3$.

Gravitational collision efficiencies Col_g of unity correspond to the collision cross sections being equal to the geometric cross sections. It is well known that hydrodynamic interactions between particles can yield collision efficiencies much less than unity, especially for particles that are unequal in size. The problem of collisions between falling (spherical) aerosols has been the object of much detailed theoretical and experimental study, and may be more complex than can be represented by the simple expressions normally used in aerosol codes. In CONTAIN, the user can specify a value of Col_g ; however, the default value is almost always used in practice and is given by

$$\text{Col}_g = 1.5 \frac{d_j^2}{(d_i + d_j)^2} \quad (4-6)$$

where d_j is the smaller of the two aerosol particle diameters. Bunz, Koyro, and Schoeck (1983) and Dunbar and Ramsdale (1984), as cited in Reference Wil87, have argued that using 0.5 instead of 1.5 as the coefficient in Equation (4-6) gives a better representation and that other corrections are needed when the size ratio d_i/d_j is less than about 2 and/or d_i is greater than about $20 \text{ } \mu\text{m}$.

Gravitational collision efficiencies have been a subject of considerable study in atmospheric and aerosol sciences, but much less attention has been paid to turbulent agglomeration collision

efficiencies. As described in Reference Wil87, the treatment of turbulent agglomeration in CONTAIN is based upon that of Saffman and Turner (1956), who assumed unit collision efficiencies. However, in CONTAIN, Col_{T2} (the turbulent inertial collision efficiency) is set equal to Col_g , although Col_{T1} is assumed to be unity. The rationale for these choices is discussed in Reference Wil87.

Examination of the relations for the agglomeration kernels in the proportionalities of Equation (4-5) shows that the effects of collision efficiencies, aerosol shape factors, and turbulence are coupled together in a highly nonlinear fashion. The dependence upon the various parameters differs among the different agglomeration mechanisms, and the net effects are strongly size-dependent. Hence, it is possible to give only a few generalizations of the effect to be expected.

All the agglomeration processes are enhanced by large values of the agglomeration shape factor γ , with the effect being largest for turbulent shear agglomeration and smallest for Brownian agglomeration. Large values of the dynamic shape factor reduce all the kernels (calculational coefficients) except the turbulent shear kernel, which is unaffected. Hence, large values of the shape factors enhance the relative importance of turbulence, especially for the turbulent shear effect.

The agglomeration model used in CONTAIN receives temperature, pressure, and mass flow rate information from the UC atmosphere model. The agglomeration model then calculates β coefficients and sends the resulting coefficients to the aerosol dynamics model (Equation (4-3)).

4.2.2 Condensation and Evaporation

The condensation or evaporation of water on containment aerosols is calculated in CONTAIN as part of the aerosol behavior model. The aerosol condensation and evaporation model treats the condensation and evaporation of water from and to the surfaces of particles. Therefore, diffusiophoresis is not treated in this model, because diffusiophoresis deals with aerosol deposition resulting from condensation of water vapor onto structural surfaces. Diffusiophoresis is treated in the deposition model discussed in Section 4.2.3.

The rate equation for diffusion of water vapor to and from an aerosol is not the equation used in the MAEROS stand-alone code, but is one taken from Reference Bye65. It accounts for both the diffusivity of water vapor in air and the conduction of the heat of condensation away from the aerosol. The rate of condensation on an aerosol 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 4-2. The coefficients ${}^1G_{\ell,k}$ and ${}^2G_{\ell,i}$ in Equation (4-3) are related to the

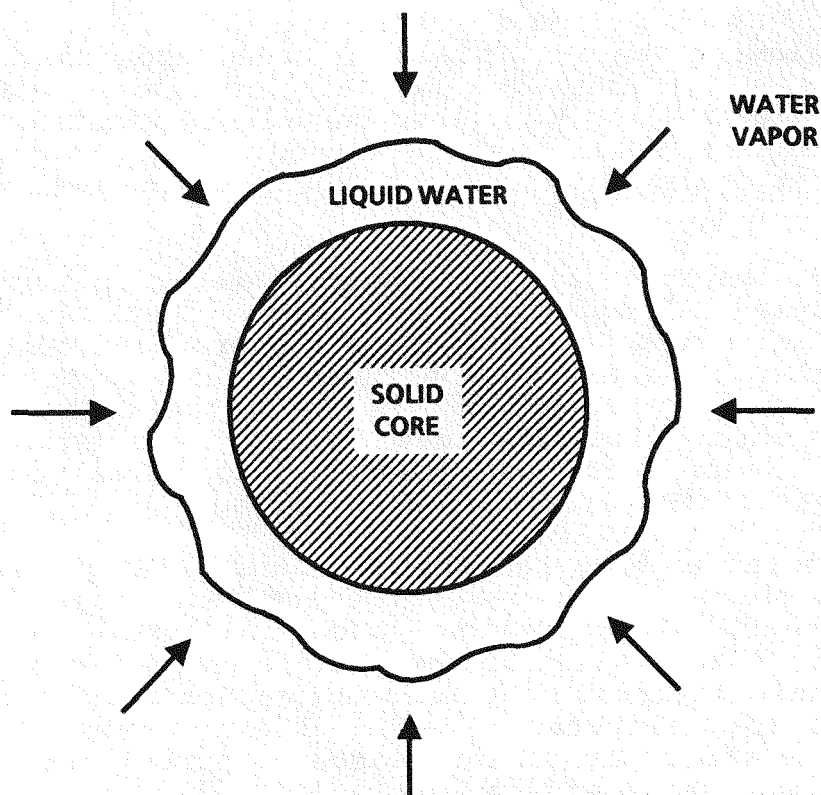


Figure 4-2. Model for Water Condensation on Aerosols

condensation rate. The Runge-Kutta integration method is used to calculate the condensation rate.

Two solution methods are used for evaporation. For high superheat, when aerosol water evaporation 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 aerosol rate poses problems, because the discontinuous change in rate at dryout causes the Runge-Kutta integrator to become inefficient. Therefore, when the Runge-Kutta method is used during evaporation, the solid materials are assumed to inhibit evaporation when the water mass and the solid mass are comparable. The coefficients ${}^2\overline{G}_{\ell-1,k}$ and ${}^3\overline{G}_{\ell-1,k}$ in Equation (4-3) are related to this evaporation rate. The mass flow during evaporation is assumed to be

$$W_{d, \text{evap}} = 1.037 W_d \tanh(2m_{\ell w}/m) \quad (4-7)$$

where W_d is the uninhibited evaporation rate from a spherical aerosol and $m_{\ell w}$ and m are the aerosol's water mass and total mass, respectively. 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 decrease if the particles have grown. 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 section. The mass added is typically much less than the error tolerance used in integrating the masses in each size section.

Both the condensation and evaporation rates of water on an aerosol are driven by the steam mass available in the atmosphere. Because condensation of water in CONTAIN is also coupled with condensation of water in aerosol, pool, and heat structure, the available steam mass condensed onto the aerosol is transferred from the intercell flow model. On the other hand, the evaporation of water from an aerosol is done within the aerosol model.

Once the steam mass is calculated, the actual condensation and evaporation rates are calculated using a slight variant of the Mason Equation presented in Reference Bye65:

$$\xi(m) = 4\pi r(SSat-1) \left[\frac{M_{wvap} h_{lg}}{k_{gas} R T^2} + \frac{1}{\rho_{sat} D} \right]^{-1} \quad (4-8)$$

where

- $\xi(m)$ = mass condensation/evaporation rate on particles of mass m (kg/s),
- r = particle radius (m),
- $SSat$ = supersaturation,
- M_{wvap} = molecular weight of water,
- h_{lg} = latent heat of vaporization (J/kg),
- k_{gas} = gas thermal conductivity (W/m-K),
- R = universal gas constant (J/kgmole-K),
- T = temperature (K),
- ρ_{sat} = saturated steam density (kg/m³), and
- D = steam diffusivity (m²/s).

If $\xi(m)$ is negative, evaporation is occurring; otherwise, if $\xi(m)$ is positive, condensation is occurring.

ρ_{sat} is calculated from the atmospheric condition. These thermodynamic calculations are described in Section 3.4. Note that m in Equation (4-8) is dependent on the $4\pi r$ factor. Therefore, this factor goes into the integrals for the G coefficients presented in the aerosol dynamics model (Equation (4-3)).

4.2.3 Deposition

Containment aerosols can deposit or settle onto containment surfaces and structures. Deposition occurs through four processes: gravitational settling, diffusion to surfaces, thermophoresis, and diffusiophoresis. Of these natural depletion processes, gravitational settling is often the dominant mechanism, although phoretic effects may be significant in some cases. In general, particle diffusion is considered to be a relatively unimportant deposition process. For some ESF decontamination calculations, a fifth process, inertial impaction, is included.

For postaccident aerosols in containment, the gravitational deposition removal mechanism is governed by the following particle settling equation:

$$v_s = \frac{d_p^2 \rho_p g C_m}{18 \mu \chi} \quad (4-9)$$

where

$$\begin{aligned} v_s &= \text{the downward settling terminal velocity (m/s);} \\ d_p &= \text{the particle diameter (m);} \\ \rho_p &= \text{the particle density (kg/m}^3\text{);} \\ g &= \text{acceleration of gravity = 9.8 m/s}^2\text{;} \\ C_m &= \text{the Cunningham slip correction, which reduces the} \\ &\quad \text{Stokes drag force to account for noncontinuum} \\ &\quad \text{effects, is expressed as} \\ &= 1 + \frac{2\lambda}{d_p} [\text{slip} + 0.4 \exp(-1.1 d_p / 2\lambda)] \text{ (dimensionless)} \end{aligned}$$

where

$$\begin{aligned} \lambda &= \text{mean free path of air at 298K} \sim 0.069 \cdot 10^{-6} \text{m;} \\ \text{slip} &= \text{slip factor (1.257);} \\ \mu &= \text{viscosity of air at 298K} \sim 1.8 \cdot 10^{-5} \text{(N}\cdot\text{s/m}^2\text{);} \\ &\quad \text{and} \\ \chi &= \text{dynamic shape factor.} \end{aligned}$$

One basic restriction of this model is that the aerosol particle Reynolds number Re must be much less than 1. This physically means that inertial effects of the flow may be neglected. This Reynolds number is not to be confused with the moving intercell mass (air, steam, aerosol particles) Reynolds number, which is typically much greater than one.

Another aerosol deposition mechanism results from diffusion of aerosols in a concentration gradient, that is, from a higher to a

lower concentration region. The diffusive deposition velocity is given by

$$v_{\text{diff}} = \frac{\sigma T C_m}{3\pi\mu d_p \Delta} \quad (4-10)$$

where

v_{diff} = diffusion deposition velocity (m/s);
 σ = Boltzmann Constant = $1.38 \cdot 10^{-23}$ (J/s-m²K⁴);
 T = atmosphere temperature (K);
 μ = viscosity (N·s/m²); and
 Δ = user-specified diffusion boundary layer thickness (m).

It is assumed that there is no gas velocity perpendicular to the deposition surface. This mechanism is most effective for smaller aerosol particle sizes.

Thermophoresis is another aerosol deposition mechanism, which results from the force exerted on aerosol particles by temperature gradients in containment. The thermophoretic deposition velocity v_{therm} is given by

$$v_{\text{therm}} = \frac{1.5 \mu C_m (C_t \text{Kn} + k_{\text{gas}}/k_p) \nabla T}{\chi \rho_{\text{gas}} T (1 + 3 C_m \text{Kn}) (1 + 2 C_t \text{Kn} + k_{\text{gas}}/k_p)} \quad (4-11)$$

where

Kn = $2\lambda/d_p$ (Knudsen number),
 k_{gas}/k_p = ratio of thermal conductivity of gas over that for aerosol particle k_p , and is user-specified,
 ∇T = structure surface temperature gradient (K/m),
 ρ_{gas} = gas density (kg/m³),
 T = wall temperature, and
 C_t = constant associated with the thermal accommodation coefficients (~1).

Still another aerosol deposition mechanism is diffusiophoresis. Diffusiophoresis occurs because aerosols suspended in a nonuniform mixture of gases will experience a force resulting from the concentration gradients of the gas components. This process can be activated by gas or vapor diffusing in air. If the vapor, for example water vapor, is denser than air, the water vapor molecules will impart a greater momentum to an aerosol particle from the side of higher water vapor concentration, which forces the aerosol particle in the direction of the diffusion of the heavier molecules. Water vapor condensing (or evaporating) from a surface is only one, but an important, producer of diffusiophoresis.

Stokes drag is also produced by the aerodynamic (Stefan) flow near condensing/evaporating surfaces [Hin82].

The aerosol deposition velocity equation for water vapor is the combination of diffusiophoresis forces and competing (opposite) Stokes drag attributable to Stefan flow.

$$v_{\text{dep}} = \left[\frac{\gamma_1 \sqrt{M_w}}{\gamma_1 \sqrt{M_w} + \gamma_2 \sqrt{M_w}} \right] \left(\frac{\dot{m}_{\text{tr}}}{\rho_w A_{\text{ap}}} \right) \quad (4-12)$$

where

$$\begin{aligned} M_w &= \text{molecular weight of water (kg/kgmole),} \\ \dot{m}_{\text{tr}} &= \text{mass rate of water condensed/evaporated to/from} \\ &\quad \text{the aerosol particle to/from the atmosphere} \\ &\quad \text{(kg/s),} \\ A_{\text{ap}} &= \text{outer surface area of an aerosol particle (m}^2\text{),} \\ \rho_w &= \text{density of water film boundary layer immediately} \\ &\quad \text{adjacent to the aerosol particle (kg/m}^3\text{), and} \\ \gamma_1 \text{ and } \gamma_2 &= \text{aerosol intermediate factors, defined as:} \\ \gamma_1 &= \frac{P_{\text{sat}}(T_{\text{ap}})}{P_{\text{gas}}} \end{aligned} \quad (4-13)$$

and

$$\gamma_2 = 1 - \gamma_1 \quad (4-14)$$

where

$$\begin{aligned} P_{\text{sat}}(T_{\text{ap}}) &= \text{water saturation pressure evaluated at the} \\ &\quad \text{aerosol temperature } T_{\text{ap}} \text{ (Pa); and} \\ P_{\text{gas}} &= \text{atmospheric gas pressure (Pa).} \end{aligned}$$

An equation similar to Equation (4-12) is calculated with the heat and mass transfer for the heat structures (see Section 6.4). This velocity is an example of a model generating a tightly coupled interface variable between models. The velocity calculated in Equation (4-12) is away from the surface for evaporation, and toward the surface for condensation.

With these four velocities defined, CONTAIN uses them to calculate the aerosol removal rate term $\mathcal{R}$ (kg/m³·s) in Equation (4-3). The $\mathcal{R}$ term includes the processes from four physical deposition

mechanisms: gravity, diffusion, thermophoresis, and diffusio-phoresis, which is defined as

$$\bar{\mathcal{R}} = \sum_{j=1}^{N_{str}} \sum_{k=1}^{N_a} \sum_{\ell=1}^m Dep_{j,\ell} Q_{\ell,k} \quad (4-15)$$

where

- N_{str} = total number of heat structure surfaces and/or pool surfaces for aerosol deposition in cell i ;
- N_a = total number of aerosol material components;
- m = total number of aerosol sections;
- $Dep_{j,\ell}$ = pseudo-deposition rate for the heat structure j for aerosol section ℓ (s^{-1}); and
- $Q_{\ell,k}$ = aerosol density for section ℓ of component k (kg/m^3).

$Dep_{j,\ell}$ in Equation (4-9) is defined as

$$Dep_{j,\ell} = \frac{A_j}{V_i} (v_g + v_{diff} + v_{therm} + v_{dep}) \quad (4-16)$$

where

- A_j = heat structure surface j (m^2), and
- V_i = cell volume i (m^3).

The first three velocity terms in Equation (4-16), which represent the three deposition velocities, are computed by multiplying the deposition coefficients with their forcing functions. First, these coefficients are integrated from a form similar to Equations (4-9) to (4-11) for a range of the user-defined minimum/maximum aerosol temperatures and pressures. Thus, a table of deposition coefficients is generated for later usage. Based on the current condition of the aerosol, these coefficients (AC terms in Equation (4-17)) are interpolated from this table.

The interpolated sectional deposition coefficients CF_i for the deposition mechanism i are given by

$$CF_i = (1-F_T)(1-F_p)AC_{11,i} + F_pAC_{12,i} + F_T(1-F_p)AC_{21,i} + F_pAC_{22,i} \quad (4-17)$$

where

- AC_{11,i} = the aerosol coefficient for the deposition mechanism i for the lowest atmospheric temperature (T_{min}) and pressure (P_{min}),
- AC_{12,i} = the aerosol coefficient for the deposition mechanism i for the lowest atmospheric temperature (T_{min}) and highest pressure (P_{max}),
- AC_{21,i} = the aerosol coefficient for the deposition mechanism i for the highest atmospheric temperature (T_{max}) and lowest pressure (P_{min}), and
- AC_{22,i} = the aerosol coefficient for the deposition mechanism i for the highest atmospheric temperature (T_{max}) and pressure (P_{max}).

And F_T and F_P in Equation (4-17) are defined as

$$F_T = \left(\frac{T_{\text{gas}} - T_{\text{min}}}{T_{\text{max}} - T_{\text{min}}} \right) \quad (4-18)$$

and

$$F_P = \left(\frac{P_{\text{gas}} - P_{\text{min}}}{P_{\text{max}} - P_{\text{min}}} \right) \quad (4-19)$$

where

- T_{gas} = cell temperature (K), and
- P_{gas} = cell pressure (Pa).

The deposition velocities in Equation (4-16) are computed by multiplying these coefficients CF_i with their forcing functions. For the gravitational deposition, the forcing function is the direction of air/aerosol mass flow (that is, up or down). The diffusion deposition forcing function is Δ (that is, diffusion boundary layer thickness). The thermophoresis deposition forcing function is ∇T (that is, temperature gradient at surface).

In CONTAIN, the user should note that aerosols will not deposit onto a structure surface if the outer face of the structure is specified to be adiabatic or outside of the cell in which the structure is defined, even if aerosol particles are present in the cell where the outer face resides. The outer surface of a ceiling structure is considered a floor deposition area and 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. 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.

Direct natural deposition (such as settling) into the LC is not modeled; however, aerosol mesh losses may accumulate in a LC pool. When this happens the coolant component of the aerosol is added to the mass of water in the pool. Also, aerosols may accumulate in the pool through the action of CSs, ICs, or FCs: the engineered safety systems.

4.3 Sources

Additional input to the aerosol dynamics model includes the source term S in Equation (4-3). These sources may include aerosols from the LC (for example, core-concrete interactions) or aerosol removal by other models (for example, ESFs). Descriptions of the ESF models are given in Section 6. The source terms carry units of mass per size group l and component k , so they are directly added to the appropriate aerosol inventory each timestep.

Sources may also be explicitly specified by the user. Such user-supplied sources may be introduced directly into the atmosphere or through BWR vents. When introduced through BWR vents, the aerosols can be size-dependent and can pass through a suppression pool to be scrubbed should the vents be submerged. This simulation is explained in the following section.

4.4 Aerosol Scrubbing Model

Two models are available for scrubbing aerosol materials passing through suppression pool vents; an adaptation of the SPARC code [Owc85a] and the model taken from the VANESA code [Pow86], which is referred to in CONTAIN as SCRUB. These models are also used for the SRV discharge model. The SCRUB model is also used in conjunction with CORCON-MOD2/VANESA. These models calculate the decontamination factors that arise from the scrubbing that 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 because of 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, that is, the discussion 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 that 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 (for example, to simulate elliptical bubbles with enhanced scrubbing) or a smaller value (for example, 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 [Owc85a], 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 caused by 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 Owc85a. 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 because of 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 FPs hosted by these aerosols. Note that the scrubbing of FPs not hosted by aerosols, such as vapor phase iodine, is not modeled. These FPs pass through the pool without being affected. The targeted release and acceptance formalism may be useful in simulating iodine scrubbing.

5.0 FISSION PRODUCT BEHAVIOR MODELS

In a reactor accident, a principal concern is the risk associated with potential release of radionuclides from the containment system to the outside environment. This section describes the FP behavior models used in CONTAIN 1.1 to estimate this potential source term. The term "fission product" is used in CONTAIN to represent all radionuclides, including actinides and other neutron activation products.

FP behavior is treated in CONTAIN by a set of models that includes the FP linear decay chain model, the FP decay heating model, the FP targeted release and acceptance model, and the FP liquid transport model.

CONTAIN depends on input from the user for the initial inventory and location of FPs. From that point on, CONTAIN tracks FP decay and determines the inventories of each isotope. FP parent-daughter relationships are defined in the input by specifying the decay chain structure as a series of linear chains. The decay constants and initial masses are also specified in the input. Only beta and gamma decay schemes can be modeled because CONTAIN 1.1 assumes decay creates no mass changes. Although a large number of decay chains can be specified, normally only a selected subset of radionuclides is of interest for radiological or transport reasons. These important radionuclide decay chains are typically specified explicitly, and the remaining FP inventory is handled in a generic way for decay heat analysis. FPs are associated with various "hosts," or repositories. A host can be gas, aerosol, heat structures, or a LC layer or pool.

Some hosts, such as the UC atmosphere gas or aerosol, are mobile, while others, such as the wall surfaces, are fixed. In general, the initial introduction of FPs onto various hosts is specified by the user. CONTAIN then tracks the transport of the FPs according to a variety of mechanistic and nonmechanistic models enumerated below.

One way in which FPs are transported is through the movement of the mobile hosts. FPs can be tracked as individual nuclides and/or as user-defined FP groups (such as elemental or compound groups). Transport of FPs associated with atmospheric hosts (gases and aerosols) is modeled mechanistically. Except for removal of gaseous iodine species by CSSs, the removal of gaseous FPs from the atmosphere is not modeled mechanistically. Further transport of FPs, once removed from the atmosphere, is generally not modeled, with the exception of that resulting from condensate films draining from heat-transfer structures and that resulting from pool-to-pool liquid transport. Simple, yet partially mechanistic, models are available for the latter processes. The code tracks the location and movement of FPs throughout the containment system. If a breach of containment occurs to a cell that represents the outside environment, the code will predict the extent of FP releases from containment.

FP masses, as treated by CONTAIN, do not influence the dynamics of their hosts, except through possible heating effects. Thus, FPs associated with aerosol hosts will not influence aerosol dynamics. In effect, FPs are treated as massless. Therefore, the intercell flow of FPs is governed primarily by the movement of gas and aerosol by the intercell flow model and by the liquid transport model for FPs that are present in liquid pools.

In addition to transport with hosts, FPs can transfer among hosts. This process is controlled by the targeted release and acceptance model. User-specified transfer rates within the targeted release and acceptance formalism in CONTAIN provide a flexible, nonmechanistic way to simulate the change in the affinity of a FP for its host when it decays. Transfer rates can depend on the host temperatures; however, no mechanistic models are provided for the determination of these transfer rates. User-specified transfer rates may also be useful in modeling other processes, such as, revaporization, which can be modeled to be a function of temperature, see Section 5.3.

CONTAIN also includes a FP heating model for lumped stationary FPs in the LC. Decay heating can be included for both individual decay chains and the balance of FP decay heat. A decay heating model ensures that the sum of the decay power from all inventories equals the ANSI-standard decay power appropriate to the reactor operating power and fuel burnup [Ame79].

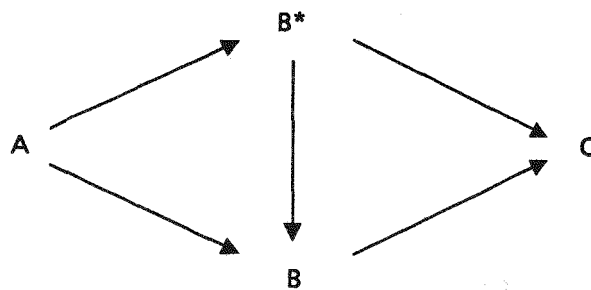
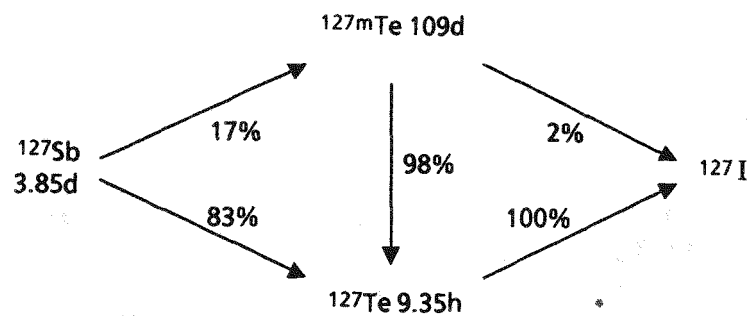
Section 5.1 discusses the FP linear decay chain model. Section 5.2 describes the models for FP heating. Section 5.3 discusses the targeted release and acceptance model, and Section 5.4 details the FP liquid transport model. The intercell transport of FPs hosted to gases and aerosols is discussed in Section 3.6.

5.1 Linear Decay Chain

The decay of FPs and the accumulation of decay product daughters are modeled in CONTAIN using the techniques 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 treated independently so only the masses in one chain are needed to solve for the effects of decay at any given time.

The system shown in Figure 5-1 is an example of a branching and merging decay chain formulated in terms of the three linear chains shown at the bottom of the figure. Because the same FP can appear in more than one linear chain, the rules for determining initial masses and half-lives to be used in the linear chains must be carefully specified by the user. The CONTAIN User's Manual [Mur89] describes the initialization of the linear decay chain model. A brief description of the rules also follows here.

Initialization of the model requires input of decay constants and initial masses. The decay constants appropriate for each linear



1. A → B* → B → C
2. A → B* → C
3. A → B → C

Figure 5-1. Example of FP Linear Decay Chains Derived from a Branched Decay Chain

chain can be determined from the branching ratio and the parent decay constant.

$$\lambda_1 = \lambda BR_1$$

where

$$\begin{aligned}\lambda &= \text{decay constant of parent,} \\ \lambda_1 &= \text{decay constant for branch 1, and} \\ BR_1 &= \text{branching ratio for branch 1.}\end{aligned}$$

The branching ratios and decay constants are tabulated in most core inventory code libraries, and are based on data provided in ENDF/IV or V listings [Koc81].

Consider the decay of ¹²⁷Sb in Figure 5-1. The decay constant of the parent, ¹²⁷Sb, is 0.18 day⁻¹. The branching ratio for the dominant branch to ¹²⁷Te is 0.83. That is, 83% of the disintegration of ¹²⁷Sb results in ¹²⁷Te. The decay constant for this branch is

$$0.83 (0.18 \text{ day}^{-1}) = 0.15 \text{ day}^{-1}.$$

Similarly, the decay constant for the branch to ^{127m}Te is

$$0.17 (0.18 \text{ day}^{-1}) = 0.03 \text{ day}^{-1}.$$

When a complex chain is reduced to a set of linear chains, the isotopic inventory must be apportioned to each chain according to inventory factors. These factors are determined from the products of the branching ratios for the linear chain.

These factors, one for each isotope in each chain, are then multiplied by the isotopic mass inventory to obtain isotopic mass per chain. The factors themselves are calculated by multiplying together the branching ratios per isotope for each chain. Some chain segments will be seen to be identical. Inventory factors for the repeated isotopes in identical segments are divided equally among the isotopes.

For the example in Figure 5-1, the inventory factors *F* are calculated as follows:

For linear chain 1,

$$\begin{aligned}F_A &= (0.17) (0.98) = 0.166 \\ F_{B^*} &= 0.98 \\ F_B &= 1.0/2 = 0.5.\end{aligned}$$

For linear chain 2,

$$\begin{aligned}F_A &= (0.17) (0.02) = 0.0034 \\ F_{B^*} &= 0.02.\end{aligned}$$

For linear chain 3,

$$\begin{aligned} F_A &= 0.83 \\ F_B &= 1.0/2 = 0.5. \end{aligned}$$

In addition, 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 FP decay are linear, a source of FPs that occurs after the start of the problem can be taken into account by adding the source masses to existing masses. The user must specify the external sources and times initially; code calculated (internal) sources are added automatically.

The mathematical description of this kind of decay can be decoupled into linear differential equations if each is fed by a single parent and each decay is assumed to be beta or gamma (massless). The resulting equations [Eng68] follow:

$$m_1 \xrightarrow{\lambda_1} m_2 \xrightarrow{\lambda_2} m_3 \cdots m_j \xrightarrow{\lambda_j} \cdots m_n \quad (5-1)$$

$$\frac{dm_1}{dt} = -\lambda_1 m_1 + S_1$$

$$\frac{dm_2}{dt} = \lambda_1 m_1 - \lambda_2 m_2$$

⋮

$$\frac{dm_j}{dt} = \lambda_{j-1} m_{j-1} - \lambda_j m_j + S_j$$

⋮

$$\frac{dm_n}{dt} = \lambda_{n-1} m_{n-1}$$

where

$$\begin{aligned} m_j &= m_j(t) = \text{mass (kg) of isotope } j \text{ present at time } t, \\ \lambda_j &= \text{decay constant (s}^{-1}\text{) for the } m_j \text{ isotope,} \\ dm_j/dt &= \text{rate of change (kg/s) of the nuclide; and} \\ S_j &= \text{source of nuclide } j \text{ from intercell flow and/or} \\ &\quad \text{external sources (kg/s).} \end{aligned}$$

To model this decay process, CONTAIN defines the one-sided Laplace transform for a class of functions $f(t)$, as is established in Reference Eng68, for $t \geq 0$:

$$L[f(t)] = \int_0^{\infty} f(t) e^{-st} dt \equiv F(s) \quad (5-2)$$

where s is a complex variable and L is the Laplace transform operator.

If the Laplace transform is taken on both sides of Equation (5-1), using the rules of Laplace transform theory, a solution can be obtained for use in CONTAIN:

$$m_n(t) = \sum_{k=1}^n \sum_{m=0}^k \prod_{j=k}^n \lambda_j \sum_{i=k}^n \frac{e^{-\lambda_i t}}{\prod_{\substack{m=k \\ m \neq i}}^n (\lambda_m - \lambda_i)} \quad (5-3)$$

This model receives user-specified information, such as FP decay constant (λ) and FP initial source inventory $\begin{bmatrix} 0 \\ m \\ k \end{bmatrix}$. Equation 5-3 then is used to calculate the mass of each nuclide remaining after decay over a timestep for use by other FP models, such as the FP heating model.

5.2 Fission Product Decay Heating

FP behavior is coupled to the thermal-hydraulics models in CONTAIN through the effects of FP decay heating. The FP heating model in CONTAIN calculates the amount of energy deposited in the atmosphere and heat structures resulting from the absorption of the beta and gamma nuclear radiation. The energy associated with the decay of FPs hosted to the gas and to aerosols is assumed to be deposited in the atmosphere. The energy associated with the decay of FPs on structure surfaces is assumed to heat the structure surface. The decay energy of FPs in the LC layers is assumed to be distributed uniformly throughout each layer, with the exception of the concrete layer where it is always deposited into the uppermost node.

The decay of each radioisotope is modeled according to user-specified decay chains, half-lives, and decay powers. This provides the following two features:

1. The daughter products may be a different element, and may be released and accepted among hosts at different rates.
2. The heat of the radioactive decay is deposited at the location of the appropriate host. (This is a simplifying assumption.)

However, it is usually undesirable to specify in detail all of the radioisotopes that would contribute to decay heating, as this would require a large amount of input. Normally, only a selected subset of radioisotopes is of interest for radiological reasons, and it is these radioisotopes that are typically specified by species or, if desired, FP groups. The remaining decay heat from the reactor fuel can be handled in a different way. The ANSI/ANS-5.1-1979 standard "American National Standard for Decay Heat Power in Light Water Reactors" [Ame79] is the basis for the FP decay heat quantities used in this model. The power associated with the specified individual radioisotopes is subtracted from this total power, and the remaining power is then deposited in a number of locations (coolant pool, atmosphere, etc.) according to fractions specified in the user input. This formulation greatly reduces the computational time [Wil87].

For FP decay chain elements representing individual radionuclides, the user can specify a constant decay power in watts per kilogram. To accommodate the representation of FP groups, a time-dependent decay power option is used. 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

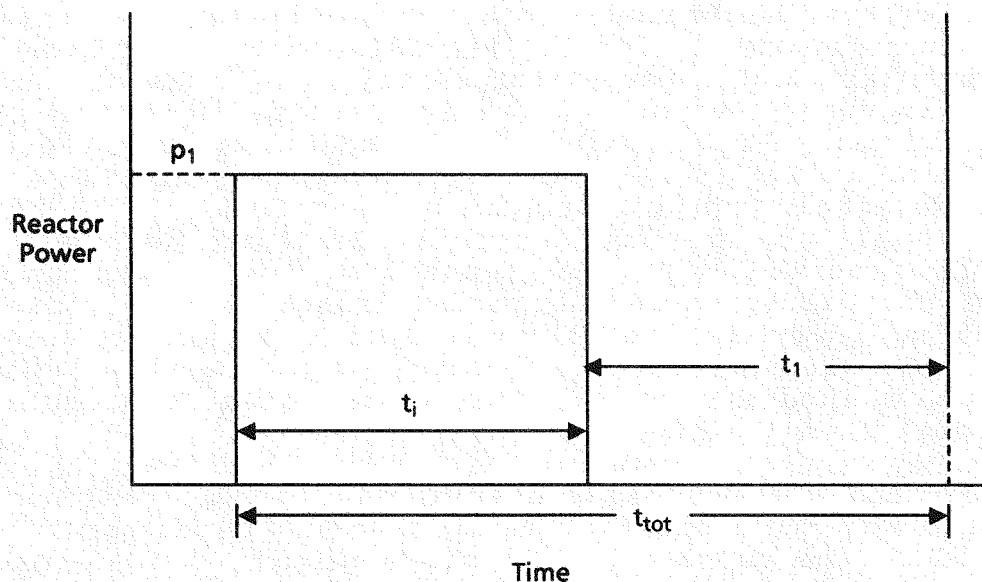
$$p' = a_1 (e^{-a_2 t}) + a_3 (e^{-a_4 t}) \quad (5-4)$$

where t is time in seconds and a_2 and a_4 are inverse seconds s^{-1} .

A coefficient not specified defaults to zero; for example, if only three coefficients (a_1 , a_2 , and a_3) are given, a_4 will be zero. Note that at $t = 0$ second, p' calculated by Equation (5-4) generally represents decay power for that element at shutdown.

The ANS-5.1 decay heat model [Ame79] describes the total FP energy deposition rate resulting from alpha, beta, and gamma emissions, as a function of time after a reactor abruptly shuts down, such as after a reactor scram. The model taken from the ANS-5.1 methodology is that for the thermal fission of ^{235}U and ^{239}Pu , and the fast fission of ^{238}U , which is appropriate for LWR applications.

The FP heat model used by CONTAIN assumes that the reactor power level was constant over a discrete time period prior to scram, as depicted by the histogram in Figure 5-2. This model distributes the balance of the FP decay power, that is, total FP decay power minus that associated with the decay power from user-specified FP decay chains, to various LC layers or the LC pool, as defined by the user. This makeup power can be used as decay heat source for the core-concrete interactions using the CORCON-MOD2/VANESA models, if they were invoked. Once this power is apportioned to the core-concrete interaction, CONTAIN can model the decay heat that results from the generation of FPs hosted on the aerosols and gaseous FPs from the core-concrete interaction. This modeling requires mapping the user-specified FPs against those released from the VANESA



p_1 = Average reactor power

t_i = Total operating time interval, including intermediate intervals at zero power, seconds

t_1 = Time after shutdown or severe accident; cooling time, seconds

t_{tot} = Total time after start of reactor power

Figure 5-2. Reactor Power and Decay Time Intervals

model. CONTAIN also monitors the decay heat of FPs released from the LC layers in events not involving core-concrete interaction and FPs from the pool-to-pool transport. The code internally adjusts the makeup power in the LC to account for the decay heat leaving the LC in a situation such as a core-concrete interaction. Although any FP heat from LC hosts is added to appropriate locations, the makeup power must remain in the cell. This model also verifies that the decay power from individual FPs does not exceed the decay power for the entire core.

CONTAIN models FP decay heat using calculations found in the standard decay heat tables in the appendices of Reference Ame79.

$$P_{fp} = (F_{LWR})(P_{ANS}) \quad (5-5)$$

where

P_{fp} = total reactor core FP decay heat power (W),
 F_{LWR} = LWR reactor power factor, and
 P_{ANS} = calculated decay heat power (W), obtained using the American National Standard tables [Ame79].

The p_{ANS} in Equation (5-5) is defined as

$$P_{ANS} = [P_{dh} + P_{UN}] F_{scale} \quad (5-6)$$

where

P_{dh} = decay heat power from FP of ^{235}U , ^{239}Pu , and ^{238}U (W);
 P_{UN} = decay heat power from FP of ^{239}U and ^{239}Np (W); and
 F_{scale} = FP scale factor, which is a constant = 0.947.

The limitations of the ANS decay heat model include the following:

1. It is not applicable for decay time greater than 10^9 seconds.
2. It is specifically for LWRs.
3. It is a core-average decay heat model.
4. Fissionable nuclides other than ^{235}U , ^{238}U , and ^{239}U are accounted for by treating them as ^{235}U .

This model must be initialized by specifying the reactor operating time and power before the accident, and the time after the accident that the CONTAIN analysis starts. This model distributes calculated decay energy to UC and LC locations.

5.3 Targeted Release and Acceptance of Fission Products

Users can select to release FPs from their specific locations, such as structure, aerosol, and/or fuel, to other user-specified targets or hosts, such as the UC atmospheric gas. This formalism is known and modeled in CONTAIN as the targeted release and acceptance model.

Modeling of the release and acceptance phenomena is made possible through an inventory scheme in which FPs are assigned to various hosts. The user should assign FPs to a host based primarily on the chemical affinity and physical characteristics of the FP. These assignments may be made for the initial FP inventory and for time-dependent sources of FPs. If CORCON-MOD2 is being used, certain targeted and release hosts are not allowed (for example, LC layers). As described in Section 5.2, for tracking purposes VANESA constituents may be assigned as CONTAIN FPs to CONTAIN aerosol hosts through the option described in the CONTAIN User's Manual [Mur89].

The UC atmospheric gas and each component of the suspended aerosols are always hosts in every cell. The code automatically defines surfaces of heat transfer structures and LC layers as hosts. Both surfaces of each structure and each LC layer are taken to be individual FP hosts. This includes the upper LC-model layer that represents the atmosphere. Therefore, each cell will generally have a different number of FP hosts. A dummy host is also provided in each cell to allow the modeling of FP holdup.

The transport of CONTAIN host materials within the cell may cause the FP to change hosts; for example, aerosol deposition causes a FP attached to the aerosols to become attached to the deposition surface. A semimechanistic model for the washdown of FPs from structure surfaces to a pool is available. In general, however, host changes need to be specified by the user through the targeted release and acceptance formalism described below.

In this formalism, the user can specify transfer rates for individual FPs between any number of host pairs. For a given host pair i, j , the fractional transfer rates per second $r_{i \rightarrow j}$ for a particular FP may depend on the host temperature T_i or T_j according to the following expressions:

$$r_{i \rightarrow j} = \left\{ \begin{array}{ll} a \exp(-b/T_i) & \text{for } T_i \geq T_{\text{threshold}} \\ 0 & \text{for } T_i < T_{\text{threshold}} \end{array} \right\} \text{ if } a > 0 \quad (5-7)$$

$$r_{j \rightarrow i} = \left\{ \begin{array}{ll} |a| \exp(-b/T_j) & \text{for } T_j > T_{\text{threshold}} \\ 0 & \text{for } T_j < T_{\text{threshold}} \end{array} \right\} \text{ if } a < 0$$

where a , b , and $T_{\text{threshold}}$ are user-specified parameters that define the threshold temperature below which the release rate or the transfer rate is set to zero. FPs are assumed to transfer at mass rates proportional to the amount of FP mass present. For example, the simple case of the transfer between one pair of hosts at the fractional rate, $r_{i \rightarrow j}$ per second is represented by the coupled equations:

$$\frac{dm_i}{dt} = -r_{i \rightarrow j} m_i, \quad \frac{dm_j}{dt} = r_{i \rightarrow j} m_i \text{ if } a > 0 \quad (5-8)$$

$$\frac{dm_j}{dt} = -r_{j \rightarrow i} m_j, \quad \frac{dm_i}{dt} = r_{j \rightarrow i} m_j \text{ if } a < 0 \quad (5-9)$$

where

m_i represents the FP mass of the i^{th} host, and
 m_j represents the FP mass of the j^{th} host.

For simple coupled equations like those given in Equation (5-8), FP mass redistributions are calculated using the analytic solution.

The trivial solution, where each host is involved in only one targeting equation, is given by

$$m_i(t) = m_i(0) e^{-r_{i-j}t} \quad (5-10)$$

$$m_j(t+\Delta t) = m_j(t) + m_i(t)(1 - e^{-r_{i-j}\Delta t}) \quad (5-11)$$

where Δt is the CONTAIN calculation timestep, and $a > 0$.

For $a < 0$,

$$m_j(t+\Delta t) = m_j(t) e^{-r_{j-i}\Delta t} \quad (5-12)$$

$$m_i(t+\Delta t) = m_i(t) + m_j(t)(1 - e^{-r_{j-i}\Delta t}) \quad (5-13)$$

In addition to this trivial case, other cases involving FP release from one host to more than one other host can be solved in this direct fashion. Likewise, this solution is applicable to the case where multiple hosts are releasing the same FP to a common host. The only requirement is that no one host is releasing and accepting the same fission chain element. If the sets I and J are defined as

I = family of all releasing hosts for a FP and
J = family of all accepting hosts for a FP,

then mathematically, $I \cap J = 0$ is the requirement for the following decoupled solution to be valid:

$$s_i = \sum_j r_{i \rightarrow j} \quad (\text{sum of all release rates from host } i \text{ to all receiving hosts } j) \quad (5-14)$$

$$m_i(t+\Delta t) = m_i(t) e^{-s_i \Delta t} \quad (\text{for } i \in I) \quad (5-15)$$

$$m_j(t+\Delta t) = m_j(t) + \sum_i \frac{r_{i \rightarrow j} m_i(t) [1 - e^{-s_i \Delta t}]}{s_i} \quad (\text{for } j \in J) \quad (5-16)$$

where $j \in J$ means j is a member of (or is contained in) the set J, and the same is true for $i \in I$.

Certain targeting scenarios are not so simple. They lead to equations that are more highly coupled. More complex coupled equations are solved by a highly accurate exponential operator

method [Lee80]. The general target problem is written in matrix form as

$$\frac{d\vec{m}}{dt} = \mathbf{A} \vec{m} \quad (5-17)$$

where $\vec{m}$ is a vector of all FPs on hosts, and $\mathbf{A}$ is a matrix of release rates from one host to another.

The Ash exponential operator method [Lee80, Was83] is used to transmute the $\mathbf{A}$ matrix forward in time (analogous to scalar exponentiation) to give the solution

$$\mathbf{m}(t + \Delta t) = [e^{\mathbf{A}\Delta t}]_{\mathbf{m}(t)} \quad (5-18)$$

This method was chosen over implicit finite difference methods because of its ability to solve the highly coupled and large global timestep case reliably and within a reasonable computer time [Was83]. Even though the implicit method was slightly more efficient than Ash (when using one time node), preliminary computations indicate as much as 50% error in mass calculation can result from such a violation of the characteristic timestep.

If the equations are decoupled, the direct solution method is used. Otherwise, the coupled matrix is solved using the operator method.

Targeted release rates are associated with FP names and are applied to all fission chain elements having the specified name. Therefore, all chain elements having the same FP name will transfer at the same rate. For example, when a release rate is defined for nuclide C in Figure 5-1, the masses of the C elements in chains 1, 2, and 3 are all transferred at the same specified rate.

To illustrate the flexibility of the targeted release formalism when coupled with FP decay, consider the following example:

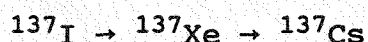
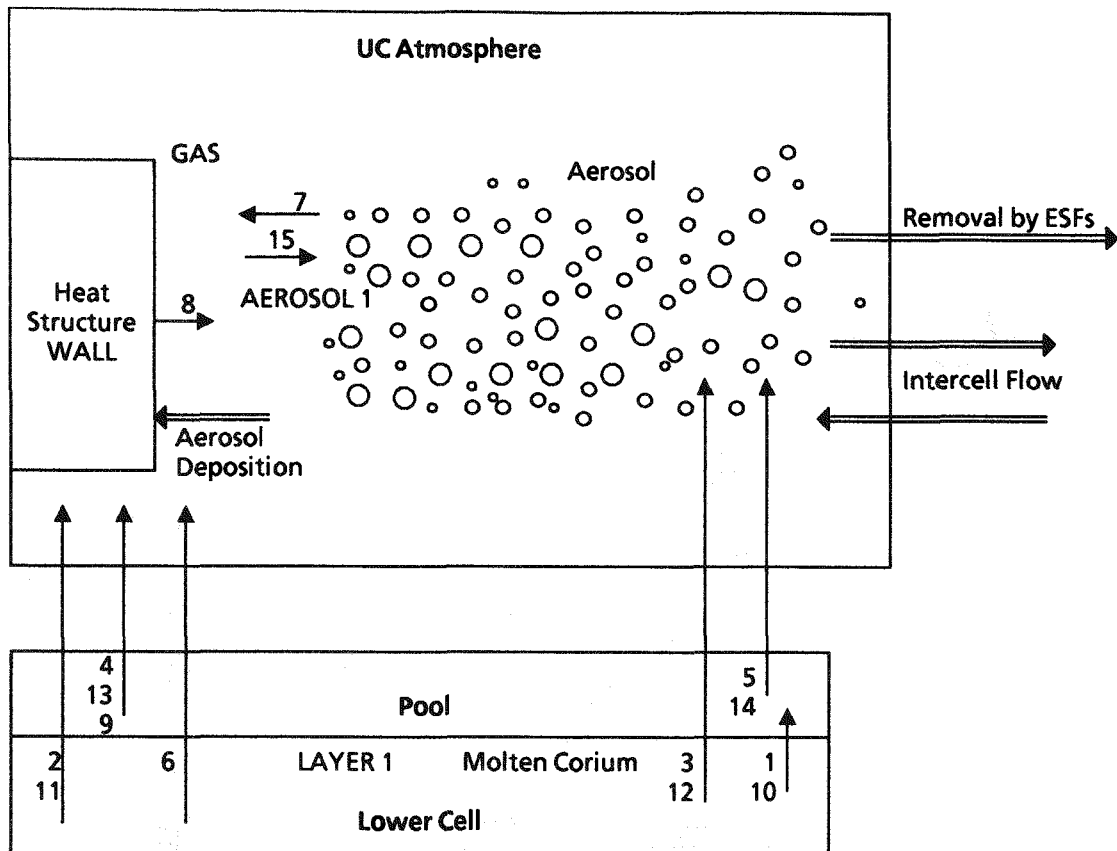


Figure 5-3 illustrates how the targeted release processes fit into the overall FP transport picture. In the example, all the initial mass is assumed to be iodine and hosted to the first LC layer (molten corium), and it is further assumed that a water pool exists above the corium layer. Decay processes govern the formation of xenon and, eventually, cesium. Targeted release processes affect the mass distribution among host materials. Intercell flow transports FPs hosted to the gas and aerosols to and from other cells in multicell problems (See Section 3.6). Finally, FPs in aerosol form deposit on the heat structures (such as walls).



- ESFs = Engineered safety features
 UC = Upper cell
 ==> = Processes simulated by other source and removal models
 ==> = Process simulated by targeted release and acceptance model

Figure 5-3. Example of FP Redistribution by Targeted Release and Acceptance Model for FPs Initially Located in the LC Fuel Layer (Numerical key on arrows corresponds to the process numbers in Table 5-1.)

In CONTAIN input descriptions, the hosts involved in this illustrative problem are called GAS (for the UC atmosphere), AEROSOL 1 (for aerosol component 1), WALL (for the surface of the wall heat structure), and LAYER 1 (for a LC layer representing corium), and POOL (for the overlying water pool).

Table 5-1 lists the target and release processes simulated in this example. The release rates in Table 5-1 simulate a variety of processes that may occur within a cell. It is assumed that melted corium is represented by Layer 1. The gaseous iodine and xenon are assumed to transfer from the fuel to the atmosphere (processes 2 and 6) at the rate of 0.1% per second. Based on current research, the transfer rate of cesium vapor (process 11) is assumed to be two orders of magnitude lower (10^{-5}). The rapid release of iodine and cesium from molten fuel in the form of aerosols (processes 3

Table 5-1
Illustrative FP Targeted Release Rates

Process	Nuclide	From	To	Rate (s ⁻¹)	Process Represented
1.	¹³⁷ I	LAYER 1	POOL	10 ⁻¹	Dissolution (Scrubbing)
2.	¹³⁷ I	LAYER 1	GAS	10 ⁻³	Vaporization
3.	¹³⁷ I	LAYER 1	AEROSOL 1	10 ⁻¹	Aerosolization
4.	¹³⁷ I	POOL	GAS	10 ⁻⁵	Partitioning
5.	¹³⁷ I	POOL	AEROSOL 1	10 ⁻⁵	Aerosolization
6.	¹³⁷ Xe	LAYER 1	GAS	10 ⁻³	Outgassing
7.	¹³⁷ Xe	AEROSOL 1	GAS	5.0	Rapid gas escape
8.	¹³⁷ Xe	WALL	GAS	5.0	Rapid gas escape
9.	¹³⁷ Xe	POOL	GAS	1.0	Rapid gas escape
10.	¹³⁷ Cs	LAYER 1	POOL	10 ⁻¹	Dissolution (Scrubbing)
11.	¹³⁷ Cs	LAYER 1	GAS	10 ⁻⁵	Vaporization
12.	¹³⁷ Cs	LAYER 1	AEROSOL 1	10 ⁻¹	Aerosolization
13.	¹³⁷ Cs	POOL	GAS	10 ⁻⁵	Partitioning
14.	¹³⁷ Cs	POOL	AEROSOL 1	10 ⁻⁵	Aerosolization
15.	¹³⁷ Cs	GAS	AEROSOL 1	10 ⁻¹	Adsorption

and 12) is assumed to occur at the rate of 10% per second. Iodine and cesium can be trapped in the pool (processes 1 and 10) and xenon generated in the pool by decay processes can be released to the UC atmosphere (process 9). Any xenon hosted to the aerosols or to the wall of the structure (as a result of iodine decay) is assumed to be transferred to the gas at an essentially instantaneous rate (500%/s) (processes 7 and 8). Some iodine and cesium is assumed to be aerosolized from the pool to the UC atmosphere (processes 5 and 14) at a slow rate (10^{-5} s^{-1}). Partitioning of iodine and cesium from the pool to the UC atmosphere (processes 4 and 13) is modeled at a rate of 10^{-5} s^{-1} .

Finally, cesium hosted to the gas (as a result of release from the fuel or decay of xenon in the gas) is assumed to adsorb on the aerosols at the rate of 10% per second (process 15).

Because no default values are provided, the user must specify source and destination FPs, release rates, and host-target relationships. This model supplies FP locations to UC models and aerosol behavior models.

5.4 Liquid Transport of Fission Products

This model simulates FP cross-cell transport by liquids to pools or to floor surfaces of structures. The FPs are assumed to be well mixed in the pool liquid. The materials transported in liquid pathways between repositories of coolant liquid are restricted to the coolant and to FPs carried by the coolant. Although materials such as deposited noncoolant aerosols are not transported, the transport of FPs along with the coolant allows the user to assess the radiological inventories and the decay heating resulting from such transport.

If the user has specified that the overflow mass, which occurs from aerosol mesh losses or condensate (with or without FPs) runoff from structures, is to be ignored, the FPs are placed into a waste (overflow) cell. Otherwise, the FPs (if any) go to the LC pool with the condensate. If no pool exists (for example, because the expelled in-vessel steam could not condense or has not condensed), the FPs are transported to floor structures. If no floor structures or atmospheric source hosts exist, then the FP mass goes to the waste cell. This waste cell should not be confused with the BWR drywell, which is also sometimes called an overflow cell.

The transport of FPs in liquid pathways occurs in two instances. FPs present on structure surfaces as the result of aerosol deposition and other mechanisms may be transported with the condensate film draining from the surfaces. In addition to vapor condensation, coolant aerosol deposition may also contribute to the film. FPs deposited in coolant pools may also be transported along with the coolant in the flow between pools.

Part of the user input specifies transport efficiency factors that determine the transfer rate of FPs relative to the transfer rate of coolant. Only those FPs assigned a finite value in the input will be transferred with the condensate runoff and the coolant flow between pools. The value of any transport efficiency factor is defined as the ratio of the FP fraction transferred from a repository per timestep, to the fraction of liquid transferred from that repository. Thus an efficiency factor of 1.0 will ensure movement of all FPs associated with the transported coolant.

The transport efficiency factors are assigned by FP name and apply globally to liquid pathway transfers of the FP. Fission chain elements that have the same FP name are automatically assigned the same liquid pathway transport efficiency factor.

6.0 EXPLICIT CELL MODELS

Sections 3, 4, and 5 describe the major phenomenological models in the CONTAIN code, including intercell flow and atmosphere thermal-hydraulic behavior, aerosol behavior, and FP decay, heating, and transport. Section 3 also describes the models for suppression pool behavior and the boiling of coolant pools. CONTAIN includes a number of support models to simulate various phenomena occurring within the containment in addition to the major models described in Sections 3, 4, and 5. These support models provide sources and sinks of mass and energy to the intercell flow and thermal-hydraulics modeling done by the implicit flow solver. In a few cases, they can also directly alter the thermodynamic state (used as a flow solver initial condition) of the atmosphere between flow solver integration steps. These models are denoted "explicit cell models" because of the explicit manner in which they couple to the flow solver.

Phenomena treated by the explicit cell models include evaporation and condensation of coolant onto structures, convective heat transfer between the atmosphere and structures, radiation heat transfer, hydrogen and carbon monoxide deflagrations, heat conduction within structures, heat and mass transfer resulting from the operation of ESFs, and pool-to-pool liquid redistribution. The mass sources and sinks associated with these processes are identified in Table 1-1, and the energy sources and sinks are identified in Table 1-3. Note that the source, so, and sink, si, terms defined in Section 1.4 are combined for convenience here. The governing equations given in the remainder of this chapter describe the explicit terms identified in these tables. The explicit mass terms that are defined in this section are:

- m_{bn} = sources and sinks of gases resulting from hydrogen and carbon monoxide combustion. The constituents affected by this model are: H_2 , CO , O_2 , H_2O , and CO_2 ;
- m_c = coolant mass sinks resulting from condensation or coolant mass sources resulting from evaporation; and
- m_{esf} = mass sinks resulting from operation of ESFs. This includes added or removed coolant, aerosol removal, and volatile iodine scrubbing.

The explicit energy terms that are defined in this section are:

- q_{bn} = hydrogen and carbon monoxide deflagration energy sources,
- q_c = convection and condensation/evaporation energy exchanges,
- q_{esf} = energy exchange resulting from operation of spray, FC, and IC ESFs, and
- q_r = radiation energy exchange.

The organization of Section 6 is as follows. Section 6.1 describes how CONTAIN calculates the bulk thermodynamic properties of the atmosphere and the dimensionless parameters used in the heat and mass transfer correlations. Section 6.2 discusses the hydrogen and carbon monoxide deflagration model, which was adopted from the HECTR code. Section 6.3 describes the explicit cell models for heat and mass transfer between the atmosphere and structures, including convection, condensation and evaporation, and radiation. Although modeling for the LC is not explicitly addressed in Section 6.3, the associated LC governing equations are basically the same as those presented herein with a few minor differences resulting from the different module interfaces. Section 6.4 describes the heat conduction model for structures. Again, the same model and governing equations are used for heat conduction in the LC; therefore, the LC is not discussed. Section 6.5 discusses the ESFs and LC liquid redistribution models.

Note that this document does not include an explicit discussion of the LC models. However, selective models that also apply to the LC as well as interfaces between the atmosphere and LC are discussed throughout this section. Corium-concrete interactions are also not discussed here; because, as explained earlier, these models have been directly imported from the stand-alone CORCON-MOD2 code and are documented in the CORCON-MOD2 manual [Col84].

6.1 Material Properties

Internal to the CONTAIN code is a library of physical properties for 50 standard materials that can be used in the modeling of containment systems. This library provides temperature-dependent specific enthalpy, specific heat, density, viscosity, and thermal conductivity for a variety of materials commonly found in nuclear reactor containments under severe accident conditions. Table 6-1 lists the standard materials available in CONTAIN and the corresponding name of each material in the library.

In addition to this library of material properties, the user may define new materials and their properties through tabular input. It is also possible to redefine the properties of one or more of the 50 internally defined standard CONTAIN materials through tabular input. These tables are temperature-based and must be given in standard CONTAIN units. The user must ensure that the tables cover the entire range of temperatures that are anticipated to be encountered in a given problem. If the temperature extends beyond the specified range, the enthalpy tables are linearly extrapolated beyond their limits. For all other properties the endpoint values are assumed for out-of-range temperatures.

Table 6-1
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

The material property library includes temperature-dependent functions for the following properties:

k	Thermal conductivity (solids, liquids, gases),
h	Specific enthalpy (solids, liquids, gases),
c _p	Specific heat capacity at constant P (solids, liquids),
c _v	Specific heat capacity at constant V (gases),
ρ	Density (solids, liquids), and
μ	Viscosity (gases)

As indicated in the above list, viscosity functions are not included for solids, and gas densities are determined from the ideal gas law. A complete listing of the property functions for each of the 50 materials in the CONTAIN 1.1 library is beyond the scope of this document. Moreover, these functions have undergone major revisions since CONTAIN 1.1. Refer to Reference Val88 for

the correlations in CONTAIN 1.1 and those developed for later versions of CONTAIN. The water enthalpy function used in CONTAIN was obtained from Reference Rey79.

6.1.1 Material Properties for Coolant

Coolant is the only atmosphere material in CONTAIN that is modeled to undergo phase changes. Water phase changes are included for modeling the melting of ice in the IC ESF model, condensation of steam onto structures and aerosols, pool boiling, and the evaporation of water films. The correct phase of water and the heat of fusion is automatically taken into account in the enthalpy function of water. The enthalpy function for water vapor as a function of temperature used in CONTAIN was obtained from Reference Rey79.

CONTAIN also performs the necessary calculations to determine the saturation pressure of vapor at a given temperature, and the temperature corresponding to saturated vapor at a given pressure. The latter function is determined by numerically inverting the saturation pressure function. The vapor saturation pressure function as a function of temperature was obtained from Reference Rey79.

Water mass and energy sources are accounted for as described in the conservation of mass equation in Table 1-2 and the conservation of energy equation in Table 1-3.

6.1.2 Bulk Thermodynamic Properties

This section describes the equations used in CONTAIN to obtain bulk material properties when two or more material components are present. In general the following weighted averaging method is used to obtain mixture properties in CONTAIN

$$\overline{MP} = \frac{\sum (MP_i \cdot WF_i)}{\sum WF_i} \quad (6-1)$$

where

$\overline{MP}$ = the weighted average property,
 MP_i = the value of the property for component i, and
 WF_i = the weighting factor for component i.

The weighting factor is described below for each property.

Bulk Gas Thermal Conductivity ($\bar{k}$) This property uses a weighting factor based on the number of moles of each component, that is, mole fraction

$$WF_i = \frac{Mo_i}{Mo_{tot}} \quad (6-2)$$

where

Mo_i = number of moles of component i, and
 Mo_{tot} = total moles of all components.

Bulk Gas Viscosity ($\bar{\mu}$) This property uses a weighting factor based on the mass of each component, that is,

$$WF_i = \frac{m_i}{m_{tot}} \quad (6-3)$$

where

m_i = mass of component i, and
 m_{tot} = total mass of all components.

Bulk Gas Specific Heat at Constant Volume This property uses a weighting factor that is based on the product of the component mass and the square root of the molecular weight, that is,

$$WF_i = \frac{m_i (Mo_i)^{1/2}}{\sum [m_i (Mo_i)^{1/2}]} \quad (6-4)$$

Additional mean values that are used include:

Bulk Density ($\bar{\rho}$)

$$\bar{\rho} = \frac{m_{tot}}{V} \quad (6-5)$$

where V = atmosphere volume. Note that this bulk density is not actually used in the calculation of intercell flow. The implicit inertial flow model uses the densities of the individual species in the upstream cell as explained in Section 3. The above calculated bulk density is calculated for output and for use in the transport property calculations described in Section 6.1.3.

Bulk Ratio of Specific Heats

$$\bar{\gamma} = 1 + \frac{R M o_{\text{tot}}}{m_{\text{tot}} C_v} \quad (6-6)$$

where R is the universal gas constant.

6.1.3 Transport Property Dimensionless Parameters

This section gives the equations for the dimensionless parameters used primarily in the convection and condensation models. The equations used to calculate the Prandtl number, Grashof number, Reynolds number, Schmidt number, and Sherwood number are given below and in the nomenclature list.

The Prandtl number Pr is calculated from

$$\text{Pr} = \frac{\mu c_p}{k} \quad (6-7)$$

where

μ = viscosity of the fluid (kg/m-s),
 c_p = specific heat (at constant pressure) of the fluid (J/kg-K), and
 k = thermal conductivity of the fluid (W/m-K).

The Grashof number Gr is calculated using

$$\text{Gr} = \frac{L^3 g \max(|\Delta T|, 10^{-4}) \left(\frac{\rho}{\mu}\right)^2}{T_{\text{BL}}} \quad (6-8)$$

where

L = length of a convective heating surface (m);
 g = acceleration of gravity (m/s^2);
 ρ = density of the fluid (kg/m^3);
 ΔT = temperature difference between the atmosphere and heat structure surface (such as a wall), calculated as
 $= T_{\text{gas}} - T_{\text{wall}}$
 T_{gas} = temperature (K) of the atmospheric gas and
 T_{wall} = temperature (K) of heat structure surface;
 and
 T_{BL} = film temperature,
 $= \frac{T_{\text{gas}} + T_{\text{wall}}}{2}$ (6-9)

The Reynolds number Re is calculated using

$$Re = \frac{\rho L v_{conv}}{\mu} \quad (6-10)$$

where v_{conv} is the convective velocity (m/s). Normally CONTAIN uses a natural convection correlation for convection heat transfer that does not depend upon Re . However, a forced convection correlation that depends on Re can be used as an option. The forced convection option requires that convective velocity v_{conv} be specified by the user.

The Schmidt number Sc is calculated using

$$Sc = \frac{\mu}{\rho D_{atm}}$$

with

$$\begin{aligned} D_{atm} &= \text{diffusivity of water vapor in air} \\ &= \frac{(4.4784 \cdot 10^{-6}) T_{BL}^{2.334}}{P_{gas}} \end{aligned} \quad (6-11)$$

where P_{gas} is the bulk atmosphere pressure.

Other dimensionless numbers used in the course of a CONTAIN calculation include the Nusselt number Nu and the Sherwood number Sh . The correlations used to calculate the Nusselt number are discussed in Section 6.3.2 on convection heat transfer. The Sherwood number is defined in Section 6.3.3 on condensation mass transfer modeling. All such dimensionless groups are summarized in the nomenclature list.

6.2 Hydrogen and Carbon Monoxide Burning

This section describes the hydrogen and carbon monoxide burn model in the CONTAIN code. Under certain accident conditions, hydrogen and/or carbon monoxide gases can build to sufficient concentrations to cause deflagrations to occur within the containment. The conditions under which a deflagration may occur have been measured experimentally and corresponding models for combustion based on these observations have been implemented into the HECTR computer code [Din86]. The burn model in CONTAIN is derived from the HECTR code and includes the HECTR burn-model update. Note that there are several implementation-specific differences between the CONTAIN and HECTR treatments. In addition, CONTAIN does not model continuous burning, which is available in HECTR. The deflagration ignition and propagation criteria, flame speed correlation, combustion

completeness correlation, and flame propagation criteria are basically the same as in HECTR.

The chemical reactions that occur during a deflagration are



Both of these reactions are exothermic, and the energy released is deposited into the atmosphere. The following expression gives the energy released in a burn as a function of the rate at which moles of combustibles are consumed:

$$q_{\text{bn}} = (2.86 \cdot 10^8 \dot{N}_{\text{H}_2} + 2.83 \cdot 10^8 \dot{N}_{\text{CO}}) \cdot \Delta t_{\text{bn,tot}} \quad (6-14)$$

where $\dot{N}_{\text{H}_2}$ is the burn rate of hydrogen moles, $\dot{N}_{\text{CO}}$ is the burn rate of carbon monoxide moles, and $\Delta t_{\text{bn,tot}}$ is the total burn time. Note that q_{bn} in Equation (6-14) corresponds to the explicit cell burn energy defined in Table 1-3. The m_{bn} explicit cell mass source defined in Table 1-2 accounts for changes of the H_2 , CO , O_2 , H_2O , and CO_2 constituents. The calculation of these sources is described in Section 6.2.3. Section 6.2.1 below describes the correlations used to determine whether a deflagration will occur by ignition or propagation from another burning region. Section 6.2.2 gives the equations used to calculate the hydrogen and carbon monoxide deflagration flame speed and corresponding total burn time, $\Delta t_{\text{bn,tot}}$, given the initial molar concentrations. Section 6.2.3 describes the burn rate equations and the explicit cell mass changes, m_{bn} , resulting from the burn.

6.2.1 Deflagration Ignition and Propagation Criteria

The burn model initiates a deflagration when minimum threshold concentrations of combustible gas and oxygen are exceeded and the time is within the specified time window during which burns are allowed. A burn can also propagate from an adjacent burning cell when conditions are favorable. The user can define a time window for allowable burns to account for the presence or absence of ignition sources, such as igniters, sparks from electrical equipment, etc. The burn continues for a time that is based on either an internally calculated flame speed or a user-specified burn time. The ignition and propagation criteria used in CONTAIN are described in this subsection. The flame speed correlation is described in Section 6.2.2.

Note that the default burn-parameter models are based on experiments performed with ignition sources. As a result, the user must employ judgment regarding a burn without continuous ignition sources because when, for example, higher concentrations might exist before accidental ignition.

The molar concentrations required for igniting 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 mole fractions of hydrogen (X_{H_2}) and of carbon monoxide (X_{CO})

$$X_{H_2} + FX_{CO} \geq X_{Cgas}^{crit} \quad (6-15)$$

where

- X_{Cgas}^{crit} = is the threshold (or critical) mole fraction for ignition to be initiated;
F = is an empirical parameter that accounts for the presence of both hydrogen and carbon monoxide.

Values for F in Equation (6-15) are derived from empirical values of the threshold for the two limiting cases in which only H_2 or only CO are present. Values of X_{Cgas}^{crit} and the associated values of F for spontaneous ignition, and for downward, upward, and horizontal propagation are given in Table 6-2. Table 6-2 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/or water vapor for inerting.

For the default values in Table 6-2, a burn is spontaneously initiated if the mixed mean effective combustible mole fraction is $\geq 7\%$, the oxygen mole fraction is $\geq 5\%$, and the sum of the carbon dioxide and water vapor mole fractions is $\leq 55\%$. Note that the concentration limits specified for propagation apply to the adjacent cells, not the cell in which the burn originates.

Note that by default the oxygen and diluent limits are the same for ignition and propagation from any of the directions listed. The code does allow each of these default limits to be overridden by user-specified values. A fixed burn time can also be specified by the user to override the burn time that is normally calculated from the flame speed as described in Section 6.2.2. Also, the user can specify the fraction of initial combustible gas left following a burn, or, CONTAIN can calculate it internally from a correlation based on the initial concentration as described in Section 6.2.3. Note that the final combustible concentration may never be reached, for example, if the burn is oxygen-limited.

Table 6-2
Default Ignition and Propagation Limits

		Combustibles (H ₂ +F*CO)	Oxygen O ₂	Diluent (H ₂ O+CO ₂)
<u>Limits</u>	F	[X _{Cgas} ^{crit}]	[X _{O₂} ^{crit}]	[X _S ^{crit}]
Ignition	0.541	≥ 0.07	≥ 0.05	≤ 0.55
Upward propagation	0.328	≥ 0.041	≥ 0.05	≤ 0.55
Horizontal propagation	0.435	≥ 0.06	≥ 0.05	≤ 0.55
Downward propagation	0.600	≥ 0.09	≥ 0.05	≤ 0.55

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. However, propagation through BWR suppression pool vents is not allowed. The criteria in Table 6-2 for the propagation of a burn to another cell depend on whether that cell is located above, alongside, or below the originating cell. The relative locations of the cells are specified through the cell elevation variable, which has a default value of zero. For horizontal propagation to occur between two cells, their elevations must be identical. If the elevation of cell i is greater than that of 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, which must have a value between zero and one, delays the propagation of a burn to an adjoining cell by a fraction of the total burn time in the cell from which the burn propagates. The default time delay factor is 0.5. Because the propagation criteria have not been thoroughly verified, the performance of sensitivity studies to determine the importance of the propagation should be considered.

Figure 6-1 illustrates the burn propagation model. A flame that starts in cell 1 can propagate to cell 2 if the proper conditions exist in cell 2. The characteristic length of the cell in the flame direction in this illustration is X. As the cells are drawn, it will take half the total burn time in cell 1 for the flame to reach the passageway to cell 2, which corresponds to the default time delay factor value of 0.5. When different cell geometries or elevations are specified, the time for propagation to adjacent cells may be greater or less than half the burn time. This fact is not accounted for in the modeling, although the default delay factor may be overridden by a user-specified value.

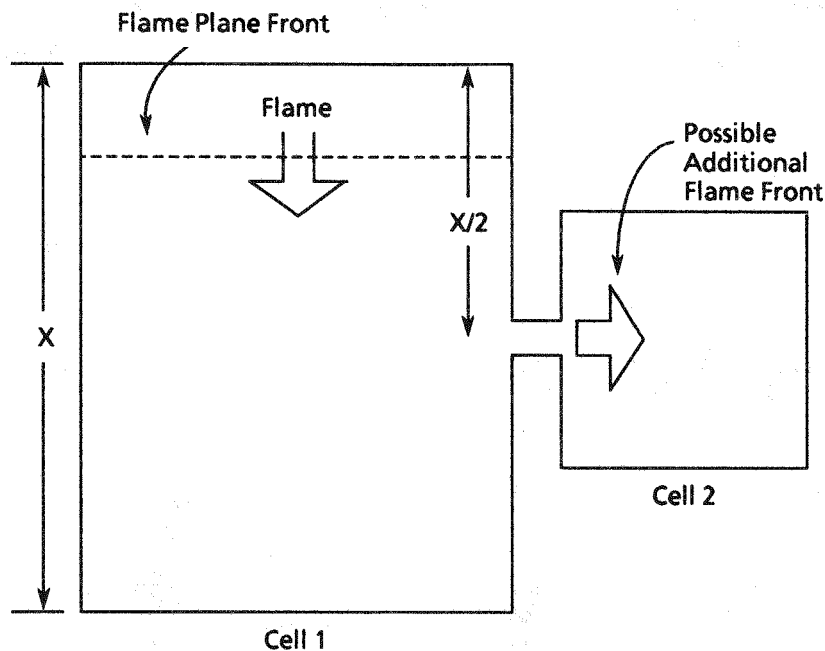


Figure 6-1. Flame Propagation Diagram

6.2.2 Flame Speed and Burn Time

All deflagrations are assumed to occur over a discrete period of time, denoted here as the burn time $\Delta t_{bn,tot}$, following ignition or propagation into another cell. The duration of each newly ignited deflagration is based on an experimentally derived flame speed correlation that depends on initial concentrations of combustible gas, oxygen, and steam. The flame speed may also be specified by the user to override the calculated value. The user may also override the burn time model altogether by providing a user-specified discrete burn time. If the burn parameters are calculated by the code, they are calculated for each burn based on the conditions existing at the start of the burn. When the burn parameters are user-specified, they are held constant throughout the calculation and apply to each deflagration that occurs. The remainder of this section describes the correlations that are used by default to calculate the flame speed and total burn time. Note that the flame speed and burn time are not allowed to vary over the course of any one burn.

The deflagration model assumes that the flame travels a characteristic distance in the compartment along a plane wave front at speed v_f . The total burn time $\Delta t_{bn,tot}$ for a given compartment is

therefore calculated by dividing the characteristic burn length L_{chbn} by the flame speed

$$\Delta t_{bn,tot} = \frac{L_{chbn}}{v_f} \quad (6-16)$$

Normally the model assumes that the characteristic burn length is equal to the characteristic cell length, which is taken to be the cube root of the cell volume. The user is allowed to override this default value and specify a characteristic burn length that is more appropriate for the specific geometry of the cell. For example, if a cell is much taller than it is wide, as opposed to cubical in shape, a longer burn length than the cube root of the volume may be more appropriate.

Flame speed v_f is calculated based on an experimentally derived flame speed correlation that depends on initial mole fractions of CO_2 and H_2O diluents and CO and H_2 combustible gases. Again, Le Chatelier's formula is used to account for both CO and H_2 in the flame speed correlation. The ignition criterion F parameter of 0.541 is used to compute the combustible gas mole fraction X_{Cgas} that is used in the flame speed correlation.

$$X_{Cgas} = X_{H_2} + 0.541 X_{CO} \quad (6-17)$$

Six different functions are used to describe the flame speed correlation. Each function corresponds to a particular range of values of the combustible gas mole fraction X_{Cgas} . The following equation gives the flame speed for $0.0 < X_{Cgas} \leq 0.1$,

$$v_f = (59.2 X_{Cgas} + 1.792) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-18)$$

where f_{O_2} = correction factor for O_2 present, and is given by

$$f_{O_2} = \min[1.0, \max(12.5 X_{O_2}, 0.5)] \quad (6-19)$$

and f_{H_2O} = correction factor for H_2O present, and is given by

$$f_{H_2O} = \min(1 - 4.53 X_{H_2O} + 5.37 X_{H_2O}^2, 0.05) \quad (6-20)$$

The remaining functions use the same correction factor for oxygen given in Equation (6-19); however, different factors are used as noted below for the steam correction factor for X_{Cgas} values greater than 20 percent.

For $0.1 < X_{Cgas} \leq 0.2$,

$$v_f = (172.88 X_{Cgas} - 9.576) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-21)$$

For $0.2 < X_{Cgas} \leq 0.3$,

$$v_f = (50 X_{Cgas} + 15) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-22)$$

where f_{H_2O} in the above expression is defined as

$$f_{H_2O} = (1 - 4.53 X_{H_2O} + 5.37 X_{H_2O}^2) (3 - 10 X_{Cgas}) + (1 - 1.29 X_{H_2O}) (10 X_{Cgas} - 2) \quad \text{for } X_{H_2O} \leq 0.4 \quad (6-23a)$$

$$f_{H_2O} = 0.15 - 0.5 X_{Cgas} + (1 - 1.29 X_{H_2O}) (10 X_{Cgas} - 2) \quad \text{for } X_{H_2O} > 0.4 \quad (6-23b)$$

For $0.3 < X_{Cgas} \leq 0.4$,

$$v_f = (45 - 50 X_{Cgas}) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-24)$$

where f_{H_2O} in the above expression is defined as

$$f_{H_2O} = 1 - 1.29 X_{H_2O} \quad (6-25)$$

For $0.4 < X_{Cgas} \leq 0.6$

$$v_f = (55 - 75 X_{Cgas}) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-26)$$

where f_{H_2O} is given by Equation (6-25).

For $X_{Cgas} > 0.6$,

$$v_f = (48.58 - 64.3 X_{Cgas}) f_{O_2} f_{H_2O} \quad (m/s) \quad (6-27)$$

where f_{H_2O} is again given by Equation (6-25).

6.2.3 Burn Rate

Section 6.2.1 presented the equations that are used to determine the ignition and propagation of a deflagration. The equation used to calculate the total burn time of a deflagration event was then presented in Section 6.2.2. This final subsection of the deflagration model describes how the burn time is applied to determine the burning rate and the masses consumed.

The basic approach taken to determine the burning rate is to estimate the number of moles of combustibles and oxygen available to burn over the remainder of the burn time. The number of moles available to participate in the burn is determined from the number of moles present at a given point during the burn. An adjustment is made to account for sources and other containment processes that may change the inventory in the cell. Finally, the burn is limited by the mole fraction of combustibles or oxygen that must remain at the end of the burn. The burning rate is then set assuming a steady depletion rate of the most limiting constituent over the remaining burning time.

The actual processing of the deflagration always begins at the start of a global timestep. Thus, if one of the ignition criteria described in Section 6.2.1 is met, the cell will begin to burn at the start of the next global timestep. Before the deflagration begins, the model determines the minimum mole fraction of combustibles that can remain at the end of the burn. This minimum unburned mole fraction for hydrogen, $(X_{H_2})_{final}$, and carbon monoxide $(X_{CO})_{final}$ are given by,

$$X_{Cgas} = (X_{H_2})_{initial} + 0.600(X_{CO})_{initial} \quad (6-28)$$

$$X_f = \min[1, \max(0.005, 1.87956 - 23.4320 X_{Cgas})] \quad (6-29)$$

$$(X_{H_2})_{final} = (X_f)(X_{H_2})_{initial} \quad (6-30)$$

$$(X_{CO})_{final} = (X_f)(X_{CO})_{initial} \quad (6-31)$$

The $(X_{H_2})_{initial}$ parameter is the mole fraction of hydrogen before the burn starts. Note that the hydrogen concentration at the actual burn initiation may be slightly different than at the time when the ignition criteria were checked and it was decided to initiate the burn. This occurs because the cell conditions could slightly change, for example, because of flow from another cell.

The $(X_{CO})_{initial}$ parameter is the mole fraction of carbon monoxide gas before the burn starts. Again, this may differ from the value of X_{CO} used earlier. Note that the 0.600 downward propagation constant is used in Le Chatelier's formula (Equation (6-28)) because it is the largest of the burn direction options.

The chemical reaction rate is adjusted each burn timestep to account for intercompartment flows and source injection, so that the burn finishes at the predetermined time with the correct final mole fraction of combustible gases. Consumption or production of combustible gases and oxygen by other phenomenological processes modeled in CONTAIN are also accounted for in this adjustment. Note that intercompartment flow adjustments are only made at the end of the global timestep; however, the burn model automatically reduces the global timestep accordingly to force problem stability and to force flow adjustments to occur in the burn model at a reasonable frequency. This interaction between the intercell flow model and the burn model should not be confused with the capability to represent long continuous burns over periods of changing conditions within the containment. The CONTAIN model treats each deflagration as a discrete event, and the burn time of that event is fixed once the deflagration is calculated to occur.

The burn rate of combustibles is calculated by estimating the total number of moles remaining in the cell at the end of the burn, Mo_{unbn} . This value is updated as time progresses toward the end of the deflagration total burn time, $\Delta t_{bn,tot}$, using the following balance equation

$$Mo_{unbn} = \frac{Mo_{tot} + \Delta t_{bn} \left[\frac{dMo_{H_2O}}{dt} + \frac{dMo_{N_2}}{dt} + \frac{dMo_{O_2}}{dt} + \frac{dMo_{CO_2}}{dt} \right]}{[1 - (0.5)(X_{H_2}) - (0.5)(X_{CO})]} + \frac{(0.5) \left[(\Delta t_{bn}) \left(\frac{dMo_{H_2}}{dt} + \frac{dMo_{CO}}{dt} \right) - Mo_{tot} [(X_{H_2})_{initial} + (X_{CO})_{initial}] \right]}{[1 - (0.5)(X_{H_2})_{final} - (0.5)(X_{CO})_{final}]} \quad (6-32)$$

where

- Mo_{unbn} = estimate of the remaining moles of gas at the end of the total burn time, $t_{bn,tot}$,
- Δt_{bn} = time remaining before the end of the total burn time is reached,
- Mo_{tot} = moles of gas before the end of the burn,
- $\frac{dMo_i}{dt}$ = molar source rate resulting from other phenomena during the burn time.

The unburned mole fractions of hydrogen $(X_{H_2})_{final}$ and carbon monoxide $(X_{CO})_{final}$ are defined in Equation (6-30) and (6-31), respectively.

Note that Equation (6-32) is only an approximation of the end molar content of the cell since it does not account for changes that might occur in the source rates. Also, the addition or removal of gas species other than oxygen, hydrogen, steam, carbon monoxide, carbon dioxide, and nitrogen are not accounted for.

An estimate of the number of moles of hydrogen remaining at the end of the burn F_{H_2} readily follows from Equation (6-32).

$$F_{H_2} = MO_{unbn}(X_{H_2})_{final} \quad (6-33)$$

The number of moles available to burn Res_{H_2} for the remainder of the burn time is given by the initial moles of hydrogen, plus any anticipated hydrogen sources, minus the number of moles that must remain after the burn. Putting this into equation form, Res_{H_2} is given by

$$Res_{H_2} = MO_{H_2} + \Delta t_{bn} \left[\frac{dMO_{H_2}}{dt} \right] - F_{H_2} \quad (6-34)$$

An analogous approach is used to calculate the moles of carbon monoxide and oxygen available to participate in the burn for the remainder of the deflagration total burn time.

$$F_{CO} = MO_{unbn}(X_{CO})_{final} \quad (6-35)$$

$$Res_{CO} = MO_{CO} + \Delta t_{bn} \left[\frac{dMO_{CO}}{dt} \right] - F_{CO} \quad (6-36)$$

$$F_{O_2} = MO_{unbn}(X_{O_2})_{final} \quad (6-37)$$

$$Res_{O_2} = MO_{O_2} + \Delta t_{bn} \left[\frac{dMO_{O_2}}{dt} \right] - F_{O_2} \quad (6-38)$$

where X_{O_2} is the present value of the oxygen molar fraction.

Note that $(X_{O_2})_{final}$ is 0.05 (if there is sufficient combustible gas) by default, but the value can be changed by the user.

Finally, the total moles of combustible gas available for burning over the remainder of the burn time is

$$(Res_{Cgas})_{avail} = (Res_{H_2})_{avail} + (Res_{CO})_{avail} \quad (6-39)$$

If $(Res_{Cgas})_{avail}$ is greater than $2 (Res_{O_2})_{avail}$ (two moles of oxygen are required to burn one mole of combustible gas), then the burn will be oxygen limited. In this case, the moles of hydrogen to combust will be reduced as

$$(Res_{H_2})_{burn} = (Res_{H_2})_{avail} \frac{2(Res_{O_2})_{avail}}{(Res_{Cgas})_{avail}} \quad (6-40)$$

and the carbon monoxide moles for combustion will also be reduced by the same factor:

$$(Res_{CO})_{burn} = (Res_{CO})_{avail} \frac{2(Res_{O_2})_{avail}}{(Res_{Cgas})_{avail}} \quad (6-41)$$

The molar burn rate for hydrogen $\dot{N}_{H_2}$ is

$$\dot{N}_{H_2} = \frac{Res_{H_2}}{\Delta t_{bn}} \quad (6-42)$$

and the molar burn rate of carbon monoxide $\dot{N}_{CO}$ is

$$\dot{N}_{CO} = \frac{Res_{CO}}{\Delta t_{bn}} \quad (6-43)$$

where again, Δt_{bn} is the burn time remaining in the total burn time.

These bounding rates are used in Equation (6-14) to calculate the deflagration energy release. They also are used to determine the explicit cell level mass sources in Equation (3-14) resulting from deflagrations. The molar rates given in Equation (6-42) and (6-43)

are converted to mass rates of hydrogen, carbon monoxide, oxygen, steam, and carbon dioxide.

$$\dot{m}_{H_2} = \dot{N}_{H_2} \cdot M_{H_2}$$

$$\dot{m}_{O_2} = \left[\frac{1}{2} \dot{N}_{H_2} + \frac{1}{2} \dot{N}_{CO} \right] \cdot M_{O_2}$$

$$\dot{m}_{H_2O} = - \dot{N}_{H_2} \cdot M_{H_2O}$$

$$\dot{m}_{CO_2} = - \dot{N}_{CO} \cdot M_{CO_2}$$

6.3 Heat and Mass Transfer

This section describes the models used in CONTAIN to calculate heat and mass transfer between the atmosphere and heat structures. In addition, these models are used to calculate the heat and mass transfer in the IC and the FC and with the LC pool. The models described include those for radiation and convective heat and mass transfer, which includes condensation and evaporation. The heat conduction model within heat structures is discussed in Section 6.5.1.

Figure 6-2 shows the heat transfer configuration assumed for the mass and heat transfer calculation. Even though the figure depicts radiation, convection, and condensation, these processes are modeled separately in an explicit manner. Because the condensable vapor must diffuse through a region of noncondensable gas and depleted condensable vapor concentrations, a gas boundary layer in the atmosphere contributes the principal resistance to condensation. For most calculations, it is sufficient to determine only this boundary layer resistance. However, this resistance can occasionally become quite small, and it is therefore desirable to include the thermal resistance of the condensate film and of a layer of oxide or paint on the heat structure surface. Note that there have been improvements to the CONTAIN modeling in this area, see Appendix A. Figure 6-3 provides a schematic representation for the various resistances affecting heat and mass transfer to structures. This illustration should not be taken as literally equivalent to a thermal circuit because convection is driven by a temperature difference, whereas condensation is driven by a partial pressure difference.

Section 6.3.1 describes the convective heat transfer model between the atmosphere and the heat structures. Section 6.3.2 describes the mass transfer model between the atmosphere and the heat structures and the total convective heat and mass transfer heat

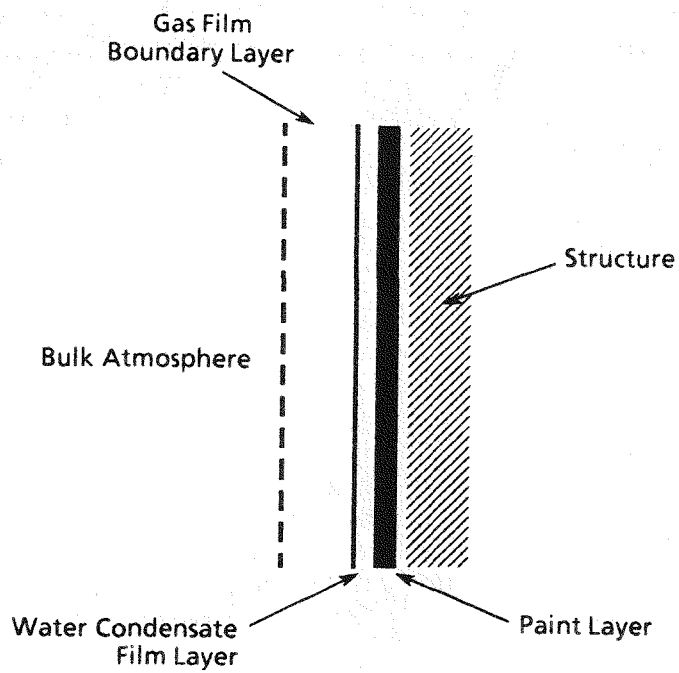


Figure 6-2. Heat Transfer Configuration (not to scale)

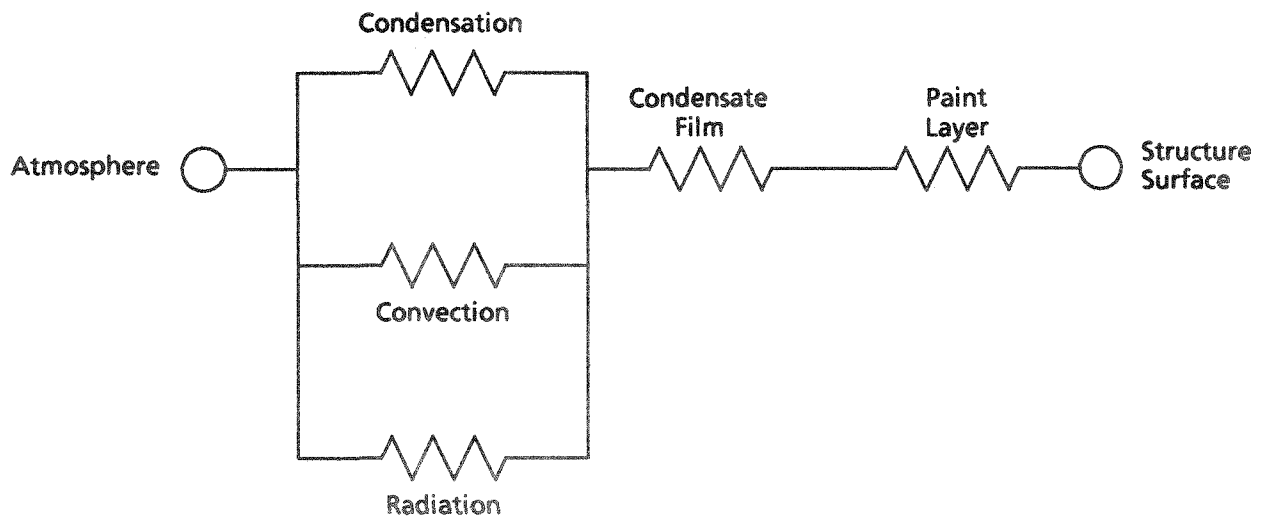


Figure 6-3. Equivalent Circuit for the Heat Transfer Configuration of Figure 6-2

flux calculations. Section 6.3.3 describes the thermal radiation heat transfer models.

6.3.1 Convective Heat Transfer

The convective heat transfer flux between the atmosphere and the heat structure is given by

$$q_{\text{conv}} = h_{\text{conv}} (T_b - T_i) \quad (6-44)$$

where

$$\begin{aligned} q_{\text{conv}} &= \text{convective heat transfer flux (W/m}^2\text{)}, \\ T_b &= \text{bulk atmospheric temperature (K)}, \\ h_{\text{conv}} &= \text{convective heat transfer coefficient (W/m}^2\text{-K)}, \text{ and} \\ T_i &= \text{temperature at the atmosphere-liquid film interface (K)}. \end{aligned}$$

Section 6.3.2 discusses the procedure used to account for the effects on energy transfer of the convected sensible heat transfer, mass transfer, liquid-film resistance, and surface-coating resistance.

The convective heat transfer coefficient h_{conv} is related to the Nusselt number Nu by

$$h_{\text{conv}} = Nu \frac{k}{L} \quad (6-45)$$

where

$$\begin{aligned} k &= \text{thermal conductivity of the gas-vapor mixture in the} \\ &\quad \text{atmosphere (W/m-K)}, \text{ and} \\ L &= \text{characteristic length as user-defined (m)}. \end{aligned}$$

Three standard correlations are available in CONTAIN for determining Nu in Equation (6-45) for either forced or natural convection regimes.

By default the code uses a natural convection correlation. For vertical walls, downward facing ceilings, which are colder than the atmosphere, and upward facing floors, which are warmer than the atmosphere, the following turbulent correlation is used:

$$Nu_c = 0.13 Gr Pr^{0.33}$$

The following laminar correlation is used for downward facing ceilings, which are warmer than the atmosphere, and upward facing floors, which are colder than the atmosphere.

$$\text{Nu}_c = 0.27 \text{Gr} \text{Pr}^{1/4}$$

In situations where forced flow conditions are believed to exist, the user must give a table that specifies either a gas velocity or a Nusselt number as a function of time. If velocity is given, then the Reynolds number will be computed using Equation (6-10). The forced convection correlation

$$\text{Nu}_f = 0.037 \text{Re}^{0.8} \text{Pr}^{0.33}$$

will then be used to calculate the Nu number. Note, however, that this Nu_f will only be used if it exceeds the value determined using the appropriate natural convection correlation.

Finally, the Nu number used in the convection model for structures can be specified directly by the user in a table as a function of time. Such values are not overridden by the natural convection correlation. To summarize,

$$\begin{aligned} \text{Nu} &= \text{Max} (\text{Nu}_c, \text{Nu}_f) \text{ if velocity or Re is given,} \\ &= \text{Nu}_c \text{ if no options are given, and} \\ &= \text{Nu}_{\text{user}} \text{ if the user specifies Nu directly.} \end{aligned}$$

A similar approach is used in the convection model for the LC upper surface; however, there are insignificant differences in the correlations.

For all outer surfaces facing another cell's atmosphere the following assumptions are made: the convective heat transfer coefficient, h_{conv} in Equation (6-45), is assumed to have a constant value of $6.08 \text{ W/m}^2\text{-K}$; and condensation on heat structures and the formation of the condensate films are ignored. Because of this limitation, structures that divide two containment compartments are best modeled if they are divided in half and modeled as separate structures in the respective cells. A consequence of this strategy is that heat conduction between the two cells cannot be modeled. This limitation of the CONTAIN code has been corrected in later CONTAIN versions. (See Appendix A.)

6.3.2 Mass Transfer

Mass transfer, which governs condensation and evaporation of vapor at the heat structure surfaces, is driven by the partial pressure difference of the condensable vapor. If a condensate film layer exists on the structure surface, the partial pressure of the non-condensable gas at this film layer will be higher than that of the

bulk mixture (see Figure 6-4 for illustrations and definitions). This condition occurs because the noncondensable gas is carried with the vapor toward the interface where it accumulates. The increase in the partial pressure of the noncondensable gas produces a driving force for diffusion of the noncondensable gas away from the surface. This force opposes the motion of the bulk mixture (sum of noncondensable gas and vapor) towards the surface. As shown in Figure 6-4, the total pressure of the bulk mixture remains constant, the vapor partial pressure at the interface is lower than that in the bulk mixture when the process is condensation. The vapor partial pressure at the interface is higher than that in the bulk mixtures when the process is evaporation.

For the example in Figure 6-4, both the molar fluxes ($\text{kgmole}/\text{m}^2\text{-s}$) of noncondensable gas J_{nc} and condensable vapor J_{vap} passing through the interface are given by Reference Col81:

$$D \frac{\partial C_{nc}}{\partial y} + C_{nc} v_J = J_{nc} \quad (6-46)$$

and

$$D \frac{\partial C_{vap}}{\partial y} + C_{vap} v_J = J_{vap} \quad (6-47)$$

where

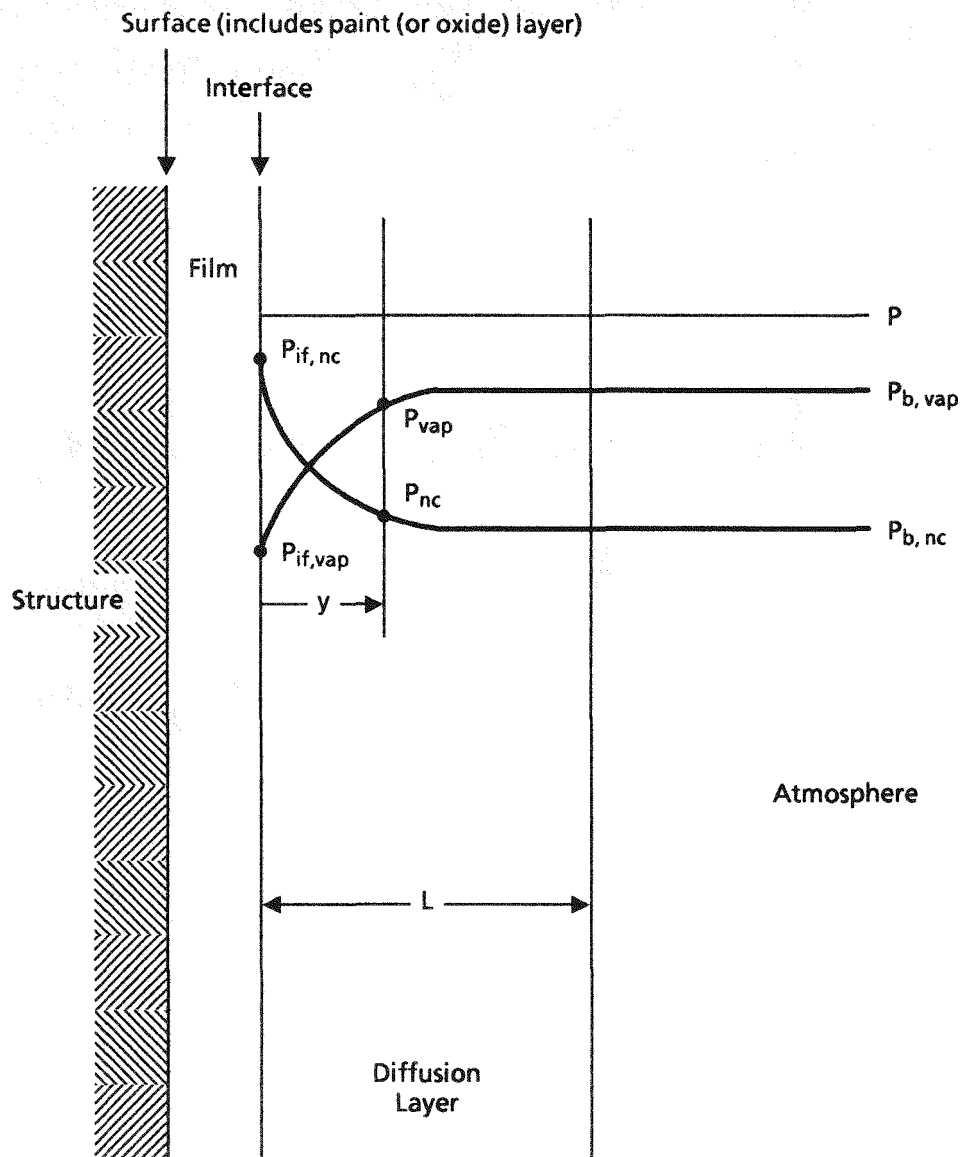
- D = diffusion coefficient (m^2/s),
- C_{nc} = molar concentration of noncondensable gas ($\text{kgmole}_{nc}/\text{m}^3$),
- v_J = drift-flux velocity of the bulk mixture toward the interface (m/s), and
- C_{vap} = molar concentration of vapor ($\text{kgmole}_{vap}/\text{m}^3$).

The following relations will be used:

$$\frac{\partial P_{nc}}{\partial y} = - \frac{\partial P_{vap}}{\partial y} \quad (6-48)$$

and

$$\frac{\partial C_{nc}}{\partial y} = - \frac{\partial C_{vap}}{\partial y} \quad (6-49)$$



- L = diffusion length,
- P = total pressure,
- $P_{b,vap}$ = partial pressure of vapor in the bulk mixture (atmosphere),
- $P_{b,nc}$ = partial pressure of noncondensable gases in the bulk mixture (atmosphere),
- P_{nc} = partial pressure of noncondensable gas at distance y from the interface,
- P_{vap} = partial pressure of vapor at distance y from the interface,
- $P_{if,nc}$ = partial pressure of noncondensable gas at the interface, and
- $P_{if,vap}$ = partial pressure of vapor at the interface.

Figure 6-4. The Influences of Noncondensables on Interface Resistance

Substituting Equations (6-48) and (6-49) into Equation (6-47) results in

$$J_{\text{vap}} = C_{\text{vap}} v_J - D \frac{\partial C_{\text{nc}}}{\partial y} \quad (6-50)$$

Combining Equation (6-46) and Equation (6-50) results in

$$J_{\text{vap}} = -D \frac{\partial C_{\text{nc}}}{\partial y} \left[\frac{C_{\text{vap}}}{C_{\text{nc}}} + 1 \right] \quad (6-51)$$

Substituting the relation $\partial P_{\text{nc}} / \partial y = R T \partial C_{\text{nc}} / \partial y$ into Equation (6-51) results in

$$J_{\text{vap}} = -\frac{D}{R T} \frac{\partial P_{\text{nc}}}{\partial y} \left[\frac{C_{\text{vap}}}{C_{\text{nc}}} + 1 \right] \quad (6-52)$$

It can be shown that $(P_{\text{vap}}/P_{\text{nc}}) + 1 = (C_{\text{vap}}/C_{\text{nc}}) + 1$. Combining this with the assumption that $P_{\text{vap}} + P_{\text{nc}} = P$, Equation (6-52) can be rewritten as

$$J_{\text{vap}} = -\frac{D}{R T} \frac{\partial P_{\text{nc}}}{\partial y} \frac{P}{P_{\text{nc}}} \quad (6-53)$$

Integrating Equation (6-53),

$$J_{\text{vap}} \int_0^L dy = -\frac{D}{R T} P \int_{P_{\text{if,nc}}}^{P_{\text{b,nc}}} \frac{\partial P_{\text{nc}}}{P_{\text{nc}}} \quad (6-54)$$

yields

$$J_{\text{vap}} = \frac{D P}{R T L} \ln \left[\frac{P_{\text{if,nc}}}{P_{\text{b,nc}}} \right] \quad (6-55)$$

To solve Equation (6-55), the interface condition must be known. However, this condition is not usually known and an iterative procedure is required. For containment applications, the condensate film resistance is expected to be quite small relative to other resistances in series with it. Therefore, the film

resistance is neglected* and the iterative procedure is bypassed by making use of the zero order and first-order Taylor series expansions in $(T_{if} - T_s)$, where T_{if} is the temperature of the film surface and T_s is the structure surface temperature. The zero order term in the Taylor expansion is T_s . Thus, Equation (6-55) can be approximated in terms of the vapor mass flux j ($\text{kg}/\text{m}^2\text{-s}$) with the zero order term denoted by subscript 0:

$$j_{\text{vap},0} = K_g M_{\text{vap}} (P_{b,\text{vap}} - P_{s,\text{vap}}) \quad (6-56)$$

where

- K_g = mass transfer coefficient ($\text{kgmole}/\text{m}^2\text{-s-Pa}$), which is defined further below;
- M_{vap} = molecular weight of the vapor (kg/kgmole);
- $P_{s,\text{vap}}$ = saturation pressure of vapor at the structural surface (Pa); and
- $P_{b,\text{vap}}$ = saturation pressure of vapor at the bulk temperature (Pa).

K_g in Equation (6-56) is defined as the mass transfer coefficient ($\text{kgmole}/\text{m}^2\text{-s-Pa}$), which is given by

$$K_g = \frac{Sh P D}{R T P_{nm} L} \quad (6-57)$$

where

- Sh = Sherwood number,
- P = cell pressure (Pa),
- D = diffusivity, see below (m^2/s),
- R = universal gas constant ($\text{m}^3\text{-Pa}/\text{kgmole-K}$),
- T = arithmetic average of T_b and T_s (K),
- P_{nm} = defined below (Pa), and
- L = diffusion length (m).

In Equation (6-57), D is the mass diffusivity of vapor in the noncondensable gas given by

$$D = \frac{4.4784 \cdot 10^{-6} T^{2.334}}{P} \quad (6-58)$$

*These procedures have been improved in subsequent versions of CONTAIN, see Appendix A.

P_{nm} is the logarithmic mean pressure which is defined as

$$P_{nm} = - \frac{P_{b,vap} - P_{s,vap}}{\ln \left[\frac{P - P_{b,vap}}{P - P_{s,vap}} \right]} \quad (6-59)$$

and the Sherwood number Sh for the bulk mixture is given by

$$Sh = Nu (Sc/Pr)^{1/3} \quad (6-60)$$

Equation (6-56) is also used for the LC pool, which is treated as a floor with a characteristic length equal to the square root of the pool area and a structure surface temperature equal to the pool temperature.

To account for the effects of the changing condensate film layer depth, the next term in the Taylor series expansion ($T_{if} - T_s$) must be included. This term is not applied to pool condensation.*

The first order Taylor series expansion requires the saturation pressure $P_{if,vap}$, which is given by

$$P_{if,vap} = P_{sat}(T_s) + \frac{dP_{sat}(T_s)}{dT} (T_{if} - T_s). \quad (6-61)$$

Then, a correction term is subtracted from Equation (6-56) to yield the first order vapor flux $j_{vap,1}$ term:

$$j_{vap,1} = j_{vap,0} - \frac{B \Delta T}{h_{v\ell}} \quad (6-62)$$

where

$$B = K_g M_{vap} \frac{dP_{sat}(T_s)}{dT} h_{v\ell} \quad (6-63)$$

where dP_{sat}/dT is the temperature derivative of the saturation pressure evaluated at T_s ; and

ΔT = temperature of the interface between the atmosphere and the liquid film (K); and

*Improvements have been added in this area, see Appendix A.

$h_{v\ell}$ = difference between the vapor enthalpy at the bulk atmosphere temperature T_b and the liquid enthalpy at the surface temperature T_s (J/kg).

The film-to-wall heat transfer coefficient h_{flm} is defined as

$$h_{flm} = \frac{1}{r_{paint} + r_{flm}} \quad (6-64)$$

where

r_{paint} = thermal resistance of the paint layer on the structural surface assumed to be $5 \cdot 10^{-4}$ s-m²-K/J, and
 r_{flm} = thermal resistance of the condensate layer on the structural surface,

$$= \frac{m_{tr}}{k_\ell \rho_\ell A_s}$$

m_{tr} = the amount of vapor condensed on the structural surface (kg),

k_ℓ = thermal conductivity of the liquid (W/m-K),

ρ_ℓ = density of the liquid (kg/m³), and

A_s = surface area of the structure (m²).

Note that the vapor condensation mass transfer rate to the structural surface with an area A_s is given by

$$\frac{dm_{tr}}{dt} = J_{vap,1} A_s \quad (6-65)$$

As indicated in Figure 6-4, the heat flux from the atmosphere to the liquid-film interface is equated to the heat flux through the liquid h_{eff} from Equation (6-64):

$$q_1 = q_{m,1} + q_{c,1} = h_{eff} \Delta T \quad (6-66)$$

where the 1 subscripts mean that these are first-order values.

Equation (6-67) can be solved to obtain

$$\Delta T = \frac{q_0}{h_c + h_{flm} + J_0 c_p + B} \quad (6-67)$$

where c_p is the specific heat of the liquid at the temperature T_{wall} . The corrected fluxes are then obtained by substituting Equation (6-67) for ΔT into Equations (6-62) and (6-66).

6.3.3 Thermal Radiation

In CONTAIN, the user can choose from two radiative heat transfer models. The first model is the net enclosure radiation model. This model allows for simultaneous calculations of radiative heat transfer among the UC atmosphere, all heat structures and the uppermost layer of the LC. With this model, radiation transfer between surfaces is modeled as well as radiation between the atmosphere and heat structure inner surfaces. The second model is the simple radiation model. As the name implies, this model only treats the direct radiative heat transfer between the atmosphere and the heat structures, and between the atmosphere and the uppermost layer of the LC. Within this model, the user can establish radiative heat transfer from the atmosphere to both the inner and outer surfaces of a heat structure if they are both within the cell. Both radiation models account for the optical properties of the atmosphere based on the emissivity of H₂O vapor, CO₂, and CO. A simple parametric model is also available to account for the absorptivity of aerosols present.

Section 6.3.3.1 describes the net enclosure radiation model and Section 6.3.3.2 discusses the simple radiation model. Lastly, the radiative emissivity models used in CONTAIN are presented in Section 6.3.3.3.

6.3.3.1 Net Enclosure Radiation Model. This model was adapted from a formulation for gray surfaces in Reference Sie81. A basic assumption is that the atmosphere is completely surrounded by heat transfer surfaces, which can include the uppermost layer of the LC. The surrounding surfaces can be at different temperatures with automatic accounting for secondary (surface-to-surface) reflections. Aerosols in the atmosphere can be modeled to absorb energy.

According to Kirchhoff's law, the outgoing radiation flux, q_j for structural surface j is given by

$$q_j = \frac{\epsilon_j}{1 - \epsilon_j} (\psi_j - B_j) \quad (6-68)$$

where

ϵ_j = user-input emissivity of structural surface j ,
 ψ_j = radiosity of structural surface j (W/m²), and
 B_j = Planck blackbody radiation of structural surface j (W/m²).

When a water film is present on a surface, the code automatically sets the emissivity of that surface to that of water (0.94).

In Equation (6-68), B_j is defined as

$$B_j = \sigma T_j^4 \quad (6-69)$$

where

σ = Stefan-Boltzmann constant ($\text{W/m}^2\text{-K}^4$), and
 T_j = Temperature for structural surface j (K).

The radiosity, ψ_j in Equation (6-68), is calculated by solving a series of linear equations simultaneously.

$$\psi_j - (1 - \epsilon_j) \sum_{k=1}^N F_{jk} (1 - \epsilon_{m,jk}) \psi_k = \epsilon_j B_j + (1 - \epsilon_j) \sum_{k=1}^N F_{jk} \epsilon_{m,jk} B_{\text{gas}} \quad (6-70)$$

where

N = number of the structural surfaces in the enclosure,
 F_{jk} = user-input view factor from surface j to surface k (the fraction of radiation from surface j that is directed toward surface k),
 $\epsilon_{m,jk}$ = emissivity of atmospheric gas mixture that is calculated by the code internally, and
 B_{gas} = Planck blackbody radiation for the atmospheric gas (W/m^2).

In Equation (6-70), $\epsilon_{m,jk}$ is a function of the user-input beam length L_{jk} between surfaces j and k . The calculation of $\epsilon_{m,jk}$ is discussed in Section 6.3.4.3. In Equation (6-62), B_{gas} is calculated by

$$B_{\text{gas}} = \sigma T_{\text{gas}}^4 \quad (6-71)$$

where T_{gas} = atmospheric gas temperature in the enclosure (K).

Because the temperatures (surfaces and atmospheric gas) of the enclosure are known, the radiosity of each surface, which is based on Equation (6-70), can be solved linearly. The code internally solves these equations with a standard linear equation solver.

Note that Equation (6-70) can be simplified to solve for the point at which the atmospheric gases (other than CO_2 , CO , and H_2O vapor)

become transparent. Thus, $\epsilon_{m,jk}$ in Equation (6-70) becomes zero and Equation (6-70) becomes

$$\psi_j = (1 - \epsilon_j) \sum_{k=1}^N F_{jk} \psi_k + \epsilon_j B_j \quad (\text{W/m}^2) \quad (6-72)$$

When calculating the gas-mixture emissivity, if the user has not input the beam length L_{jk} between heat structures for the net enclosure radiation model, CONTAIN will calculate it by default as

$$L = \frac{3.6V}{\sum_{i=1}^N A_{s,i}} \quad (6-73)$$

where

$$\begin{aligned} V &= \text{cell volume (m}^3\text{), and} \\ A_{s,i} &= \text{area (m}^2\text{) of the structural surface } i. \end{aligned}$$

For the view factor between heat structures, the user only needs to supply the one directional view factor (from structure i to j). Then, the code will calculate the view factor in the opposite direction (from structure j to i) according to the following equation:

$$A_{s,i} \cdot F_{ij} = A_{s,j} F_{ji} \quad (6-74)$$

where

$$\begin{aligned} F_{ij} &= \text{view factor from structural surface } i \text{ to } j, \\ F_{ji} &= \text{view factor from structural surface } j \text{ to } i, \text{ and} \\ A_{s,j} &= \text{area (m}^2\text{) of the structural surface } j. \end{aligned}$$

If corium-concrete interactions are being modeled (with CORCON-MOD2), a derivative of the layer radiative heat flux with respect to the layer surface temperature T_{ly} is calculated as

$$\frac{dq_r}{dT} = \frac{dq_1}{dT} + 4 \frac{dq_2}{dT} T_{ly}^3 \quad (6-75)$$

where

$$\frac{dq_1}{dT} = \frac{q_{low} - q_{ly}}{T_{low} - T_{ly}} - \frac{dq_2}{dT} \alpha_1 \quad (6-76)$$

and

$$\frac{dq_2}{dT} = \frac{T_{ly}(q_{hi} - q_{low}) - T_{low}(q_{hi} - q_{ly}) + T_{hi}(q_{low} - q_{ly})}{(T_{low} - T_{ly})(T_{hi} - T_{ly})(\alpha_1 - \alpha_2)} \quad (6-77)$$

where

$$\begin{aligned} \alpha_1 &= (T_{low} + T_{ly}) (T_{low}^2 + T_{ly}^2), \\ \alpha_2 &= (T_{hi} + T_{ly}) (T_{hi}^2 + T_{ly}^2), \\ T_{low} &= 0.98 T_{ly}, \\ T_{hi} &= 1.02 T_{ly}, \\ q_{ly} &= \text{the radiative heat flux evaluated at } T_{ly}, \\ q_{low} &= \text{the radiative heat flux evaluated at } T_{low}, \text{ and} \\ q_{hi} &= \text{the radiative heat flux evaluated at } T_{hi}. \end{aligned}$$

Equation (6-75) is used by the CORCON-MOD2 module to estimate the effective heat transfer coefficient between the corium pool and the atmosphere.

6.3.3.2 Simple Radiation Model. The simple radiation model in CONTAIN calculates the radiative heat transfer between the heat structures and the atmosphere, between the atmosphere and the uppermost LC layer, and between the uppermost LC layer and heat structures. Because this model is relatively simple in contrast to the net enclosure radiation model, secondary reflections between surfaces are treated only in an approximate fashion. Also, direct radiation between structure surfaces is not modeled. Unlike the net enclosure radiation model, the simple radiation model permits radiative heat transfer from the atmosphere to both inner and outer surfaces of a heat structure if they are both within the cell.

Unlike the net enclosure radiation model, the simple radiation model employs an iterative technique in the calculation of radiative energy exchange with the atmosphere. This total radiative heat transfer to the atmosphere is given by

$$q_{r,t} = q_{r,s} + q_{r,ly} \quad (6-78)$$

where

$$\begin{aligned} q_{r,s} &= \text{total radiative heat transfer flux between structures to atmosphere, and} \\ q_{r,ly} &= \text{total radiative heat transfer flux between the uppermost layer of LC and the atmosphere.} \end{aligned}$$

In Equation (6-78), $q_{r,s}$ is given by

$$q_{r,s} = \sum_{j=1}^N q_{r,j} \quad (6-79)$$

where $q_{r,j}$ is the radiative heat flux between the atmosphere and structure j ; and is given by

$$q_{r,j} = \sigma \epsilon_s (\epsilon_{m,j} T_{tr}^4 - \alpha_{m,j} T_j^4) \quad (6-80)$$

where $\epsilon_{m,j}$ and $\alpha_{m,j}$ are calculated, as described in Section 6.3.3.3, as a function of user-specified beam length for surface j . T_j is the temperature of surface j . Note that Equation (6-80) also applies to the radiative heat exchange between atmosphere and the uppermost layer of the LC. T_{tr} in the above equation is an estimate of the postradiative atmosphere temperature. This value is determined iteratively.

For a gray enclosure, some of the incident radiation striking its walls is reflected back into the gas and to other parts of the enclosure. The ϵ_s parameter in Equation (6-80) accounts for this reflection.

For CONTAIN, ϵ_s is calculated as

$$\epsilon_s = \frac{\epsilon_j + 1}{2} \quad (6-81)$$

where ϵ_j is the emissivity of surface j . For a water film on a surface, a value of 0.94 is used for ϵ_s .

An iteration for calculating the equilibrium atmospheric temperature T_{tr} (T_a below) takes into account the sensible heat added by $q_{r,t}$ in the atmosphere. This equilibrium temperature is used for calculating the radiative heat flux for the LC.

The radiative heat transfer Q_r is found from the following analysis. The energy changes of the atmosphere over a computational timestep Δt is written as follows.

$$M_a c_a (T_a^{n+1} - T_a^n) = -Q_r + M_a c_a \Delta t \chi^{n+1} - M_a c_a d \Delta t \Delta T_a \quad (6-82)$$

The semi-implicit atmosphere temperature obtained from this procedure on the previous cycle is T_a^n and the new semi-implicit

atmosphere temperature is T_a^{n+1} . The value of ΔT_a refers to the change in the actual atmosphere temperature in this cycle, T_{aa}^n , and T_a^n .

$$\Delta T_a = T_a^n - T_{aa}^n \quad (6-83)$$

This value is used as a measure of the amount of "other" heat transfer that is taking place as a result of processes not explicitly accounted for in the radiative heat transfer model, such as convective heat transfer. The value χ^{n+1} in Equation (6-82) is obtained from

$$\chi^{n+1} = \chi^n - b \Delta t \Delta T_a \quad (6-84)$$

with $\chi^0 = 0$. The coefficients b and d are artificial damping parameters that control the rate at which this method will accommodate a change in the atmosphere energy balance. In the current implementation, $d = 0.5 \text{ (s}^{-1}\text{)}$ and $b = (0.25/\Delta t) \text{ (s}^{-1}\text{)}$.

In addition to $q_{r,t}$, the simple radiation model calculates the radiative heat flux between the LC and heat structures. This heat flux $q_{\ell y, j}$ is calculated as

$$q_{\ell y, j} = F(1 - \alpha_{\text{gas}}) F_{\ell y, j} \sigma (T_j^4 - T_{\ell y}^4) \quad (\text{W/m}^2) \quad (6-85)$$

where

- α_{gas} = absorptivity of the gas mixture in the atmosphere,
- $F_{\ell y, j}$ = user-specified view factor between the structural surface j and the uppermost layer ℓy of the LC,
- $T_{\ell y}$ = the temperature of the uppermost layer ℓy of the LC (K), and
- F = a factor that should be 1.0 but is incorrectly programmed in CONTAIN 1.1 to be ϵ_s . This has been corrected in later versions of the code, see Appendix A.

6.3.3.3 Radiative Properties. Both the net enclosure and simple radiation models require the radiative properties of the atmosphere gas mixture (such as H_2O vapor, CO_2 , CO and aerosols). The Modak radiative property model is used by default to calculate these properties [Mod79]. If only water vapor is present in the atmosphere, the user can invoke the Cess-Lian water vapor radiative property model [Ces76]. This model assumes that only CO and CO_2 , if present, are transparent and do not affect radiative heat transfer. The gas mixture emittance determines the characteristics of the radiative heat transfer for the participating gas mixture

medium. This emittance is a function of the gas mixture composition, pressure, temperature, and the average optical depth of the gas mixture. This depth is also referred to as the mean optical path or beam length. For CONTAIN, this beam length is specified by the user.

The Modak radiative property model is described in Section 6.3.3.3.1. The Cess-Lian radiative property model is described in Section 6.3.3.3.2.

6.3.3.3.1 Modak Radiative Property Model. The Modak radiative property model calculates the total gas mixture emissivity and absorptivity, which takes into account the nontransparent gases (such as H₂O vapor, CO, and CO₂) and aerosol. Thus $\epsilon_{m,jk}$ and $\alpha_{m,jk}$ for beam length between surfaces j and k are given by

$$\epsilon_{m,jk} = \epsilon_p + \epsilon_{gas} - \epsilon_p \epsilon_{gas} \quad (6-86)$$

and

$$\alpha_{m,jk} = \alpha_p + \alpha_{gas} - \alpha_p \alpha_{gas} \quad (6-87)$$

where ϵ_p and α_p are, respectively, the aerosol emissivity and absorptivity, and ϵ_{gas} and α_{gas} are, respectively, the gas emissivity and absorptivity.

In Equation (6-86), ϵ_{gas} is calculated from the emissivity of the individual nontransparent gas (CO, CO₂, and H₂O vapor) with a correction for the overlapping of absorption bands from different gases. The emissivity of the individual nontransparent gas is obtained by summing over its spectral absorption bands [Edw84]. For the purpose of containment analyses, an approximate method is adapted based on the spectral emissivities and experimental results that agree to within 5%. The overlapping correction is taken to be a temperature-dependent form of Leckner's correction $\Delta\epsilon_{cw}$ [Lec72].

The emissivities (ϵ_{CO_2} , ϵ_{CO} , or ϵ_{H_2O}) of the species are fit to functions of partial² pressure P , pressure-pathlength PL, and temperature T by the expression

$$\ln \epsilon = \sum_{i=0}^2 T_i(x) \sum_{j=0}^3 T_j(y) \sum_{k=0}^3 c_{ijk} T_k(z) \quad (6-88)$$

In the above expression,

$$\begin{aligned} x &= p_1 + \frac{\ln(P)}{P_2} \\ y &= \frac{\ell_1 + \ln(PL)}{\ell_2} \\ z &= \frac{T - t_1}{t_2} \end{aligned} \quad (6-89)$$

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

$$\epsilon_g = \epsilon_{\text{CO}} + \epsilon_{\text{CO}_2} + \epsilon_{\text{H}_2\text{O}} - \Delta\epsilon_{\text{cw}} \quad (6-90)$$

where ϵ_{CO} , ϵ_{CO_2} , and $\epsilon_{\text{H}_2\text{O}}$ are the emissivities of CO , CO_2 , and H_2O , respectively, and $\Delta\epsilon_{\text{cw}}$ is the overlap correction factor for CO_2 and H_2O . The overlap correction $\Delta\epsilon_{\text{cw}}$ accounts for the 2.7- and 15- μm overlapping bands of CO_2 and H_2O . The overlap correction originally suggested by Leckner [Lec72] has been modified to include the temperature variation of $\Delta\epsilon_{\text{cw}}$ [Edw73]:

$$\Delta\epsilon_{\text{cw}} = \left| \frac{\xi}{(10.7 + 101\xi)} - \frac{\xi^{10.4}}{111.7} \right| \cdot \left\{ \log_{10} [101.3(P_{\text{CO}_2} + P_{\text{H}_2\text{O}})L] \right\}^{2.76} F(T) \quad (6-91a)$$

for $(P_{\text{CO}_2} + P_{\text{H}_2\text{O}})L \geq 1.013 \cdot 10^4 \text{ Pa}\cdot\text{m}$ and $\xi \geq 0.01$; and, otherwise,

$$\Delta\epsilon_{\text{cw}} = 0 \quad (6-91b)$$

The parameter ξ is defined by

$$\xi = P_{\text{H}_2\text{O}} / (P_{\text{H}_2\text{O}} + P_{\text{CO}_2}) \quad (6-92)$$

and $F(T)$ is given by

$$F(T) = -1.0204 \cdot 10^{-6} T^2 + 2.2449 \cdot 10^{-3} T - 0.23469 \quad (6-93)$$

In addition to ϵ_{gas} , in Equation (6-86) ϵ_p is calculated according to the method of Felske and Tien [Fél73]. This method is applicable to absorbing particles that are small enough to produce negligible scattering. Thus, the emissivity for the aerosol particle ϵ_p is given by

$$\epsilon_p = 1 - \frac{15}{\pi^4} \phi(y) \quad (6-94)$$

where ϕ is the pentagamma function, which is a function of y .

Argument y in the pentagamma function is defined as

$$y = 1 + \alpha_{\lambda_m} L_{jk} T_{\text{gas}} \lambda_m / C_2 \quad (6-95)$$

where

λ_m = reference wavelength (0.94 μm), a value representing the infrared radiation, and
 C_2 = second Planck constant, which equals $14.388 \cdot 10^{-3}$ m-K.

The term α_{λ_m} in Equation (6-95) is the absorption coefficient at the reference wavelength. The user can input this value directly into the code, or input a constant of proportionality C_{λ_m} for mechanistically calculating this value by

$$\alpha_{\lambda_m} = 4000 C_{\lambda_m} C_p \quad (6-96)$$

where C_p is the total aerosol mass concentration (kg/m^3) computed by the code.

Note that Equation (6-96) is for the aerosol cloud absorption derived by Pilat and Ensor [Pil70]. C_{λ_m} in this equation is provided to allow the user to account for the effects of wavelength, index of refraction, particle size distribution, and aerosol particle material density [Pil70]. For $C_{\lambda_m} = 1$, it corresponds approximately to soot-like particles with a density of $2000 \text{ kg}/\text{m}^3$. The user can specify C_{λ_m} based on the following relation:

$$\alpha_{\lambda_m} = \beta f_v / \lambda_m \quad (6-97)$$

where

β = a constant of proportionality,
 f_v = aerosol concentration by volume ($\text{m}^3 \text{ aerosol}/\text{m}^3 \text{ gas}$),
 and
 $= C_p / \rho_p$ (6-98)

where ρ_p is the aerosol particle material density (kg/m^3).

An asymptotic expansion representation of the pentagamma function $\phi(y)$ is given by

$$\phi(y) = y_1 + y_2 \quad (6-99)$$

where y_1 and y_2 are solved as follows.

For $y < 2.0$

$$y_2 = 6.0 \left[\frac{1}{(y+2)^4} + \frac{1}{(y+1)^4} + \frac{1}{y^4} \right], \text{ and} \quad (6-100a)$$

$$z = y + 3 \quad (6-100b)$$

For $2.0 \leq y \leq 3.0$

$$y_2 = 6.0 \left[\frac{1}{(y+1)^4} + \frac{1}{y^4} \right], \text{ and} \quad (6-101a)$$

$$z = y + 2 \quad (6-101b)$$

For $3.0 \leq y \leq 4.0$

$$y_2 = \frac{6.0}{y^4}, \text{ and} \quad (6-102a)$$

$$z = y + 1 \quad (6-102b)$$

For $y > 4.0$

$$y_2 = 0, \text{ and} \quad (6-103a)$$

$$z = y \quad (6-103b)$$

Based on the z values calculated by the above equations, y_1 in Equation (6-99) is calculated by

$$y_1 = z_3 \left[(2.0 + 3z_1) + z_2 \left\{ 2 + z_2 \left\{ -1 + z_2 \left[\frac{4}{3} + z_2(-3 + 10z_2) \right] \right\} \right\} \right] \quad (6-104)$$

where

$$\begin{aligned} z_1 &= 1/z, \\ z_2 &= 1/z^2, \\ z_3 &= 1/z^3. \end{aligned}$$

The absorptivities for the nontransparent gases and aerosol particles for Equation (6-87) are calculated in a manner similar to that used for the emissivities using Equation (6-88) through (6-104), except that T_{gas} is replaced by T_s , the structural surface temperature.

Based on these equations, the absorptivity for the nontransparent gases ($\alpha_{\text{gas},c}$) is multiplied by a factor to account for the temperature changes:

$$\alpha_{\text{gas}} = \alpha_{\text{gas},c} f_T^{0.65 - 0.2 \frac{P_{\text{vap}}}{P_{\text{tot}}}} \quad (6-105)$$

where P_{tot} = total nontransparent gas pressures, which is given by

$$P_{\text{tot}} = P_{\text{vap}} + P_{\text{CO}_2} + P_{\text{CO}} \quad (6-106)$$

6.3.3.3.2 Cess-Lian Radiative Property Model. The second radiative property model that a user can choose is the Cess-Lian model. This model is based on an analytic correlation developed by Cess and Lian and is used to calculate the steam/air emissivity and absorptivity [Ces76]. In this model, data from Hottel emittance charts [Hot67] have been fit to an equivalent single-band exponential form, which requires significantly less computation time than that for a wide-band exponential model. In CONTAIN, if the Cess-Lian radiative property model is chosen, CO and CO₂ (if present) are assumed to be transparent. Therefore, they do not contribute to the total atmospheric gas-mixture emittance. Obviously, this model should be used only when the effect of steam is dominant.

Equations to calculate $\epsilon_{m,jk}$ and $\alpha_{m,jk}$ for the Cess-Lian radiative property model are similar to those for the Modak radiative property model, except ϵ_{gas} and α_{gas} are calculated as follows.

The value of ϵ_{gas} is calculated based on the steam/air mixture as

$$\epsilon_{\text{gas}} = a_0 \left[-\exp(-a_1 \sqrt{x}) \right] \quad (6-107)$$

where a_0 , a_1 are coefficients determined from Table 6-3, with linear interpolation used to find values at intermediate temperatures.

The value of x in Equation (6-107) is calculated by

$$x = P_{H_2Ovap} L_{jk} \left(\frac{300}{T_{gas}} \right) \left\{ \frac{P_{gas} + \left[5 \left(\frac{300}{T_{gas}} \right)^{1/2} + 0.5 \right] P_{H_2Ovap}}{(101325)^2} \right\} \quad (6-108)$$

Table 6-3
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

where

P_{H_2Ovap} = partial pressure of water vapor (Pa),
 L_{jk} = beam length between surface j to k (m),
 P_{gas} = cell pressure (Pa), and
 T_{gas} = cell temperature (K).

Similar to ϵ_g , $\alpha_{gas,c}$ is calculated using Equations (6-107) and (6-110), except T_{gas} is replaced by T_s , the structural surface temperature.

With $\alpha_{gas,c}$ defined, the α_{gas} is calculated by

$$\alpha_{gas} = \alpha_{gas,c} \left(\frac{T_{gas}}{T_s} \right)^{0.45} \quad (6-109)$$

6.4 Heat Conduction

Heat transfer structures in the containment building (including walls, roof, floors, and internal structures) are major repositories of the heat released by the reactor fuel, by FPs, and by chemical reactions. The pressure and temperature of the

atmosphere are determined largely by the competition between numerous sources of heat energy and the removal of heat by transfer to the structures. CONTAIN models for heat transfer between the structures and the atmosphere take radiation, convection, condensation, and evaporation into account (see Section 6.3). Heat transfer within each structure is handled by a one-dimensional heat conduction equation for the materials specified for the structure.

Section 6.4.1 describes the types of heat structures currently available in CONTAIN. Section 6.4.2 discusses the formulation of the heat conduction models used in CONTAIN.

6.4.1 Containment Structures

This section describes the different types of structures that can be modeled with the CONTAIN code. Containment heat sinks and surfaces for radionuclide and aerosol deposition are modeled as structures. The modeling of heat transfer to structures and heat conduction in structures is discussed in Sections 6.3, 6.4, and 6.5. The behavior of some of these models depends upon structure geometry and orientation. This information is therefore specified as problem input data by the user. Each structure can consist of an arbitrary combination of different materials. Each material present in a structure must either be in the CONTAIN material library or must be a user-defined material. Nodalization of each structure for the conduction model is also the responsibility of the user. Other user input requirements for the structures are described in the CONTAIN 1.1 User's Manual [Mur89]. Note that the modeling of structures has undergone significant enhancement since the release of CONTAIN 1.1, as described in Appendix A.

All structures are modeled as one-dimensional slabs, half-cylinders, or hemispheres with the conduction equation solved in the appropriate coordinate system for the three different geometries (see Section 6.4.2). Each structure must also be designated as either a "wall", "floor", or "roof". This orientation information is used in the convection and condensation/evaporation models to select the proper natural convection heat transfer correlation (laminar or turbulent, see Section 6.3), and in the aerosol deposition model (see Section 4) to restrict gravitational forces to horizontal structures. Note that each structure in a cell can have its inner and outer surfaces in the same cell. In this case, the outer surface of a "roof" structure is actually modeled as a "floor" in the cell. Similarly, the outer surface of a "floor" structure is modeled as a "roof". The orientation of a structure does not have an effect on the conduction model.

The inner surface of a structure is always inside the cell in which the structure is defined. The outer surface of a structure may or may not be inside the same cell, at the user's option. The outer surface may also be isolated from all containment cells as explained later. The heat and mass transfer models for convection, condensation, and radiation described in the following sections

apply to all inner surfaces; however, they only apply to those outer surfaces that reside in the same cell as their respective inner surfaces. Certain modeling limitations apply to the outer structure surfaces that are located in a cell different than their respective inner surface. Such surfaces will be denoted "exterior surfaces". Exterior surfaces will normally be present in a CONTAIN calculation when a structure, usually a wall, is a physical boundary between two containment rooms, where each room is modeled as a different CONTAIN cell.

The following limitations and special considerations apply to the modeling of exterior surfaces. First, condensation and evaporation are not modeled for exterior surfaces. Second, aerosol deposition, including the deposition of aerosolized water, is not modeled for exterior surfaces. Third, the net enclosure radiation model does not include exterior surfaces in its treatment. Note that radiation is modeled for exterior surfaces in the simple radiation model. The differences between these two models are described in Section 6.4. Finally, and perhaps most importantly, convection heat transfer modeling for exterior surfaces does not use the mechanistically based natural convection Nusselt correlations nor can the forced convection model be used (see Section 6.3). Instead, the heat transfer coefficient for convection is fixed at $6.08 \text{ W/m}^2\text{-K}$ for all exterior surfaces. Note that this is a typical heat transfer coefficient value obtained using a turbulent natural convection Nusselt correlation (see Section 6.3).

An exterior surface need not actually be in thermal contact with another cell's atmosphere. That is, an exterior surface may be isolated from all containment cells with either an adiabatic or isothermal boundary condition. The heat flux is fixed at zero in the adiabatic boundary condition case. In the isothermal boundary condition case, the exterior surface is treated as if exposed to a fictitious atmosphere at a fixed user-specified temperature. Again, a fixed surface heat transfer coefficient of $6.08 \text{ W/m}^2\text{-K}$ is used between the exterior surface and the fictitious atmosphere. Any energy convected from the exterior surface is lost from the problem, and any energy convected into the surface is magically created.

If the above noted exterior surface limitations are believed to have a significant impact, such as when condensation occurs on both surfaces of a wall which separates two cells, then it may be better to divide the structure in half and put one half in each cell. An adiabatic boundary condition should then be used for the exterior surface of each half. This is a commonly used work-around to the above noted limitations for exterior surfaces. Note, however, that there will be no conduction of heat from one half of the structure to the other half when this procedure is followed. For many severe accident scenarios, the structures that divide containment rooms are sufficiently thick such that the time scale of interest in the problem is much shorter than the time required for conduction through the wall; therefore, the limitation of this work-around will not have an appreciable effect. CONTAIN 1.11 has been

improved to allow for different cells on either side of a heat structure. See Appendix A.

6.4.2 Heat Conduction Model

This section describes the CONTAIN heat conduction model for calculating structure temperatures. This model applies to each structure geometry and orientation that can be represented in CONTAIN. CONTAIN also models the conduction of heat in the basemat of the cavity when CORCON-MOD2 is not used to model corium-concrete interactions. The conduction equation solved for the cavity basemat is identical to the one used for structures; however, the boundary conditions are handled differently and there are special provisions to account for the possibility of coolant pool boiling in the LC conduction model (see Appendix D). Only the conduction model as it is applied to calculate structure temperatures is described here. Note that heat conduction is modeled internally to the CORCON-MOD2 module for problems in which corium-concrete interactions occur.

Heat conduction in structures is modeled by solving the standard one-dimensional heat conduction equation,

$$\rho(r)c_p(r) \frac{\partial T(r,t)}{\partial t} = \nabla \cdot k(r) \nabla T(r,t) + q'''(r) \quad (6-110)$$

where

$T(r,t)$ = Temperature at position r at time t ,
 $q'''(r,t)$ = volumetric energy source rate,
 $k(r)$ = thermal conductivity,
 $\rho(r)$ = density, and
 $c(r)$ = specific heat capacity.

Note that because structures are allowed to be comprised of various materials in CONTAIN, the thermal conductivity, density, and heat capacity are all functions of the spatial coordinate r , which is defined as the coordinate normal to the inner surface. For half-cylinders and hemispheres, r is the distance from the center of curvature of the half structure. Clearly the conductance term $\nabla \cdot k \nabla T$ is also dependent upon the geometry of the structure. The treatment of this term for the three geometries modeled is described in Section 6.4.2.2. The volumetric energy source rate term is zero for all locations except the surface nodes in the discrete form of the conduction equation as explained in Section 6.4.2.1 below. This section also describes the initial and boundary conditions used in the solution to the conduction equation. The conduction equation solution method is fully described in Section 6.4.2.2.

6.4.2.1 Conduction Equation Initial and Boundary Conditions. The time evolution of each structure's temperature profile is determined by solving a discretized version of the conduction equation at each timestep. Therefore, the temperature results from the previous timestep are used as the initial condition for the conduction equation for a given timestep. This approach is used for each structure at every cell timestep. The properties of the materials are evaluated at the initial temperature at the beginning of a timestep. In addition, the boundary conditions and surface node energy sources discussed below are calculated using the initial temperatures. Therefore, the coupling between the conduction model and the heat transfer models discussed in other sections is explicit.

The heat conduction equation in CONTAIN is always solved using adiabatic boundary conditions. However, this does not mean that all structures are treated as being adiabatic. The conduction model accounts for heat transfer between structures and the atmosphere through the volumetric energy sources of the surface nodes. These energy sources are set to reflect heat transfer from convection, condensation/evaporation, radiation, and FP decay heating. That is, the energy transferred by these processes to or from structures is deposited into the surface nodes. Thus, the volumetric energy source in the above conduction equation is zero for all nodes except for the surface nodes. The inner and outer surface node volumetric energy source rates can be written in equation form as,

$$\begin{aligned} q_i''' &= (Q_c + Q_r + Q_{fp})_i / V_i \\ q_o''' &= (Q_c + Q_r + Q_{fp})_o / V_o \end{aligned} \quad (6-111)$$

where subscripts "i" and "o" refer to the inner and outer surfaces and

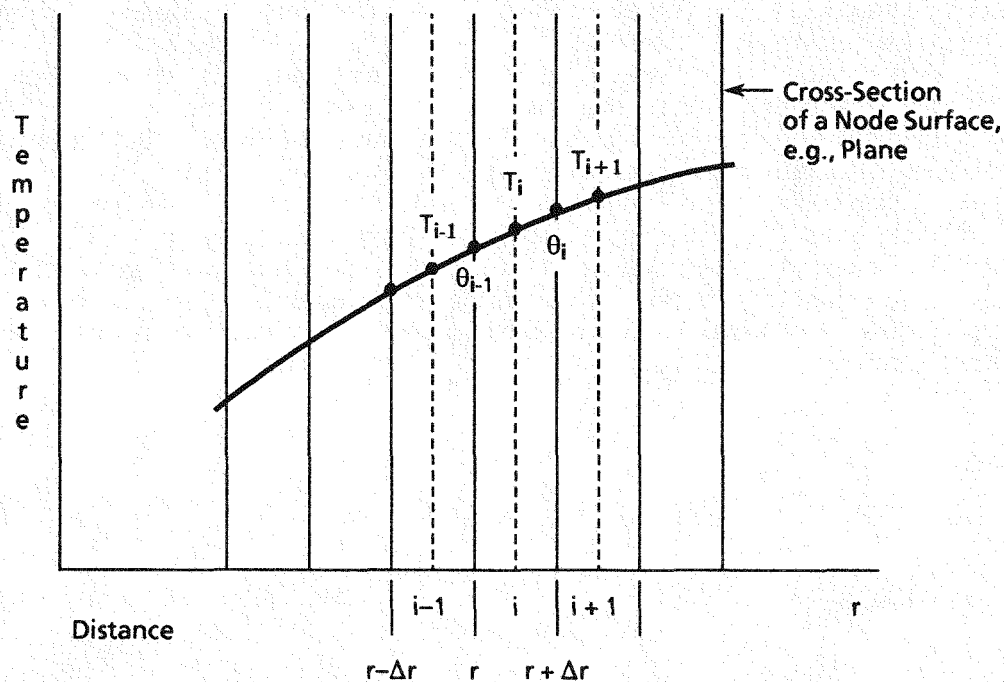
Q_c = convection and condensation energy transfer rate,
 Q_r = radiative energy transfer rate,
 Q_{fp} = FP decay heating rate,
 V_i = volume of inner node, and
 V_o = volume of outer node.

Note that q_o''' is only given by the above expression if the outer surface is not an exterior surface. Section 6.2 describes the various outer surface boundary condition treatments for exterior surfaces. Normally, exterior surfaces are specified as adiabatic, in which case q_o''' would be zero.

6.4.2.2 Heat Conduction Solution Method. This section describes the method used to solve the heat conduction equation for the three structure geometries modeled in CONTAIN. The algorithm described below is actually the one used to solve the conduction equation in CONTAIN 1.11, see Appendix A; however, the exact same method is

used in CONTAIN 1.1 for slab geometry. The solution algorithms used in CONTAIN 1.1 for half-cylinders and hemispheres are, unfortunately, incorrect. These algorithms are given at the end of this section for completeness.

The conduction equation for each structure is solved by discretizing the temperature variable in space and time. The spatial nodalization must be specified by the user, and each spatial zone must consist of only one material. There is no fundamental limit to the number of spatial nodes that a user can choose; however, care should be taken not to nodalize a structure too coarsely. The temperature distribution in a structure is therefore represented by its center node temperatures, as illustrated in Figure 6-5.



Note: Derivatives and temperature are calculated at the midpoint between nodes.

Figure 6-5. Nodes in a One-Dimensional System

A first order Taylor series expansion is used to represent the time rate of change of temperature as follows:

$$\frac{\partial T(r,t)}{\partial t} \cong \frac{T_i^{n+1} - T_i^n}{\Delta t} \quad (6-112)$$

where "i" is the structure node index at location r, and "n" is the timestep number corresponding to the beginning of the timestep at problem time t. An implicit integration scheme is used in CONTAIN to solve the discretized conduction equation. That is, temperatures in the conductance term are the end of timestep values, which are unknown at the beginning of timestep "n". This fully implicit treatment guarantees a stable solution; however, the timestep should still be chosen to be on the order of or smaller than the time constant for conduction through a node to achieve acceptable accuracy.

The conduction equation for node "i", at timestep "n" is then given by

$$\rho_i c_i \frac{T_i^{n+1} - T_i^n}{\Delta t} = \nabla \cdot k_i \nabla T_i^{n+1} + q_i''' \quad (6-113)$$

Where the subscripted material properties are the values of the property functions for the one material in node "i" at the temperature of that node at step "n". Recall that only one material is allowed to be present in a node; therefore, the properties of all nodes can be taken to be constants. Equation (6-113) is solved by integrating over the volume V_i of each node. If one then applies the divergence theorem to the conductance term, the discretized conduction equation integrated over the volume of node "i" can be expressed as

$$m_i c_i \frac{T_i^{n+1} - T_i^n}{\Delta t} = k_i (\nabla \theta_{i+1}^{n+1} A_{i+1} - \nabla \theta_i^{n+1} A_i) + q_i \quad (6-114)$$

where

A_i = area at interface "i", and

$\nabla \theta_i$ = temperature gradient at interface "i".

Notice that the density times the volume has been replaced by the total mass of the node m_i in the above equation. Also, the volumetric heating rate times the volume has been replaced by the energy deposited into the node per unit time q_i .

If the structure has been nodalized into "N" slabs, then there will be "N" such equations. The temperature gradient in this equation is approximated by the following first order Taylor expansion,

$$\nabla \theta_i \cong \frac{\theta_i - T_i^{n+1}}{\delta r} \quad (6-115)$$

where, θ_i is the temperature at the interface between nodes "i" and "i+1", and " δr " is the distance between the node midpoint and the interface (see Figure 6-5). Note that this expression is the same for all three geometries. However, the location of the node midpoint, and therefore the value of " δr " is geometry dependent. This distance is chosen such that the volume on both sides of the point are equal.

The interface temperature θ_i has still not been defined at this point. All interface temperatures can be eliminated from the equation by imposing the assumption that the heat flux on both sides of the interface between two nodes must be equal. If this is done, the temperature gradient at the interface in Equation (6-115) can be expressed in terms of differences between the center node temperatures alone. The discretized conduction equation for a given node is then given by

$$T_i^{n+1} - T_i^n = \frac{\bar{K}_{i+1} A_{i+1} \Delta t}{m_i C_i} (T_{i+1}^{n+1} - T_i^{n+1}) - \frac{\bar{K}_i A_i \Delta t}{m_i C_i} (T_i^{n+1} - T_{i-1}^{n+1}) + \frac{q_i \Delta t}{m_i C_i} \quad (6-116)$$

The $\bar{K}_i$ parameters introduced in this equation are constants that are derived by applying the flux continuity condition at the interfaces. These constants depend upon the thermal conductivity of the two regions on both sides of the interface, and the distances to the center of each node. This parameter, often called the effective conductance between node "i" and "i+1", is geometry dependent because the distances to the node centers and the interface areas are both geometry dependent. If the algebraic manipulations described above are performed, it can be readily shown that the conductances $\bar{K}_i$ and the half node thicknesses δr_i for the three geometries are given by

$$\bar{K}_i = \frac{1}{\left(\frac{k_i}{\delta r_i} \right)^{-1} + \left(\frac{k_{i+1}}{\delta r_{i+1}} \right)^{-1}} \quad (6-117a)$$

The δr_i and δr_{i+1} depend on the structure geometry.

For the slab geometry

$$\delta r_i = \delta r_{i+1} = \frac{r_{i+1} - r_i}{2} \quad (6-117b)$$

For the cylindrical geometry

$$\delta r_i = r_i \ln \left(\frac{\bar{r}}{r_i} \right) \quad (6-117c)$$

$$\delta r_{i+1} = r_{i+1} \ln \left(\frac{r_{i+1}}{\bar{r}} \right) \quad (6-117d)$$

where

$$\bar{r} = \left(\frac{r_{i+1}^2 + r_i^2}{2} \right)^{1/2}$$

For the spherical geometry

$$\delta r_i = r_i \frac{\bar{r} - r_i}{\bar{r}} \quad (6-117e)$$

$$\delta r_{i+1} = r_{i+1} \frac{r_{i+1} - \bar{r}}{\bar{r}} \quad (6-117f)$$

where

$$\bar{r} = \left(\frac{r_{i+1}^3 + r_i^3}{2} \right)^{1/3}$$

Recall from Section 6.4.2.1, that only node 1 and node "N" will have a non-zero energy term in CONTAIN even though the method can, handle non-zero values for any node. There are "N" linear coupled equations like Equation (6-116) to solve to calculate the temperature profile of a structure with "N" nodes. These equations form a set of coupled linear equations with N unknown center node temperatures. These equations are expressed in a tri-diagonal matrix solved using a standard tri-diagonal matrix solver in CONTAIN.

The last few paragraphs of this section describe the incorrect algorithm in CONTAIN 1.1 used for half-cylinders and hemispheres. In CONTAIN 1.1, cylinders and spheres use the algorithms given in Equation (6-117c) through (6-117f) with the following differences. First, the node center is placed in the middle of the node. Second, the effective conductances are given by the following expressions:

For the slab geometry,

$$\bar{K}_i = \frac{1}{\left(\frac{k_i}{\delta r_i}\right)^{-1} + \left(\frac{k_{i+1}}{\delta r_{i+1}}\right)^{-1}} \quad (6-118a)$$

For the cylindrical geometry,

$$\bar{K}_i = \frac{1}{\left(\frac{k_i}{r_{i+1}}\right)^{-1} \ln \left[\frac{r_{i+1}}{\left(\frac{r_i + r_{i+1}}{2}\right)} \right] + \left(\frac{k_{i+1}}{r_{i+1}}\right)^{-1} \ln \left(\frac{r_{i+1} + r_{i+2}}{2 r_{i+1}} \right)} \quad (6-118b)$$

For the spherical geometry,

$$\bar{K}_i = \frac{1}{\left(\frac{k_i}{\delta r_i}\right)^{-1} \left[\frac{r_{i+1}}{\left(\frac{r_i + r_{i+1}}{2}\right)} \right] + \left(\frac{k_{i+1}}{\delta r_{i+1}}\right)^{-1} \left(\frac{r_{i+1} + r_{i+2}}{2 r_{i+1}} \right)} \quad (6-118c)$$

Unfortunately, the origin of these incorrect expressions is unknown and an explanation or derivation therefore cannot be provided.

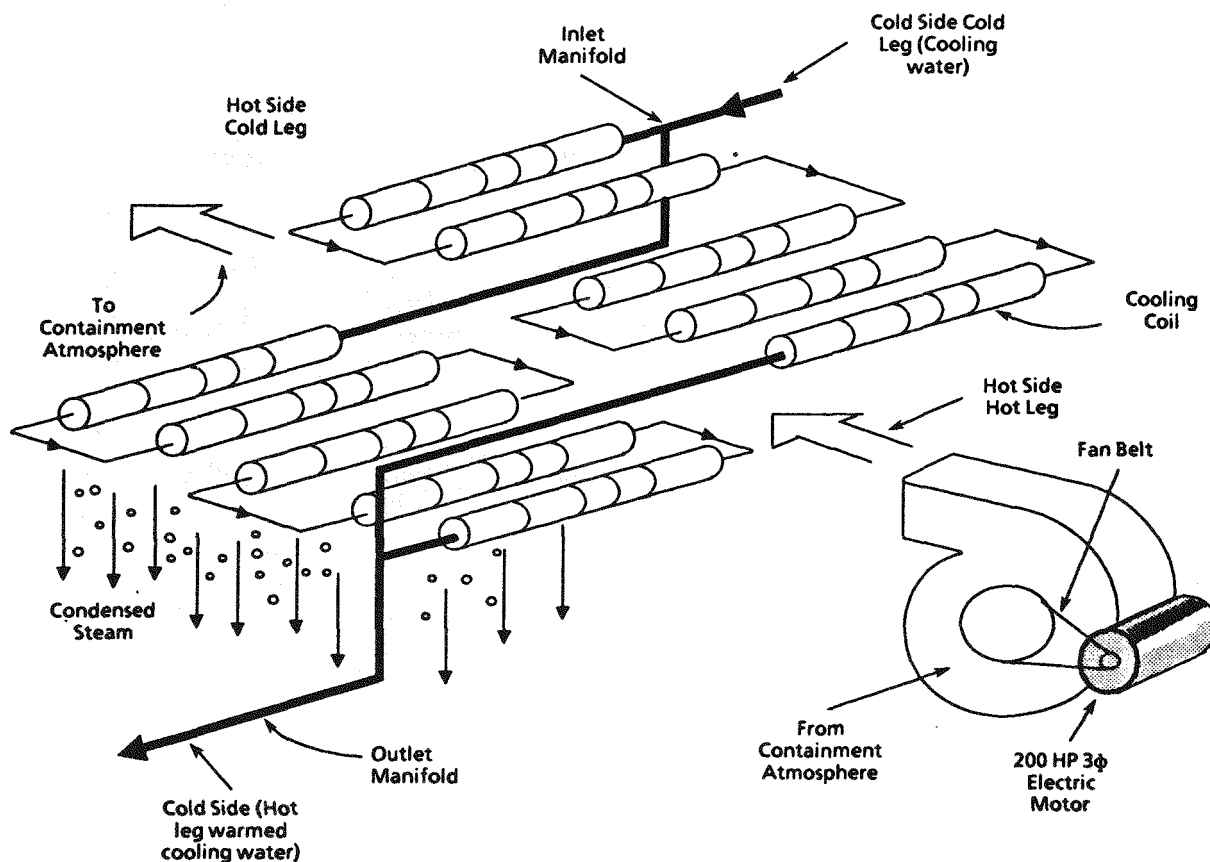
Note that the errors obtained using the CONTAIN 1.1 solution for half-cylinders and hemispheres are usually relatively small when compared to analytic solutions; however, the errors can become larger for very long-term problems. It should also be noted that very few CONTAIN applications performed to date have used half-cylindrical or hemispherical structures. Standard practice is to model such structure geometries as equivalent slabs, since the curvatures are typically very small. Finally, the conduction equation solution method used for the cavity basemat in CONTAIN 1.1 is the slab geometry algorithm described in the first part of this section.

6.5 Engineered Safety Features

The discussion of the ESFs is organized into three basic sections. They are fan cooler (FC) models, ice condensor (IC) models, and containment spray (CS) models. Associated with these models is a framework for construction of a liquid transport system that can provide sources and sinks of coolant for the ESFs. The liquid transport system models can also function independently of the basic ESF models. Note that CONTAIN models different from the ESF provide information to and receive information from the ESF models.

6.5.1 Fan Cooler Model

FCs are included in containment to provide nonemergency cooling and to augment the steam removal capabilities of the water sprays in the event of an accident. If operable during a severe accident, they could be important in reducing pressure and temperature. The cooling takes place as large-capacity fans pull the containment atmosphere across banks of finned, service-water-cooled coils, as illustrated in Figure 6-6.



Note: Arrows indicate direction of fluid flow

Figure 6-6. FC System

Each cooler has several parallel coolant paths to route water back and forth across the path of the horizontally circulated atmosphere. The coils are vertical and stacked horizontally in layered rows with the coolant entering at the back and leaving at the front, as depicted in Figure 6-7. The geometry is therefore that of a cross-flow heat exchanger (HX) with counterflow; that is, the atmosphere inlet side corresponds to the coolant outlet side. For large dry PWRs, the coolers are designed to work under normal as well as 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

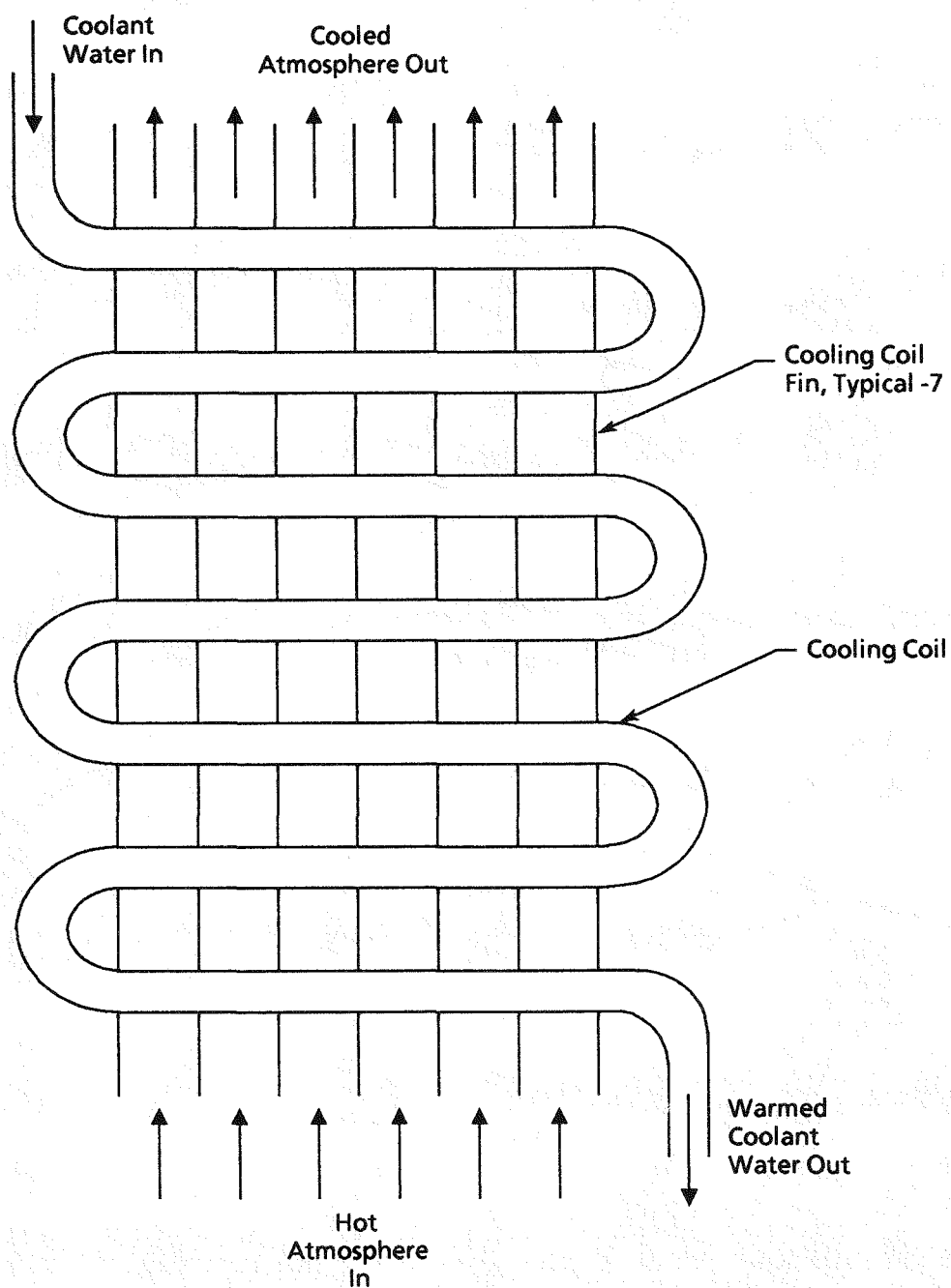


Figure 6-7. FC Geometry Depicting One Horizontal Cooling Coil (top view)

capability is in the range of 2 to $4 \cdot 10^7$ W. BWR and subatmospheric containments generally include FCs that are designed only for normal operating conditions, but the performance of such coolers may still be important following an accident.

The CONTAIN FC models do not address the FC air filters, which typically use roughing and High-Efficiency Particulate Airborne (HEPA) filters.

6.5.1.1 Fan Cooler Heat Transfer Models

CONTAIN has two FC models, the March model and a more mechanistic condense model. The simpler of the two models is the one developed for the MARCH code [Woo83].

March Model User input is required for this model for the rated cooling capacity, the rated containment inlet gas temperature, the rated coolant inlet temperature, and the rated coolant mass flow rate. 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 FCs in the Zion nuclear power plant [Zio00].

The MARCH model is simple and fast, and when used with the Zion FC characteristics, reproduces the Zion published capacity curve with reasonable accuracy. It does not address the effect of noncondensable gases other than air. Also, FP removal, condensation, and aerosol depletion are not 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 models from the simple iterative MARCH code (Model 5) are the equations that follow for the heat transfer coefficient, effective heat transfer area, and heat removal by the FC. This model does not remove water.

The heat transfer coefficient correlation [Woo83] equations are

$$h_r = 1527.0 + 2325 (X - 0.26), \quad \text{for } X \geq 0.26 \quad (6-119a)$$

$$h_r = 590.5 + 3603 X, \quad \text{for } X < 0.26 \quad (6-119b)$$

where

$$h_r = \text{FC heat transfer coefficient at rated conditions,}$$

$$X = P_{\text{gas}} / (P_{\text{gas}} + P_{\text{air}}),$$

and P_{gas} and P_{air} are the water vapor and air partial pressures at the rated containment atmosphere temperature, with the atmosphere assumed to be saturated.

The MARCH FC effective heat transfer area is then determined from

$$A_{\text{FC}} = \frac{Q_r}{h_r(T_{\text{ar}} - T_{\text{cr}}) - \frac{Q_r h_r}{8374 \cdot W_{\text{cr}}}} \quad (6-120)$$

where

A_{FC} = the effective area,
 Q_r = rated energy removal rate,
 T_{ar} = rated containment atmosphere temperature,
 T_{cr} = rated HX coolant temperature,
 8374 = twice the specific heat of water, and
 W_{cr} = rated coolant mass flow rate.

Calculations are then performed for the CONTAIN calculation by using Equations (6-119a) and (6-119b) to determine h and then Q at any other X

$$Q = \frac{h A_{\text{FC}} (T_a - T_{\text{cr}})}{\left[1. + \frac{h A_{\text{FC}}}{(8374. + W_{\text{cr}})} \right]} \quad (6-121)$$

This is the energy removed from the cell upper atmosphere. This model does not remove any condensed mass or aerosols.

Mechanistic Model The more mechanistic FC model, activated by the keyword CONDENSE, is based upon condensation mass transfer h_m and convective heat transfer coefficients for h_c that depend on the cell atmospheric conditions. The equations are given below. Note that the equations for h_m and h_c are similar to equations presented in Section 6.3 for the determination of heat and mass transfer to heat structures. 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 and a stream velocity based upon the air/steam flow rate and the cooler frontal area. The effective heat transfer area per row is an input parameter. 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 is used for heat transfer between the gas/condensate-film interface and the coolant. An approximate

value for this parameter found to be reasonable in parametric comparisons with published cooler capacity curves is $1000 \text{ W/m}^2\text{-K}$, which is also the default value.

The calculation is carried out iteratively. The steam/air mixture inlet conditions and flow rate are known. The cooling water exit temperature is first estimated from the MARCH model and the input cooler capacity. The temperature change of the cooling water because of convection 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 user-specified value. 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 FC 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.

For the calculation described above, the convective heat transfer coefficient h_c is obtained for each FC row from

$$h_c = \frac{Nu \, k_{flm}}{d_{cc}} \quad (6-122)$$

where

$$Nu = \text{Nusselt number} = 0.33 \, Re^{0.6} \, Pr^{0.33333};$$

$$Re = \text{Reynolds number} = \frac{d_{cc} \, v \, \rho_f}{\mu_f};$$

$$d_{cc} = \text{coolant coil outside diameter, which usually is inputted to account for the effect of the fins;}$$

$$\begin{aligned}
V &= W/\rho_b A = \text{velocity, and} \\
W &= \text{user-specified containment-side mass flow rate,} \\
\rho_b &= \text{bulk density of containment side fluid, and} \\
A &= \text{user-specified containment-side flow area;} \\
\rho_{flm} &= \text{air/steam density at film temperature } T_{flm}; \\
T_{flm} &= \text{film temperature} = \frac{T_a + T_c}{2}, \\
T_a &= \text{atmosphere temperature, and} \\
T_c &= \text{user-specified coolant temperature;} \\
\mu_{flm} &= \text{air/steam viscosity at } T_{flm}; \\
Pr &= \text{Prandtl number} = \frac{C_{p,flm} \mu_{flm}}{k_{flm}}; \\
C_{p,flm} &= \text{air/steam specific heat at } T_{flm}; \text{ and} \\
k_{flm} &= \text{air/steam thermal conductivity at } T_{flm}.
\end{aligned}$$

Note that each row uses updated values for T_a , T_c , and the steam mass fraction.

The condensation mass transfer coefficient h_m is obtained from

$$h_m = \frac{Sh D_{flm} \ln \frac{(1 - X_{s,c})}{(1 - X_{s,b})}}{R T_{flm} d_{cc} (X_{s,b} - X_{s,c})} \quad (6-123)$$

where

$$\begin{aligned}
Sh &= \text{Sherwood number} = Nu \left(\frac{Re}{Pr} \right)^{1/3}, \\
Sc &= \text{Schmidt number} = \frac{\mu_{flm}}{\rho_{flm} D_{flm}}, \\
D_{flm} &= \text{binary diffusivity at the film temperature,} \\
X_{s,c} &= \text{steam mole fraction at the cooling coil temperature, and} \\
X_{s,b} &= \text{steam mole fraction at bulk conditions.}
\end{aligned}$$

6.5.1.2 Fan Cooler Aerosol Deposition Model. Aerosol deposition driven by diffusiophoresis may be significant across a FC. Deposition by this process is calculated when the CONDENSE model is active. Any deposited aerosols, FPs hosted by these aerosols, and the FC condensate are routed to the pool in the cell indicated by the user. The repository in which the aerosols and FPs are placed is the same as for aerosols and FPs collected by sprays.

The diffusiophoresis (which is driven by the differential vapor pressure) deposition rate is given by the following equation:

$$\text{Dep}_{df} = \frac{\text{PR}_s (M_w)^{1/2} \frac{V}{\rho_m}}{\left[\text{PR}_s (M_w)^{1/2} + (1 - \text{PR}_s) (M_g)^{1/2} \right] m_c} \quad (6-124)$$

where

$$\text{PR}_s = \frac{P_{\text{sat}}}{P_{\text{cell}}},$$

$$P_{\text{sat}} = \text{steam saturated pressure at } T_m,$$

$$T_m = (T_{\text{cell}} + T_c) \cdot 0.5$$

where T_{cell} is the cell temperature

$$P_{\text{cell}} = \text{cell atmosphere pressure,}$$

$$M_w = \text{molecular weight of water,}$$

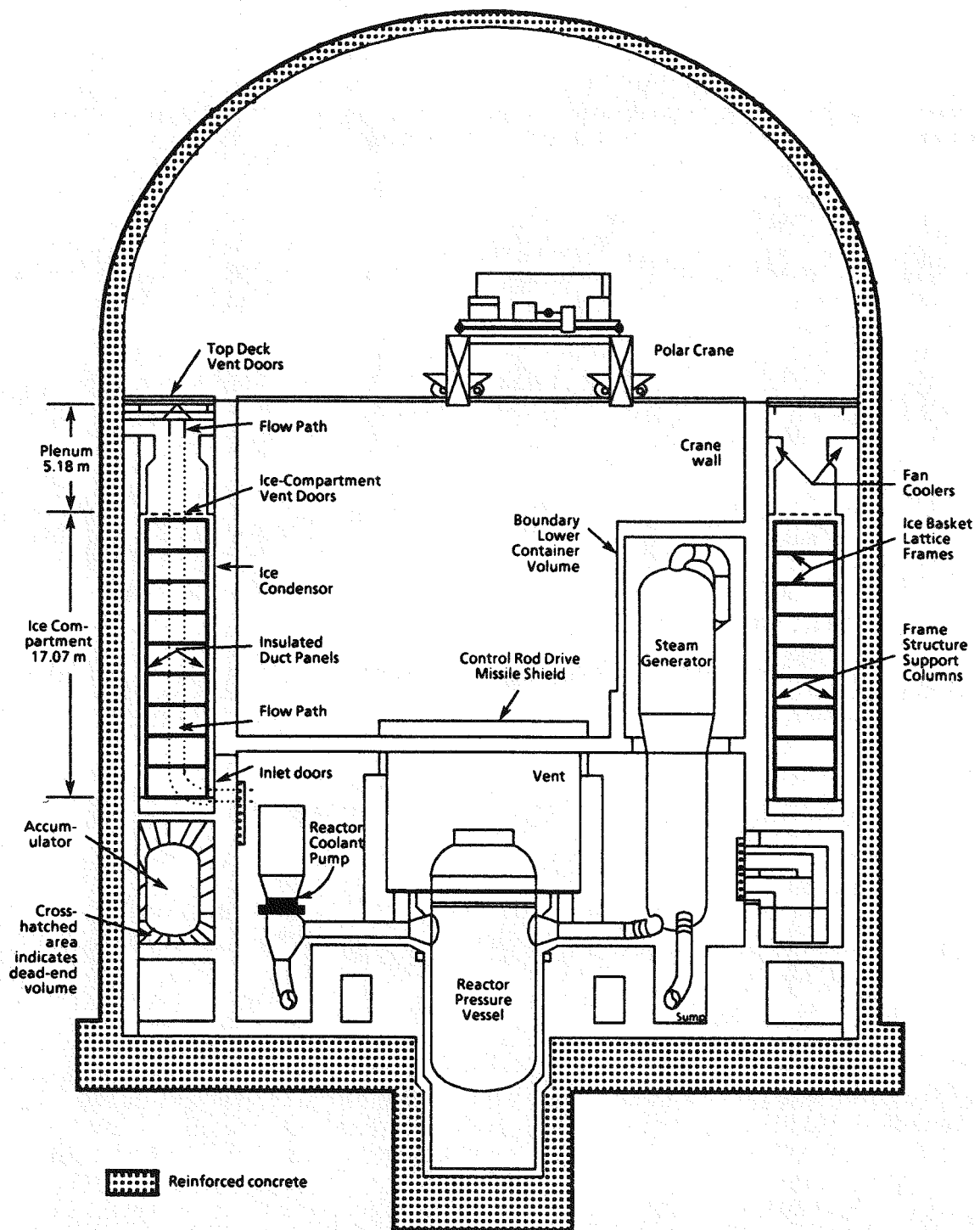
$$V = \text{cell volume,}$$

$$\rho_m = \text{steam density at } T_m \text{ and } P_s, \text{ and}$$

$$m_c = \text{mass transfer condensation rate from the equations above.}$$

6.5.2 Ice Condenser

The IC containment system is an innovation by Westinghouse Electric Corporation designed to suppress the pressure rise within a containment arising from a loss-of-coolant accident (LOCA). The design incorporates a large volume of subcooled ice that acts as a low temperature, passive heat sink. A typical IC containment is shown in Figure 6-8 and 6-9. 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 baskets 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 baskets, 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 IC, the peak pressure is



Note the flow path through the IC on the left, indicated by the dotted lines beginning at the inlet doors and ending with an arrowhead at the top deck vent doors.

Figure 6-8. Sectional View of an Ice Compartment and Containment Region Boundaries (adapted from Win83)

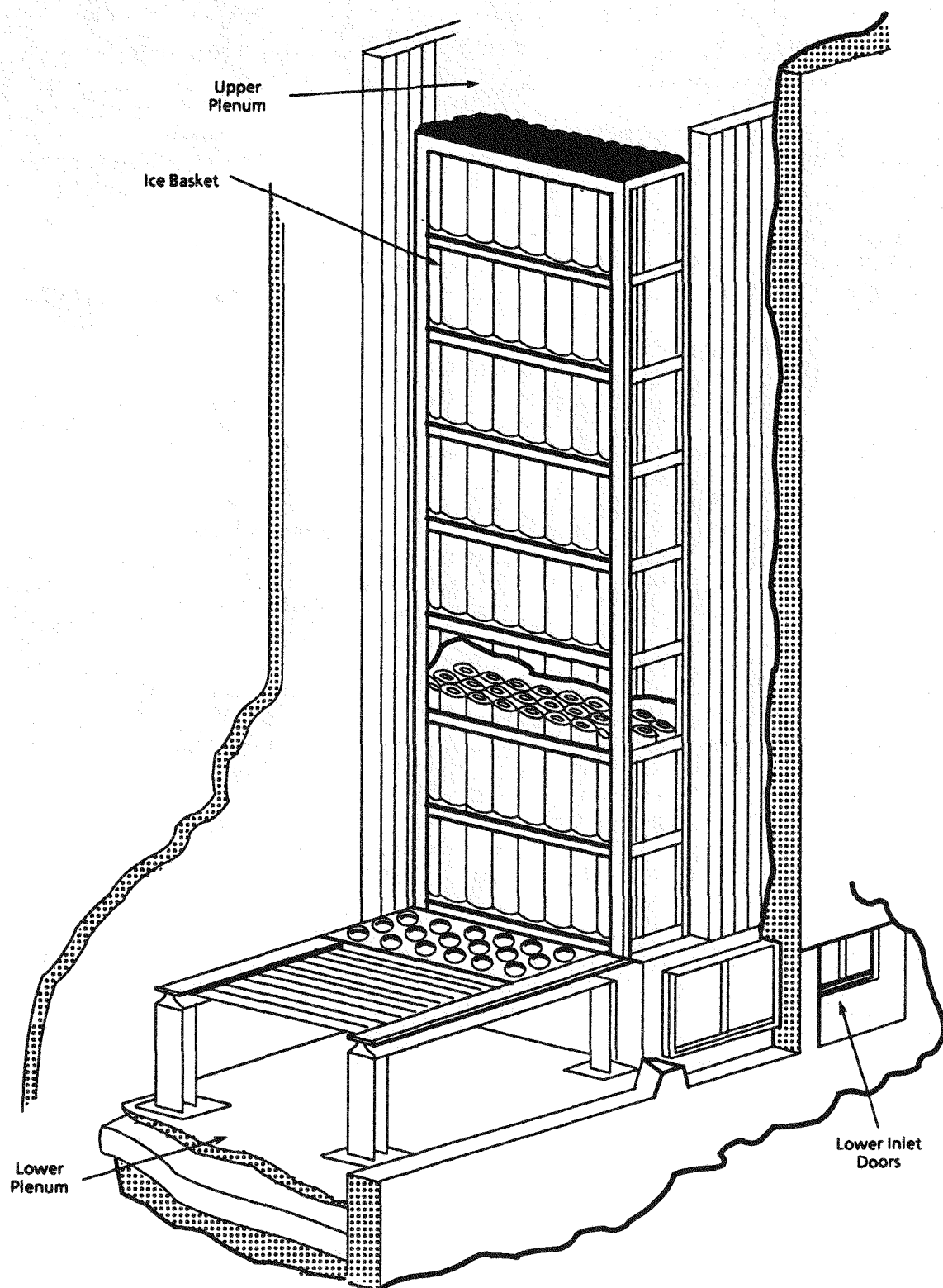


Figure 6-9. Simplified Diagram of an IC. Note that the ice baskets are perforated cylinders that are supported around their circumference by horizontal wire strips that are approximately 6 mm long and 2 mm thick.

determined largely by the accumulation of noncondensable gases in the upper compartment.

The doors opening into and out of the ice compartment are held closed by spring and gravity forces, respectively. The doors open when there is sufficient pressure difference to overcome the forces keeping the doors closed. 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.

Care should be taken in interpreting results of IC calculations, because few experimental or calculational results are available for comparison and validation of the modeling.

6.5.2.1 Ice Condenser Melting Models. Direct heat transfer to and condensation on the ice is treated in a manner similar to that for a cylindrical wall structure (see Section 6.3.2). Because the ice is contained in baskets, only the length and, hence, the heat transfer area is assumed to decrease as heat is absorbed and the ice is melted. The condensate, aerosols and associated FPs, and melted ice are diverted to the cell designated by the user to receive the residual liquid for the engineered system to which the IC is assigned (by user input). This cell is the input parameter "iclout". 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 IC system depends, to some extent, upon the temperature of this effluent, which is the input parameter "citlex". This temperature is difficult to calculate mechanistically and is therefore an input parameter.

The equations for heat and mass transfer to structures given in Section 6.3 are also used to calculate the heat and mass transfer to the ice in an IC. Both turbulent natural convection and forced convection are considered. Note that the expressions used for the Nusselt number are similar but contain a user-input multiplier that can be used to account for the roughness of the cylindrical ice columns. The default value of the multiplier is five.

The forced-convection velocity v used for the IC is based on values for the velocity into the ice condenser v_{in} and the velocity out off the ice condenser v_{out} . The v_{in} and v_{out} are based on the assumption that the flow goes through an isentropic expansion. Specifically,

$$v_{in} = \sum_{\substack{\text{flows} \\ \text{to IC}}} \frac{W F_e}{D_{IC} \rho_u} \quad (6-125)$$

where D_{IC} is the ice chest hydraulic diameter and

$$\begin{aligned} F_e &= 1 \text{ for outgoing flows,} \\ &= (P_u/P_c)^{1/\gamma_u} \text{ for incoming flows} \end{aligned} \quad (6-126)$$

ρ_u is the gas density of the upstream cell, γ_u is the specific heat ratio for the upstream cell, W is the mass flow rate, and P_u and P_c are the pressures of the upstream and downstream cells, respectively. (Here W is taken to be positive if the flow is in.) An expression similar to Equation (6-125) is used for v_{out} , except that the sum is carried over the flows from the IC.

The forced convective velocity v is chosen as follows

$$\begin{aligned} v &= v_{in} \text{ if } v_{in} > 0 \text{ and } v_{out} > 0 \\ &= v_{out} \text{ if } v_{in} < 0 \text{ and } v_{out} < 0 \\ &= ||v_{in}| - |v_{out}|| \text{ otherwise} \end{aligned} \quad (6-127)$$

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

Others require some discretion on the part of the user. Among these are the melt-condensate temperature of the water draining from the IC and the initial total IC surface area available for heat transfer. The drain temperature is dependent upon the flow rate through the compartment, and tests have produced values between 335 and 373 K. In an IC plant, there is initially over $7 \cdot 10^5 \text{ m}^2$ 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 lower plenum cell is the cell directly below, that is, upstream of the ice compartment, which may be the lower plenum or the lower compartment, depending upon the nodding scheme.

As noted above, the heat transfer to and steam condensation on the ice are treated in a manner similar to that for other heat sinks. Differences in the IC treatment include a film resistance corresponding to a fixed 0.5 mm water film and the neglect of evaporation, which is highly unlikely. Conduction within the ice is also neglected and the ice is assumed to be at a constant temperature. Heat and mass transfer from the gas flowing around the IC are assumed to melt ice as long as ice remains. Heat and mass transfer to the ice basket structures are not considered unless they are modeled separately as heat transfer structures.

Note that the model for the energy transfer from the flowing gas to the ice and melted ice water includes the following accounting:

1. The increase of the ice temperature to its freezing temperature, 273.15 K (0°C). Note that the ice is normally at approximately 264 K (-9°C).
2. The melting of the ice without any temperature rise to produce water at its freezing temperature.
3. The increase in the melted ice water temperature to above its freezing temperature. This includes the increase to the user-specified temperature at which the melted ice water exits the IC.

The heat and mass transfers to the ice and melted ice are determined by the procedures for heat structures described in Section 6.3. Note that the CONTAIN 1.11 Version includes the capability to increase the heat and mass transfers by a user-input multiplier, which can be used to account for the roughness of the cylindrical ice columns. See Appendix A.

The specific heat of the liquid water used is obtained from

$$C_{p,w} = 8370.22 - (23.2034) (T_w) + (3.18531) (10^{-2}) (T_w)^2, \text{ for } T_w \leq 600 \text{ K} \quad (6-128a)$$

$$C_{p,w} = 5915.3, \quad \text{for } T_w > 600 \text{ K} \quad (6-128b)$$

where

$C_{p,w}$ = specific heat of liquid water at constant pressure, and
 T_w = liquid water temperature (K).

The specific heat of solid ice used is $c_{ice} = 2000$.

6.5.2.2 Ice Condenser Aerosol Decontamination Models. The IC provides conditions under which significant removal of suspended aerosols from the atmosphere can occur. An aerosol removal model treating settling, impaction/interception, Brownian diffusion, diffusiophoresis, and thermophoresis is included. The model is based on the ICEDF model of Winegardner, Postma, and Jankowski [Win83], with minor modifications to make it consistent with other CONTAIN models. (Also see Reference Ow85b.) Aerosol decontamination 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.

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

The five IC FP removal mechanisms are detailed in separate sections below. Turbulent deposition is not modeled because it can be shown to have a negligible deposition effect.

The fundamental assumption of the CONTAIN FP removal model is that particles adhere irreversibly after they come in contact with a surface. In this case, the depletion process is first order with respect to airborne concentration:

$$\text{removal rate (kg/s)} = \frac{dC}{dt} = -KC \quad (6-129)$$

where

K = removal rate constant (m^3/s), and
C = airborne gas concentration (kg/m^3).

Because of low fluid velocities and the presence of water in the ice compartment, little resuspension of aerosol is expected, and the perfect sink assumption is expected to be valid. Therefore, the proportionality of removal rate to airborne concentration, as depicted in Equation (6-129), is expected to be valid.

A material balance for the aerosol in the gas phase in the ice compartment for steady state can be expressed in words as:

$$\text{input rate} = \text{deposition rate} + \text{output rate} \quad (6-130)$$

In mathematical symbols, this equation can be expressed as

$$G_i C_i = K_s C + K_I C + K_{BD} C + K_D C + K_t C + K_{td} C + G_o C_o \quad (6-131)$$

where

G = gas volumetric flow rate (m^3/s), and
C = airborne gas concentration (kg/m^3).

The subscripts have the following meaning:

i = inlet conditions,
s = settling,
I = impaction and interception,
BD = Brownian diffusion,
D = diffusiophoresis,
t = thermophoresis,
td = turbulent deposition, and
o = outlet conditions.

Note that C values identified in Equation (6-131) would have values between C_i and C_o , and, for a perfectly mixed gas phase, C could be set equal to C_o (the lowest concentration). If C is set equal to C_o , Equation (6-131) can be rearranged to solve for the fractional penetration P defined as $G_o C_o / G_i C_i$:

$$P = \frac{1}{1 + \sum_i K_i / G_o} \quad (6-132)$$

where $1 + \sum_i K_i / G_o$ is the decontamination factor (DF) for a well-mixed atmosphere. Equation (6-132) can be expected to overpredict penetration because the driving force for deposition, C, is minimized. Penetration is defined as that fraction of entering aerosol particles (by mass) that also exit (penetrate through). The DF equals the inverse of the penetration.

A minimum penetration can be predicted by considering a flow pattern in which there is negligible mixing in the direction of flow. By dividing the flow path into n segments connected in series, the overall penetration can be expressed as the product of the segment penetrations:

$$P = P_1 P_2 \dots P_n \quad (6-133)$$

Each P can be computed from Equation (6-132) by noting that the K value for each of the n regions can be obtained by dividing the overall K by the number of segments, and if n is allowed to become arbitrarily large, the penetration becomes exponential:

$$P_\infty = \exp\left(-\sum K_i / G_o\right) \quad (6-134)$$

where P_∞ is the penetration for the division of the flow path into an infinite number of series segments.

In reality, some degree of back-mixing is expected; but it is unlikely that the ice compartment will be perfectly mixed.

Therefore, actual values of P are expected to fall between predictions based on Equations (6-132) and (6-134).

Settling Deposition The removal rate constant for gravitational settling K_s is simply the product of the settling velocity and the surface area:

$$K_s = v_s A_s \quad (6-135)$$

where

v_s = particle settling velocity (m/s), and
 A_s = horizontal upward facing area (m^2).

Particle settling velocity v_s can be related to particle size and gas properties by means of Stokes' law:

$$v_s = \frac{\rho_p d_p^2 g C_m}{18\mu} \quad (6-136)$$

where

ρ_p = effective particle density (kg/m^3),
 d_p = equivalent particle diameter (of a spherical particle of equal volume) (m),
 g = gravity acceleration (m/s^2),
 C_m = Cunningham correction factor, dimensionless, and
 μ = gas viscosity ($N\cdot s/m^2$).

Combining Equations (6-135) and (6-136) leads to

$$K_s = \frac{\rho_p d_p^2 g C_m A_s}{18\mu} \quad (6-137)$$

The settling area A_s is the sum of all the horizontal areas that face upward, and would include the

- ice basket wires (strips between perforations),
- external ice horizontal area,
- available internal ice horizontal area,
- floor of ice compartment, and
- basket support structures.

Note that the Stokes' law used by the code, Equation (6-136), is valid for Reynolds numbers (with respect to flow around the particles) much less than one [Win83]. This is generally acceptable because a Reynolds number of one corresponds to an approximate diameter of 70 μm , which is relatively large. Larger particle sizes are, therefore, treated approximately.

Diffusion Deposition: Brownian Diffusion Particles exhibit a diffusivity as a result of momentum exchanges with surrounding gas molecules. For the case where the gas is isothermal and has no molecular weight gradients, the particle mobility arises from Brownian diffusion. Particles experience a net flux toward surfaces because of concentration gradients; particle capture by the surface is assumed to reduce the gas phase concentration of the particles to zero on the surface.

The efficiency of deposition depends both on the diffusivity and the fluid flow pattern past a surface. Three generic flow regimes can be identified for the ice compartment:

1. flow around the ice baskets,
2. flow parallel to surfaces, such as compartment walls, and
3. flow around the ice in the baskets.

Note that the flow around the ice baskets is modeled by assuming that the flow is around the horizontal strips used to hold the ice. See Figure 6-10.

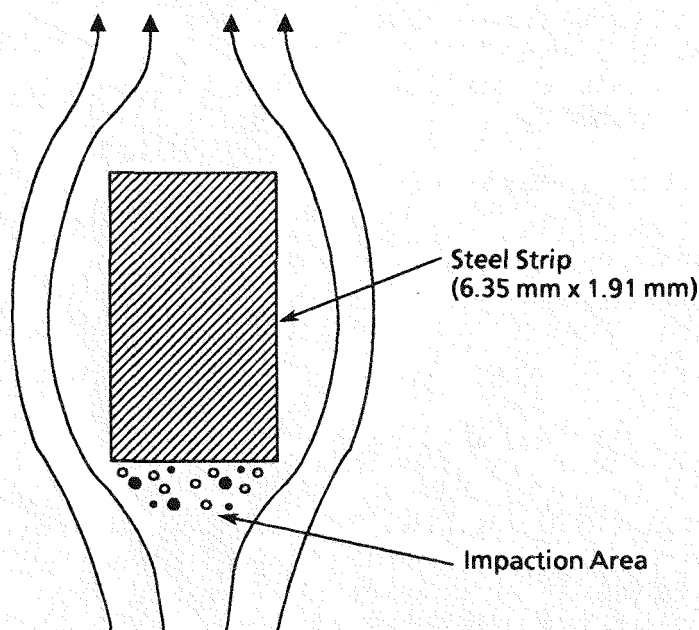


Figure 6-10. Illustration of Impaction on a Typical IC Ice Basket Horizontal Strip (based on Reference Win83)

The overall Brownian diffusion removal rate constant K_{BD} is the sum of the contributions resulting from the flow around the ice baskets, the flow parallel to surfaces, and from deposition onto the ice. Thus, K_{BD} can be expressed as

$$K_{BD} = v_I A_{BD} \epsilon_{BD} + \sum_i k_i A_i \quad (6-138)$$

where

$$\begin{aligned} v_I &= \text{gas velocity approaching the strip (m/s);} \\ A_{BD} &= \text{projected area for diffusional deposition (m}^2\text{);} \\ \epsilon_{BD} &= \text{diffusional capture efficiency,} \\ &= \frac{1}{Pe} + 1.727 \frac{Re^{1/6}}{Pe^{2/3}} \end{aligned} \quad (6-139)$$

where

$$\begin{aligned} Pe &= \text{Peclet number} \\ &= d_c v / D, \\ &\quad d_c = \text{cylinder diameter, and} \\ &\quad D = \text{particle diffusivity; and} \\ Re &= \text{Reynolds number} = \rho d_c v / \mu. \end{aligned}$$

$\sum_i K_i A_i$ accounts for the removal rate for gas flow parallel to surfaces with

$$\begin{aligned} K_i &= \text{mass transfer coefficient (m/s) to the } i^{\text{th}} \text{ surface, and} \\ A_i &= \text{surface area of the } i^{\text{th}} \text{ surface (m}^2\text{).} \end{aligned}$$

Capture of particles by horizontal basket strips is modeled by treating the strips as cylinders. For cylinders, the removal rate constant is expressed in terms of a target efficiency:

$$K_{BD} = v_I A_{BD} \epsilon_{BD} \quad (6-140)$$

Target area is calculable from the number of strips that exist and the area per strip. Effective cylindrical diameter d_c for the strip is computed by equating the cylinder perimeter to that of the rectangular strip; the equivalent diameter is 5.26 mm. A cylinder of this diameter will exhibit the same surface area and exposure time (assuming similar velocity profiles for rectangle and cylinder) and therefore appear as a reasonable simulation of the strip. For example, A_{BD} for the case of 1,944 baskets is predicted to be $3.43 \cdot 10^3 \text{ m}^2$.

The second flow regime involves the flow of gas parallel to surfaces. The surfaces include compartment walls, floor, and

ceiling, the vertical strips of the ice baskets, and probably flow along ice surfaces. The removal rate constant can be written formally as

$$K_{BD} = \sum_i K_i A_i \quad (6-141)$$

where

K_i = mass transfer coefficient to i^{th} surface (m/s), and
 A_i = surface area of i^{th} surface (m^2).

For naturally convected flows, a mass transfer coefficient can be predicted using a heat transfer/mass transfer analogy:

$$\frac{K_D L}{D} = 0.13 (\text{Gr Sc})^{1/3} \quad (6-142)$$

where

K_D = mass transfer coefficient (m/s),
 L = length of surface in direction of flow (m),
 Gr = Grashof number (defined below), and
 Sc = Schmidt number = $\mu/\rho D$.

The Grashof number used to characterize natural convection flow is

$$\text{Gr} = \frac{L^3 g \Delta \rho}{\nu^2 \rho} \quad (6-143)$$

where

g = acceleration because of gravity (m/s^2),
 ν = kinematic viscosity of gas (m^2/s),
 $\Delta \rho$ = density difference between the bulk fluid and the fluid at the surface (kg/m^3), and
 ρ = bulk fluid density (kg/m^3).

The density difference $\Delta \rho$ is the total value that would result from differences in both temperature and molecular weight.

In combining Equations (6-142) and (6-143), the length scale L cancels, making K_D independent of L . This independence of K_D with respect to L applies for turbulent flow; for the large distance applicable to ice compartments, turbulent flow is expected to occur over a large fraction of the surfaces along which naturally convected boundary layers flow.

An alternative formulation of the Sherwood number can be based on correlations for convection along surfaces. Typically, the Sherwood number varies with Sc and Re based on length. A correlating equation for flow along a flat plate is presented in Reference Win83:

$$\frac{K_D L}{D} = 0.037 Sc^{1/3} (Re_L^{0.8} - 15,500) \quad (6-144)$$

The symbols in Equation (6-144) are as previously defined except that Re_L uses the surface length (in the direction of flow) as the characteristic length.

Diffusional capture within the crushed ice itself can be viewed as an absorption process within a packed bed. For such beds a deposition velocity can be related to the Reynolds number. A first, crude estimate of diffusional deposition within crushed ice is made by assuming a flow velocity of 1 cm/s, an ice particle diameter of 0.32 cm, and nominal values for gas viscosity and density. Based on these assumptions, the deposition velocity divided by the average velocity is predicted to be 0.7 times the Schmidt number to the two-thirds power. The surface area for diffusional deposition is related to ice availability by means of the following equation:

$$S = 1.27 \cdot 10^6 \epsilon F \quad (6-145)$$

where

- S = surface area of ice available for diffusional deposition (m^2),
- ϵ = fraction of basket volume filled with solid ice, and
- F = fraction of initial surface area exposed to gas.

The numerical constant in Equation (6-145) is the total basket internal volume multiplied by the surface/volume ratio for ice as initially formed.

For sedimentation, the product ϵF could have values ranging from 0 (no ice remaining) to ~0.3, which corresponds to $\epsilon = 0.6$ (beds filled with ice fragments) and $F = 0.5$ (half of the ice facing upward). Generally, F is expected to have values significantly smaller than unity because a significant fraction of internal ice surface would be either lost (due to glaciation) or unavailable for exposure to the gas phase (closed or sealed interstitial gas pockets).

Impaction/Interception Deposition Model: Basket Strips The perforated steel baskets contain a large number of horizontal strips, around which gases flow. The individual web segments are 1.91 mm thick, 6.35 mm long (in the direction of flow), and 2.54 cm

wide. Impaction and interception on the end of a strip are pictured schematically in Figure 6-10.

The capture of particles by immersed bodies is generally characterized by an impaction efficiency, defined as the fraction of approaching particles that the body captures. The removal rate constant can be expressed as

$$K_I = v_I A_I \epsilon \quad (6-146)$$

where

$$\begin{aligned} v_I &= \text{gas velocity approaching the strip (m/s),} \\ A_I &= \text{projected area for impaction (m}^2\text{), and} \\ \epsilon &= \text{impaction efficiency.} \end{aligned}$$

The impaction efficiency is related to particle and flow parameters by means of correlations developed for cylinders. An empirical fit of impaction efficiency data presented in Reference Win83 can be expressed as:

$$\epsilon = \frac{St^2}{(St + 0.5)^2} - 0.04 \quad (6-147)$$

where St is the Stokes number, the ratio of the particle's stopping distance to the characteristic dimension of the collector surface. This is defined by

$$St = \frac{v_I \rho_p d_p^2 C_m}{9\mu d_c} \quad (6-148)$$

where d_c is the diameter of the collector cylinder.

It should be noted that the value of ϵ given in Equation (6-147) is allowed to have values of zero or greater, but cannot have negative values.

Interception efficiency of particles by the strips is related to particle size using a formula adapted from Fuchs [Win83]:

$$\epsilon_{int} = 2 \frac{d_p}{d_c} \quad (6-149)$$

The total capture efficiency resulting from impaction and interception is obtained by adding Equations (6-147) and (6-149):

$$\epsilon_I = \frac{St^2}{(St + 0.5)^2} - 0.04 + 2 \frac{d_p}{d_c} \quad (6-150)$$

The target area for impaction is the same as that for sedimentation on the basket wires and amounts to 1,240 m² for a typical plant [Win83]. The collector diameter d_c is equal to the metal thickness, 1.91 mm.

The impaction fluid velocity v_I is retained as a parameter in the model. Rough estimates of v_I can be made on the basis of the average forced-convection velocity through the compartment. Alternatively, natural-convection velocities induced by the temperature gradient between bulk gas and the ice could be estimated. Both methods lead to predicted velocities of the order of 0.3 m/s (≈ 1 ft/s).

Thermophoretic Deposition Particles experience a radiometric force when they are suspended in a gas in which a temperature gradient exists. In general, the drift velocity is directly proportional to the magnitude of the temperature gradient [Win83]:

$$v_T = -C_1 \frac{dT}{dy} \quad (6-151)$$

where

v_T = thermophoretic drift velocity (m/s),
 C_1 = a constant whose value depends on particle and gas,
 and
 dT/dy = temperature gradient in the y-direction (K/m).

The removal rate constant K_T resulting from thermophoresis is the average of the products of deposition velocities and surface area at the different elevations:

$$K_T = v_T A_T \quad (6-152)$$

where A_T is the surface area for thermophoresis (m²).

The temperature gradient that causes particle drift also causes the transport of sensible heat from the gas phase. The rate of

sensible heat loss may be related to the temperature gradient in the gas adjacent to the surface:

$$\text{heat loss rate} = -k A_T \left. \frac{dT}{dy} \right|_w \quad (6-153)$$

where k is the thermal conductivity of gas [W/m-K].

The final derived thermophoretic removal rate constant K_T can be expressed as

$$K_T = C_1 \frac{G_o}{\alpha} (B T_i - T_o) \quad (6-154)$$

where

- α = thermal diffusivity of gas at outlet conditions (m^2/s);
- B = a constant $\rho_i G_i c_{pi} / \rho_o G_o c_{po}$;
 c_p = specific heat capacity, and
 i, o = inlet and outlet, respectively;
- G = mass flow rate; and
- T = gas temperature (K).

As is evident from Equation (6-132), the penetration caused by thermophoresis depends on K_T/G_o . In addition, because G_o is a factor in Equation (6-154), gas flow rate will not play a critical role in thermophoretic capture. This finding parallels the prediction for diffusiophoresis and is as expected when one considers that the integral value of the temperature gradient (the driving force) is limited by the quantity of heat or mass that can be transferred per unit volume of gas.

The numerical value of C_1 depends on particle and gas properties, and predictive equations that account for important parameters are listed in Reference Win83. Rough estimates of C_1/α indicate that this quantity would have a numerical value of $\sim 10^{-3}/\text{K}$. Thus, for $(B T_i - T_o) = 100 \text{ K}$, K_T/G_o from Equation (6-154) is predicted to be 0.1. This corresponds to a removal efficiency of $\sim 10\%$ for thermophoresis (see Equation (6-154)). This low removal efficiency indicates that thermophoresis will not normally be a dominant particle trapping mechanism.

Diffusiophoretic Deposition The condensation of steam onto ice surfaces causes particle drift by two mechanisms: (1) net flow of gas toward the cool surface, often termed Stephan flow, which convects particles toward the surface, and (2) the gradient in steam concentration results in a molecular weight gradient that causes particles to experience a force in the direction of the gradient. For air/steam mixtures, these two mechanisms are opposing; however, the Stephan flow dominates and the particles are convected to the surface and scrubbed by the condensing steam.

The diffusiophoresis removal rate constant K_D can be expressed as

$$K_D = -v_D A_D \quad (6-155)$$

where

$$\begin{aligned} v_D &= \text{particle deposition velocity (m/s), and} \\ A_D &= \text{surface area for diffusiophoretic deposition (m}^2\text{).} \end{aligned}$$

The final derived equation governing the diffusiophoresis rate constant can be expressed as

$$K_D = 0.9 G_O \left[\frac{X_{a,o} X_{vap,i}}{X_{a,i}} - X_{vap,o} \right] \quad (6-156)$$

where

$$\begin{aligned} G_O &= \text{IC outlet gas flow rate (m}^3\text{/s),} \\ X &= \text{mole fraction,} \\ a &= \text{air,} \\ o &= \text{outlet,} \\ i &= \text{inlet, and} \\ vap &= \text{water vapor.} \end{aligned}$$

6.5.3 Containment Sprays

The CS system is a nearly universal safety feature in LWRs. This system provides the containment atmosphere with a finely divided spray of water droplets of a user-specified diameter. Heat transfer to and steam condensation on the droplets provide a rapid reduction in temperature, pressure, and FP concentration. The sprayed water collects in a sump at the bottom of the containment. Generally, the initial spray water is from a PWR refueling water storage tank (RWST) or a BWR coolant storage tank. When that source is exhausted, water is pumped from the sump, through a HX, 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. In addition, the removal of iodine and aerosols from the atmosphere because of the spray is calculated. See Section 6.5.3.10.

Figure 6-11 is a simplified model of a CS system. Its basic components include a sump pool, sump pump, HX, and RWST. All these are modeled in CONTAIN. Aerosol and volatile iodine removal by the spray is also modeled.

6.5.3.1 Pump Model. Mechanical pumps are used to circulate the containment building sump pool water up to the CS headers. The pump can be used in one of two types of systems:

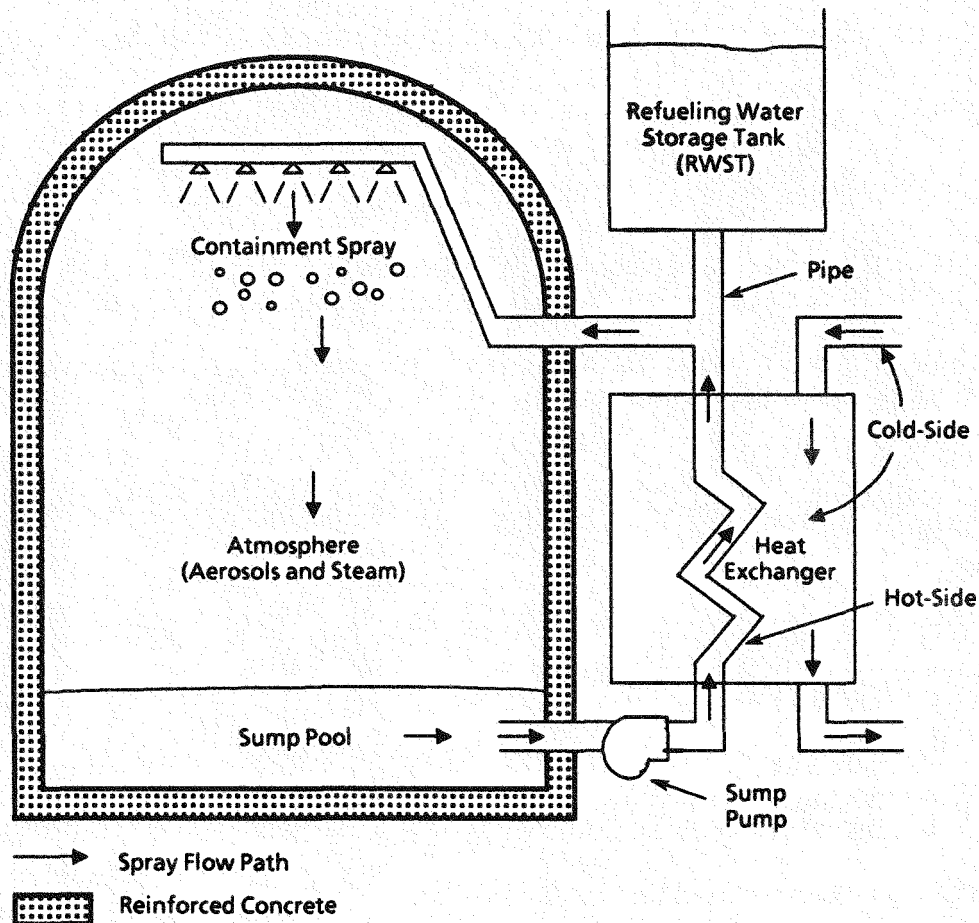


Figure 6-11. CS System

- When used by itself, the pump controls the flow of coolant liquid from one cell pool to another.
- When used in conjunction with a containment spray, the pump controls the flow of recirculated water from a pool to the sprays. When it is used in this mode in conjunction with a storage tank, the recirculation flow does not start until the storage tank water supply is exhausted.

CONTAIN models a pump using a user-specified constant mass flow rate (kg/s).

6.5.3.2 Heat Exchanger Models. The CS system typically uses a HX to cool the liquid water recirculated from the pool sump (Figure 6-11) to the CS spray nozzles.

CONTAIN uses one of four HX models corresponding to (a) a single-pass shell and U-tube geometry, (b) a cross-flow geometry with hot-side tubes and cold-side shell, (c) a counterflow geometry, and (d) a parallel flow geometry. The HXs are depicted in Figure 6-12. A

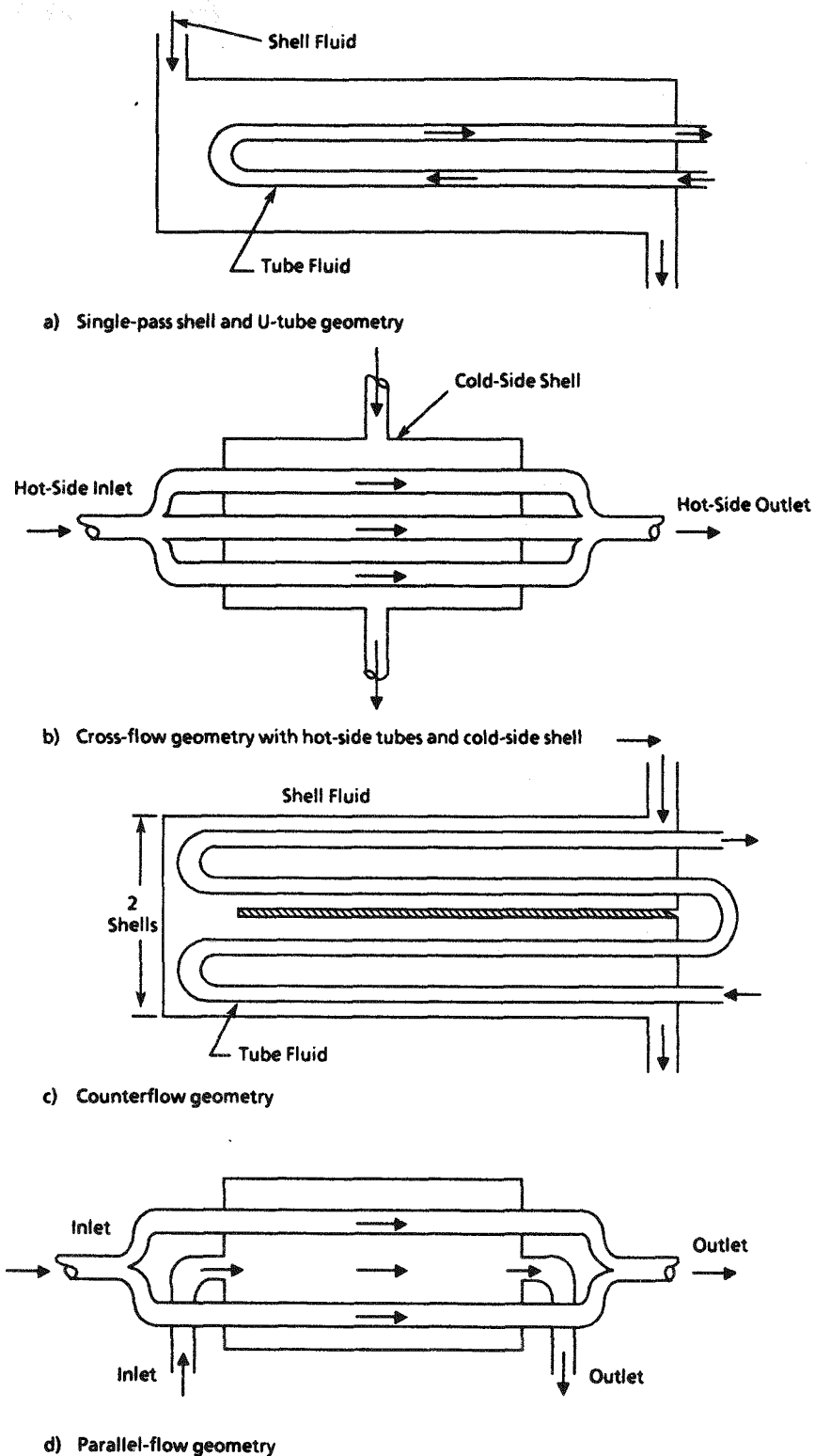
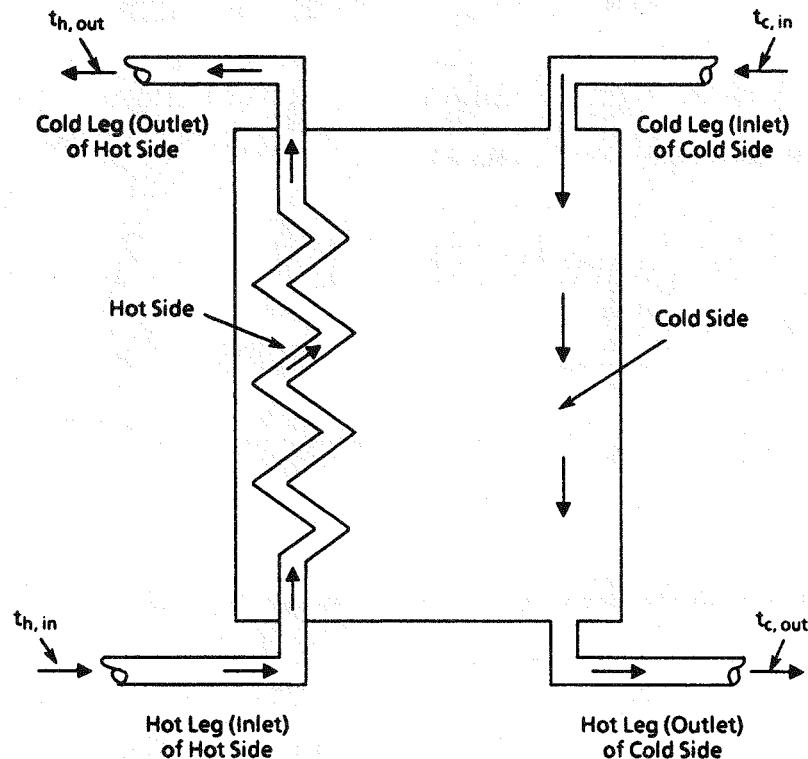


Figure 6-12. CONTAIN HX Models

nonmechanistic model with a constant user-specified hot-leg temperature drop is also available. Throughout, this section will refer to the terminology in Figure 6-13.



Note: Arrows indicate the direction of fluid flow

Figure 6-13. Simplified Schematic of Counterflow HX, Emphasizing HX Terminology

The basis for modeling the four HXs illustrated in Figure 6-12 is obtained from Reference Kay64. This method defines the HX effectiveness E as

$$\begin{aligned}
 E &= \frac{q}{q_{\max}} = \frac{\text{Cap}_h(T_{h,i} - T_{h,o})}{\text{Cap}_{\min}(T_{h,i} - T_{c,i})} \\
 &= \frac{\text{Cap}_c(T_{c,o} - T_{c,i})}{\text{Cap}_{\min}(T_{h,i} - T_{c,i})}
 \end{aligned}
 \tag{6-157}$$

where

- q = heat transfer rate (J/s);
- Cap_h = $(W c_p)_h$, the hot-side fluid capacity rate, and
 W = fluid mass flow rate, and
 c_p = fluid (water) specific heat [J/kg-K];
- Cap_c = $(W c_p)_c$, the cold-side fluid capacity rate;

Cap_{min} = the smaller of the Cap_h and Cap_c magnitudes;
 q_{max} = maximum possible transfer rate (J/s);
 $T_{h,i}$ = hot-side inlet temperature (K), that is, hot leg of the hot side in Figure 6-13;
 $T_{h,o}$ = hot-side outlet temperature, that is, cold leg of the hot side in Figure 6-13;
 $T_{c,i}$ = cold-side inlet temperature, that is, the cold leg of the cold side in Figure 6-13; and
 $T_{c,o}$ = cold-side outlet temperature, that is, the hot leg of the cold side in Figure 6-13.

In the above, the specific heat c_p is a weak function of temperature and W is a function of ρ , which is also a weak function of temperature.

It is to be noted that, given the operating conditions $T_{h,i}$, $T_{c,i}$, Cap_h , and Cap_c , the magnitude of E completely defines the heat transfer performance. If Cap_h equals Cap_{min} , then E equals a "temperature effectiveness" for cooling the hot fluid, $(T_{h,i} - T_{h,o}) / (T_{h,i} - T_{c,i})$. But, if Cap_c equals Cap_{min} , then E equals $(T_{c,o} - T_{c,i}) / (T_{h,i} - T_{c,i})$, which is the "temperature effectiveness" for heating the cold fluid. However, the general definition of effectiveness in Equation (6-157) is not a "temperature effectiveness," but rather a "heat transfer effectiveness."

The temperature ($T_{h,i}$) of the hot leg (inlet) of the hot side of the HX, that is, water temperature from the pool sump, is calculated elsewhere in CONTAIN and provided to this model. The expression $T_{c,i}$, that is, temperature of the cold leg (input) of the cold side along with the cold-side mass flow W_c , is user input. Because the ESF model supplies the hot-side mass flow rate W (from the user-specified PUMP mass flow rate), Cap_c and Cap_h both can be calculated.

From Equation (6-157), the hot leg outlet temperature $T_{h,o}$ is given by

$$T_{h,o} = T_{h,i} - \frac{E \text{ Cap}_{min}(T_{h,i} - T_{c,i})}{Cap_h} \quad (6-158)$$

The value of $T_{c,o}$ can be similarly calculated from Equation (6-157).

For the simple nonmechanistic model, the user inputs the temperature drop ΔT_{HX} only across the hot side, that is,

$$T_{h,o} = T_{h,i} - \Delta T_{HX} \quad (6-159)$$

Because $T_{h,i}$ is calculated by other ESF component models (for example, LC pool models), $T_{h,o}$ can be easily calculated from this $T_{h,i}$ and the ΔT_{HX} .

In general, it is possible to express the effectiveness of the HX as a function of Ntu, CR, and the flow arrangement, where Ntu, the number of exchanger heat transfer units, is defined as

$$Ntu \equiv \frac{AU}{Cap_{min}} = \frac{1}{Cap_{min}} \int_0^A U dA \quad (6-160)$$

where

A = user-specified effective heat transfer area (the same transfer area as used in the definition of U), and
 U = overall thermal heat transfer conductance, an input constant flow arrangement that depends on the type of HX.

And the capacity-rate CR ratio is defined as

$$CR = \frac{Cap_{min}}{Cap_{max}}$$

where Cap_{max} is the larger of the Cap_h and Cap_c magnitudes.

The following sections describe the calculations for the HX transfer effectiveness E for the four types of HXs in Figure 6-12.

Single-Pass Shell and U-Tube Effectiveness The effectiveness factor E for the HX with a single-pass shell and U-tube geometry (Figure 6-12a) is given by

$$E = 2 / \left\{ [1 + CR] + \sqrt{1 + CR^2} (1 + e^{-\Gamma}) / (1 - e^{-\Gamma}) \right\} \quad (6-161)$$

where in this case,

$$\Gamma = Ntu \sqrt{1 + CR^2} \quad (6-162)$$

Equation (6-161) was derived for one shell pass and two tube passes. All of the variables in these equations have been defined previously.

Cross-Flow Heat Exchanger Effectiveness The transfer effectiveness E for a cross-flow HX with hot-side tubes and cold-side shell (Figure 6-12b) is computed using the following:

If $Cap_{max} = Cap_h$,

$$E = 1 - \exp(-\Gamma) \quad (6-163)$$

where $\Gamma = CR[1 - \exp(-Ntu CR)]$.

Otherwise,

$$E = CR[1 - \exp(-\Gamma)] \quad (6-164)$$

where $\Gamma = CR[1 - \exp(-Ntu)]$.

Here, as before, $Ntu = AU/Cap_{min}$.

This model assumes that one fluid is mixed, the other unmixed.

Counterflow Heat Exchanger Effectiveness The counterflow HX effectiveness E (Figure 6-12c) is calculated using the following:

$$E = \frac{1 - \exp[-Ntu(1 - CR)]}{1 - CR \exp[-Ntu(1 - CR)]} \quad (6-165)$$

where $Ntu = AU/Cap_{min}$ is based on the minimum capacity rate.

Parallel Flow Heat Exchanger Effectiveness The calculations for the parallel flow HX effectiveness E (Figure 6-12d) follow.

If the absolute value of $(CR - 1) \leq 0.002$,

$$E = \frac{Ntu}{1 + Ntu} \quad (6-166a)$$

Otherwise,

$$E = \frac{1 - \exp[-Ntu(1 + CR)]}{1 + CR} \quad (6-166b)$$

6.5.3.3 Valve Model. The valve model is used only by itself in a single-component system to control transfer of coolant liquid from the pool of a donor cell to that of a recipient cell. 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 the donor cell and the recipient cell exceeds the inputted pressure difference, the flow path is opened, and the flow is characterized by the flow area and a flow loss

coefficient, 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 open and close at five user-specified times. The times are alternating opening and closing times with the valve assumed to be initially closed and the first time specified assumed to be an opening time. If the valve is to be initially open, the first time entry in the array should be the problem start time. No defaults are available for valve input parameters.

The mass flow rate for a given pressure difference is determined from

$$\Delta P = \sum K \frac{(W/A)^2}{2\rho} \quad (6-167)$$

where

ΔP = pressure difference, including liquid water head,
 $\sum K$ = sum of all irreversible flow losses,
 W = mass flow rate,
 A = flow area, and
 ρ = liquid water density.

6.5.3.4. Pipe Model. The pipe component is used like the valve model (see Equation (6-167)), 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, the inside diameter, and a total irreversible loss factor, equal to the sum of the Moody friction factor, entrance and exit loss factors, and any other form loss factors.

6.5.3.5. Orifice. This is a model for a square-edged orifice component used only by itself in a single-component system to control the transfer of coolant liquid from a pool in the donor cell to that of the recipient cell. The flow is pressure- and gravity-driven, with the driving pressure calculated from the gas pressures and the elevation difference between the bottom 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 is used [Flo79]. Input parameters that describe the geometry of the orifice are the orifice minimum diameter and the ratio of the orifice minimum diameter to the free stream diameter. No defaults are provided for these parameters.

The flow equation is similar to Equation (6-167) except that the loss coefficient is based on a squared-edge orifice loss coefficient that depends on (a) the ratio of the orifice diameter to the upstream pipe diameters and (b) the Reynolds number.

6.5.3.6. Refueling Water Storage Tank. The RWST is used primarily to supply makeup water for the new and spent-fuel pool used during the refueling of the LWR reactor fuel. It can also be used to supply water for the CS. It is connected with the CS system through valves and pumps to the CS nozzles. In CONTAIN, the RWST provides an initial amount of water to supply the containment spray. The CS system then can acquire its water from the containment building pool sump (Figure 6-11).

The user supplies the plant specifics of initial mass of RWST water, water temperature, and the constant mass flow rate at which the water is delivered to the CS.

6.5.3.7 Containment Spray Aerosol Removal Model. For the purpose of discussing the depletion of airborne FPs by CS washout, the FPs can be divided into the following groups [Lew77]:

- noble gases,
- molecular iodine (I_2),
- methyl iodide (CH_3I) and other gaseous organic iodine compounds, and
- aerosol particles.

The noble gases are inert and are not affected by the spray system. Iodine is the only other element likely to be in gaseous form in compartments with sprays operating. It may be present as molecular iodine (I_2), in which case it is very reactive, or as methyl iodide, CH_3I , which is gaseous but much less reactive. All remaining FPs 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 (Section 6.5.3.10) by CSs 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 the spray model itself. Additives have been adopted in PWR spray systems (but not in CONTAIN) to enhance the rate and extent of iodine removal. 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 droplet's surface. 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 partition coefficient used to calculate the molecular iodine absorption efficiency depends on the amount and type of additive used. A value of 5000 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 (for example, methyl iodide) have not been well established. A partition coefficient for organic iodides is used to model the removal rate for such relatively inert species. A value of zero is the default. Section 6.5.3.10 discusses the iodine removal models in greater detail.

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 falling time of a droplet, taking into account the droplet size and temperature as well as the aerosol size, and containment conditions such as pressure. Collection mechanisms considered in deriving the efficiency are Brownian diffusion, thermophoresis, diffusiophoresis, interception, and impaction.

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

Five collection mechanisms are used in the CONTAIN model for aerosol removal by spray droplets:

1. Interception, which arises because the finite size of the particle permits its surface to contact that of the drop, even when the particle center of mass is on a trajectory that does not intersect the drop.
2. Inertial impaction, which occurs because the particle has a finite inertia, leading the trajectory of the particle center of mass to cross the flow streamlines around the drop and thus intersect the surface of the drop.
3. Brownian diffusion, which results from molecular bombardment of the particles causing them to flow across the flow boundary layer around the drop.
4. Diffusiophoresis, which arises as a response of the particle to concentration gradients and to vapor flow toward (or from) the drop surface when condensation on (or evaporation from) the drop is occurring.
5. Thermophoresis, which results from the migration of a particle down a temperature gradient because of the effect of differential molecular impacts.

Although these effects interact to some degree, they are treated as being additive in CONTAIN. The first three effects are primarily a function of drop and particle size, while the phoretic effects

are primarily a function of temperature and humidity of the atmosphere and of the drop's temperature. The latter changes rapidly at the start of the drop's fall through the atmosphere, and particle collection is therefore integrated over the drop's fall history in CONTAIN. Under evaporating conditions, the diffusiophoretic effect becomes negative. The thermophoretic effect would also be negative in the unlikely circumstance that the drop were hotter than the atmosphere. In such cases, the total collection efficiency is still constrained to be nonnegative. Under extreme conditions (such as those resulting from hydrogen burns), the drop may completely evaporate during its fall; when this occurs, the solid residue is returned to the appropriate size section of the aerosol distribution. Figure 6-14 from Reference Ber85a is a qualitative representation of the relative collection efficiencies.

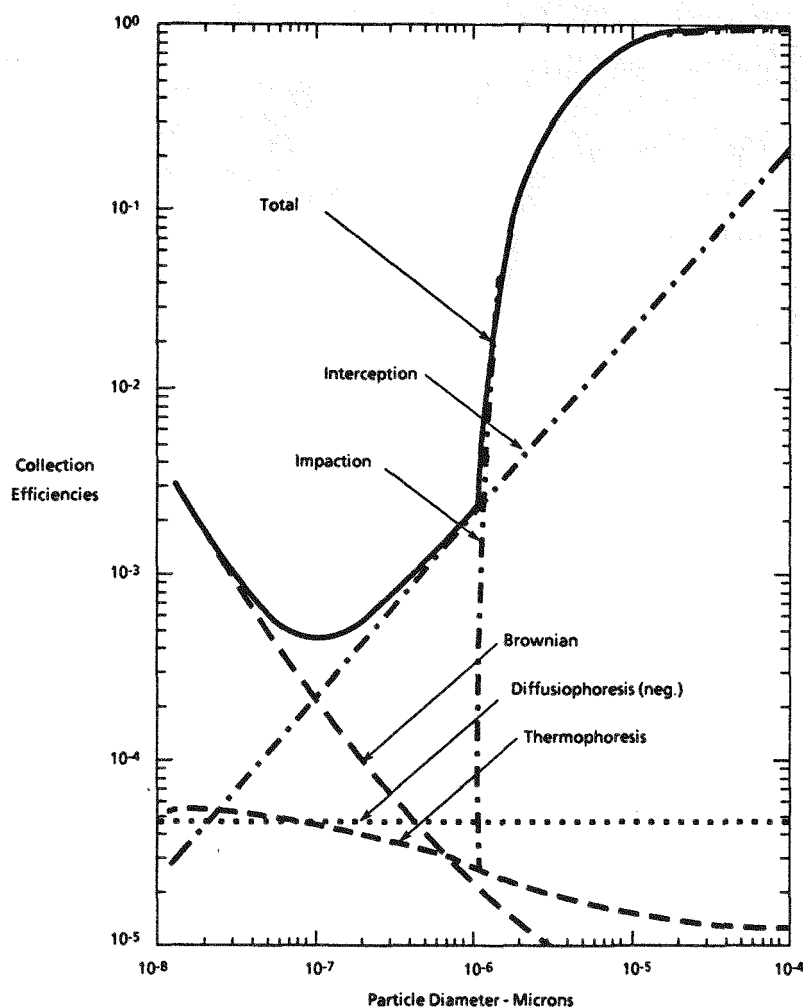


Figure 6-14. Qualitative Comparison of Aerosol Collection Efficiencies (adapted from Reference Ber85a)

The deposition rate equations below model, in sequence, these five aerosol removal mechanisms. Note that the collection efficiency E is defined by

$$E = \frac{N_p \text{ (collected)}}{(\pi D^2 / 4) H n_p} \quad (6-168)$$

where N_p (collected) is the number of particles actually collected by a drop of diameter D as it falls a height H through an atmosphere containing n_p particles per unit volume.

Interception

Viscous flow:

$$E_{I,v} = 1.5 (d/D)^2 \quad (6-169)$$

Potential flow:

$$E_{I,p} = 3d/D \quad (6-170)$$

where

$E_{I,v}$ = interception collection efficiency for viscous flow,
 d = particle diameter,
 D = spray drop diameter, and
 $E_{I,p}$ = interception collection efficiency for potential flow.

Inertial Impaction

Viscous Flow:

$$E_{II,v} = 0, \quad \text{for } St \leq 1.214 \quad (6-171a)$$

and

$$E_{II,v} = \left[1 + \frac{(0.75) \ln (2 St)}{(St - 1.214)} \right], \text{ for } St > 1.214 \quad (6-171b)$$

where

$E_{II,v}$ = impaction collection efficiency for viscous flow,
 St = Stokes number,

$$= \frac{d_p^2 \rho_p V_d}{9\mu D}, \quad (6-172)$$

ρ_p = particle density,
 V_d = drop fall velocity, and
 μ = gas viscosity.

Potential Flow:

$$E_{II,p} = 0.0, \quad \text{for } St \leq 1/12 \quad (6-173a)$$

and

$$E_{II,p} = \left(\frac{St}{St + 0.5} \right)^2, \quad \text{for } St \geq 0.2 \quad (6-173b)$$

where $E_{II,p}$ = impaction collection efficiency for potential flow.

Linear interpolation is used to obtain $E_{II,p}$ for $1/12 > St < 0.2$.

The equation for the Stokes number neglects the Cunningham slip correction, which can be important for $d \ll 1 \mu\text{m}$; however, the impaction effect is zero for such particles ($St \ll 1$) and, therefore this neglect is not very important.

As given by Fuchs [Win83] and as reproduced above, these relations make no allowance for nonspherical aerosol particles. In CONTAIN, an approximate allowance for the agglomeration and dynamic shape factors (γ and χ , respectively) is made by multiplying the ratio d/D by γ in Equation (6-169) and (6-170), and by including a factor of χ in the denominator in Equation (6-172). However, it should be noted that the sprays keep the degree of superheat in the containment atmosphere very small during most of the accident sequence. Under these conditions, water uptake is expected to lead to approximately spherical aerosol particles, with shape factors close to unity. Hence, the code default values for the shape factors were set equal to unity.

For spray drop sizes in the range of interest, the Reynolds number based on drop diameter Re_D ranges from about 15 to almost 1000. Hence, Re_D is expected always to be too large for the viscous flow relations to hold. However, it is not clear that Re_D is large enough for the potential flow relations to provide a good approximation either, except perhaps for the larger drop sizes. In this intermediate regime, no simple expression is expected to be rigorously defensible. In early work, Langmuir [Lan48] suggested a simple interpolation formula as an approximation to the impaction efficiency.

$$E_{II} = \frac{E_{II,v} + Re_D E_{II,p}/60}{1 + Re_D/60} \quad (6-174)$$

where

$$\begin{aligned} E_{II} &= \text{interpolated impaction efficiency,} \\ Re_D &= \text{Reynolds number for the drop, and} \\ &= \frac{\rho v_d D}{\mu} \end{aligned} \quad (6-175)$$

where

$$\begin{aligned} \rho &= \text{liquid density, and} \\ \mu &= \text{liquid viscosity.} \end{aligned}$$

This formula is used in CONTAIN. In addition, an equivalent interpolation formula is used for the interception efficiency. Little justification can be given for the latter, except to note that the interception efficiency is governed by the same flow patterns about the drop that govern the impaction efficiency; hence, the transition from the viscous flow limit to the potential flow limit might reasonably be expected to show a qualitatively similar dependence upon drop Reynolds number in both cases.

The expressions for the Brownian and phoretic collection efficiencies assumed in CONTAIN follow.

Brownian Diffusion

$$E_{BD} = \frac{4 D_p (2 + 0.6 Re_D^{1/2} Sc_p^{1/3})}{v_d D} \quad (6-176)$$

where

$$\begin{aligned} E_{BD} &= \text{Brownian diffusion collection efficiency;} \\ D_p &= \text{diffusivity of the particle in the atmosphere;} \\ Sc_p &= \text{particle Schmidt number;} \\ &= \nu/D_p, \text{ and} \\ \nu &= \text{kinematic viscosity; and} \\ D &= \text{drop diameter.} \end{aligned}$$

Thermophoresis

$$E_{th} = \frac{4C_{th}(2 + 0.6Re_D^{1/2}Pr^{1/3})(T_{gas} - T_{drop})}{v_d D} \quad (6-177)$$

$$C_{th} = \frac{3\mu C_m(c_t Kn + k_g/k_p)}{2\chi \rho_g T(1 + 3c_m Kn)(1 + 2c_t Kn + 2k_g/k_p)}$$

Here, Pr is the Prandtl number, T the temperature, C_m the Cunningham slip correction, Kn the Knudsen number ($2\lambda/d$, where λ is the molecular mean free path), χ is the dynamic shape factor, and k_g/k_p is the ratio of the gas thermal conductivity to the particle conductivity. The constant c_t is related to thermal accommodation. The values assumed for c_t and c_m are 1.0 and 1.37, respectively.

Diffusiophoresis

$$E_{df} = 4\check{D}_v(2 + 0.6Re_d^{1/2}Sc^{1/3}) \frac{M_1^{1/2} \ln \left[\frac{P_g - P_{vd}}{P_g - P_2} \right]}{(X_1 M_1^{1/2} + X_2 M_2^{1/2}) v_d D} \quad (6-178)$$

In Equation (6-178), $\check{D}_v$ is the vapor diffusivity in the atmosphere; Sc is the Schmidt number ν/D ; the subscripts 1, 2, and g refer, respectively, to the vapor, the noncondensable gas (treated as being dry air), and the total atmosphere; M and X are the molecular weight and the mole fraction, respectively; P is the pressure; and P_{vd} is the vapor pressure of the drop.

The expressions given above for the phoretic collection efficiencies are basically equivalent to those used to calculate phoretic deposition of aerosols upon surfaces in CONTAIN. The phoretic effects can be negative under certain conditions; for example, the diffusiophoretic effect is negative when the drop is evaporating. In such cases, the phoretic effects are still evaluated from Equations (6-177) and (6-178) and added algebraically to the other collection efficiencies. The total collection efficiency is constrained to be nonnegative, however.

6.5.3.8 Engineered Systems Overflow Model. 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 that defines the overflow cell for condensation runoff and aerosol mesh losses.) Three required input parameters indicate the overflow source 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 the overflow height in the source cell is diverted to the destination

cell during each timestep in which the condition is met. 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. There is no temperature change of the transferred liquid during the transfer.

6.5.3.9 Containment Spray Thermal-Hydraulics Models. As the CS water drops fall through the atmosphere, their diameters can increase or decrease as a result of condensation or evaporation; thus, diameter is a dynamic variable. The heat transfer and mass transfer to the spray as the drops fall are calculated. The model for these processes is basically the same as that for heat and mass transfer used elsewhere in CONTAIN, for example, for heat structures. However, 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 determination of the number of droplets 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 that 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 resulting from 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 LC pool, if present, in the cell to which the engineered system effluent is directed. The user specifies that cell as the cell for storing residual liquid from ESFs, which by default is the cell in which the spray is defined. If no LC pool is specified for that cell, the water is lost from the problem. For most situations that call for the use of containment sprays, a liquid pool can be expected to form as a result of spray droplets reaching the floor. Therefore, it is recommended that the user include a LC model with a pool in the residual-liquid cell.

When sprays are operating, containment conditions tend to approach a quasi-steady state in which the sprays are removing about as much steam and energy from the containment as the various sources are supplying to the containment. (Important exceptions to this behavior arise during and shortly after major transient inputs of steam or energy to the containment.) Likewise, the drop itself tends to reach a quasi-steady state with respect to the containment atmosphere very early in its fall, with little change in the drop parameters (such as temperature) after the first few tenths of a

meter or so of its fall. Over much of the accident history, the spray effectiveness will therefore be dominated by the drop collection efficiencies under these quasi-steady conditions.

The following subsections discuss the CS droplet models for terminal fall velocity and mass and heat transfer (as a function of time).

Water Drop Terminal Velocity and Reynolds Number Models Core spray drops are assumed to fall at constant terminal velocity speed v_t throughout their entire containment fall path.

The equation for v_t is:

$$v_t = \left[\frac{\mu_{\text{gas}} / \rho_{\text{gas}}}{D} \right] q_u \quad (6-179)$$

where

$$\begin{aligned} \mu_{\text{gas}} &= \text{atmosphere air-steam mixture viscosity,} \\ \rho_{\text{gas}} &= \text{air-steam mixture density, and} \\ D &= \text{water drop diameter,} \\ q_u &= \text{numerical factor, and} \\ &= \sqrt{82.0836 + 9.06 \sqrt{X_{\text{num1}} / D_{\text{en1}}}} \end{aligned} \quad (6-180)$$

where

$$\begin{aligned} X_{\text{num1}} &= \text{intermediate factor, calculated from} \\ &= 64.0 \rho_1 \rho_g D_g^3 \end{aligned} \quad (6-181)$$

where

$$\begin{aligned} \rho_g &= \text{atmosphere air-steam mixture density, and} \\ g &= \text{acceleration because of gravity; and} \\ D_{\text{en1}} &= 72 \mu_{\text{gas}}^2. \end{aligned} \quad (6-182)$$

This terminal velocity is used to determine where in time and fall distance to adjust information between CS and atmospheric models; for example,

$$\Delta t = \frac{\Delta H_{\text{fall}}}{v_t} \quad (6-183)$$

where

$$\begin{aligned} \Delta t &= \text{time interval, and} \\ \Delta H_{\text{fall}} &= \text{droplet fall distance.} \end{aligned}$$

Reynolds (Re) number is also calculated using v_t from

$$Re = \frac{\rho_{\text{gas}} v_t D}{\mu_{\text{gas}}} \quad (6-184)$$

where all the terms are defined previously.

Containment Spray Droplet Energy and Mass Transfer Model The heat transfer between the atmosphere and the CS droplet occurs by two processes, convection and condensation, which includes evaporation. Figure 6-15 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. For most calculations, it would be sufficient to calculate only this boundary layer resistance. Figure 6-15 illustrates the various resistances affecting heat and mass transfer to CS droplets. The figure should not be taken literally as an equivalent thermal circuit, because convection is driven by a temperature difference, while condensation is driven by a partial pressure difference. The modeling for this process is based largely on Reference Col81 and is very similar to the models presented in Section 6.3.2 for mass transfer to heat structures.

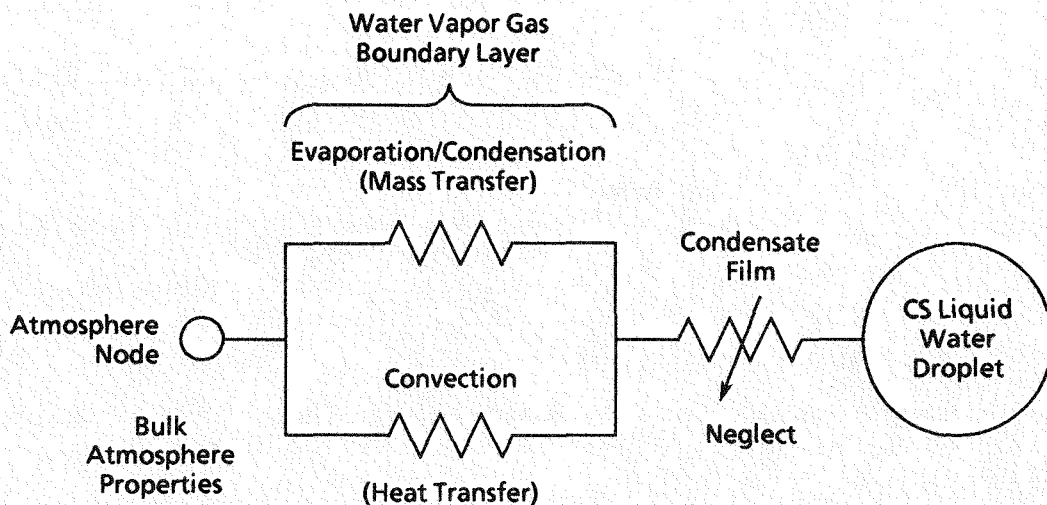


Figure 6-15. Heat Transfer Configuration

The total heat flux q (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 as follows

$$q = q_c + q_m \quad (6-185)$$

The convective heat transfer is obtained from

$$q_c = h_c(T_b - T_D) \quad (6-186)$$

where

$$\begin{aligned} h_c &= \text{convective heat transfer coefficient } (J/m^2-s-K), \text{ and} \\ &= Nu_c (k/D) \\ Nu_c &= \text{see the correlation given below,} \\ k &= \text{thermal conductivity of the gas-vapor bulk} \\ &\quad \text{atmosphere } (J/m-s-K), \text{ and} \\ D &= \text{drop diameter } (m); \end{aligned}$$

$$\begin{aligned} T_b &= \text{bulk atmosphere temperature } (K); \text{ and} \\ T_D &= \text{drop temperature } (K). \end{aligned}$$

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

$$q_m = j h_{v\ell} = j [h_v(T_b) - h_\ell(T_D)] \quad (6-187)$$

where

$$\begin{aligned} j &= \text{vapor mass flux as determined below } (kg/m^2-s), \\ h_{\ell v} &= \text{the difference in specific enthalpies for water vapor} \\ &\quad \text{at the bulk temperature and liquid water at the drop} \\ &\quad \text{temperature } (J/kg). \end{aligned}$$

The mass flux j (kg/m^2-s) at the CS drop surface is approximated by

$$j^{(0)} = K_g M (P_{vb} - P_{vw}) \quad (6-188)$$

where

$$\begin{aligned} K_g &= \text{mass transfer coefficient } (kgmole/s-m^2-Pa), \text{ which is} \\ &\quad \text{calculated from} \\ &= \frac{Sh P D_v}{R T P_{nm} L} \end{aligned} \quad (6-189)$$

where

Sh = Sherwood number,

P = UC bulk pressure (Pa),

D_v = mass diffusivity of vapor in the noncondensable gas [Bir60] (m^2/s),

R = universal gas constant ($Pa \cdot m^3/kgmole \cdot K$),

T = average of T_b and T_D (K),

(6-190)

$P_{nm} = (P_{vb} - P_{vD}) / \ln[(P - P_{vb}) / (P - P_{vD})]$ (Pa) , and

L = characteristic length (m); and

M = vapor molecular weight (kg/kgmole);

P_{vb} = partial pressure of water vapor at the bulk temperature T_b ; and

P_{vD} = saturation pressure at temperature T_D .

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

$$Sh = Nu(Sc/Pr)^{1/3} \quad (6-191)$$

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

Several standard correlations are available in CONTAIN for determining Nu in either forced or natural convection regimes. For forced convection (recall that the droplets are falling through air) around a spherical droplet [Bir60], the Nusselt numbers Nu_c and Nu_m are used. The Nusselt numbers used for calculating the convective and mass transfer heat conduction coefficients are

$$Nu_c = 2.0 + 0.60(Re_c)^{1/2}(Pr_c)^{1/3} \quad (6-192)$$

and

$$Nu_m = 2.0 + 0.60(Re_c)^{1/2}(Pr_m)^{1/2} \quad (6-193)$$

In these equations, Pr is the Prandtl number and Re is the Reynolds number. The preceding sections detail the calculations for components of these equations. Equations (6-185) through (6-193) together specify the approximations used to calculate the mass and heat fluxes to the drops.

The basic assumptions for this model are (1) pseudo-steady-state, ideal gas behavior; (2) equilibrium at the interface between the outside of the water droplet and the surrounding containment air; and (3) complete insolubility of air in water.

6.5.3.10 Iodine Removal Models. This section describes the models used to determine iodine (I_2) and methyl iodide (CH_3I) removal by the CSSs. The initial removal of I_2 by the CSSs 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 in CONTAIN to model the observed late time desorption of iodine with 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.

The depletion rate for iodine is defined as the product of an absorption efficiency (that is, the fractional saturation attained by the drop) 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 provides a simple yet effective way to treat the problem. The user can input the partition coefficient used to calculate the elemental iodine absorption efficiency. The partition coefficient depends on the amount and type of spray additive used. A value of 5000 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 compound methyl iodide (CH_3I) have not been well established. A partition coefficient for this organic iodide has been provided to allow the user to model the removal rate for such relatively inert species. A value of zero is the default.

The FPs removed by sprays, are deposited into the pool of the cell designated by the user. If a pool is not defined, the removed FPs 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 equations used to determine the iodine removal have the same form for the I_2 and the CH_3I removals. The differences are only in the diffusivities of I and CH_3I in steam, air, and liquid water. These are defined at the end of this section. Therefore, the equations that follow will simultaneously refer to both iodine dependent terms by using the subscript I to stand for either I_2 or CH_3I . To obtain the specific equation for either I or CH_3I will only require the use of the appropriate (I or CH_3I) diffusivities.

CONTAIN models iodine removal from the atmosphere by the spray drops during the cell timestep as a first order rate process expressed as

$$\frac{dm_I}{dt} = -m_I N_D IC_{final} \quad (6-194)$$

where

$$\begin{aligned} m_I &= \text{mass of iodine in the atmosphere (kg);} \\ N_D &= \text{number of drops that fall through the cell} \\ &\quad \text{atmosphere during the cell (not the fall) timestep} \\ &\quad \text{(s}^{-1}\text{);} \\ &= W_{sp}/m_D, \text{ and} \\ W_{sp} &= \text{spray mass flow rate (kg/s), and} \\ m_D &= \text{drop mass (kg),} \\ &= \frac{\pi D^3 \rho_\ell}{6}, \\ D &= \text{drop diameter (m), and} \\ \rho_\ell &= \text{liquid water density (kg/m}^3\text{); and} \\ IC_{final} &= \text{the final iodine mass in one drop (after falling)} \\ &\quad \text{divided by the total iodine mass in the} \\ &\quad \text{atmosphere.} \end{aligned}$$

Note that the iodine removal could be excessive if the cell timesteps were large. Therefore, the removal is limited as follows. Equation (6-194) is integrated over the cell timestep Δt_c to produce the following expression for F_I , the ratio of iodine mass removed to the total mass of iodine in the atmosphere:

$$F_I = \frac{\Delta m_I}{m_I} = 1 - \exp(-m_I N_D IC_{final} \Delta t_c) \quad (6-195)$$

This expression provides the control desired because large values in Δt_c will reduce the value of F_I .

The IC_{final} used above is the final value for the iodine mass in the drop per unit mass in the atmosphere after the drop has fallen through the atmosphere, with the drops assumed to initiate their fall with zero iodine mass. The final value for IC is determined by numerical integration over N fall-time increments Δt . The values for Δt are initially taken to be 1/10th of the spray fall time H/v_t , where H is the fall (compartment) height and v_t is the terminal velocity.

In equation form

$$IC_i = IC_N \quad (6-196)$$

where the IC_i are determined from the balance of the mass transfer from the gas phase to the drop surface and the mass transfer from the drop surface to the spray drop interior. Using the implicit method, the balance gives

$$IC_{i+1} = IC_i + S_I \Delta t \left[\frac{PC_I}{V} - \frac{IC_{i+1}}{V_D} \right] \quad (6-197)$$

which is solved to become

$$IC_{i+1} = \frac{IC_i V_D V + S_I PC_I V_d \Delta t}{V_D V + S_I \Delta t V} \quad (6-198)$$

where

$$\begin{aligned} V_D &= \text{drop volume} = \pi D^3/6, \text{ which can change because of} \\ &\quad \text{condensation or evaporation as the drop falls;} \\ V &= \text{atmosphere volume;} \\ S_I &= \text{parameter grouping from the mass transfer balance} \\ &\quad \text{equations,} \end{aligned}$$

$$= \frac{\pi D^2 k_{\ell I} k_{gI}}{PC_I k_{\ell I} + k_{gI}}$$

$$\begin{aligned} k_{\ell I} &= \text{mass transfer (based on mass density} \\ &\quad \text{difference) coefficient (m/s) in the spray} \\ &\quad \text{water for either } I_2 \text{ and } CH_3I, \text{ given below, and} \\ k_{gI} &= \text{mass transfer (based on mass density} \\ &\quad \text{difference) coefficient (m/s) in the gas phase} \\ &\quad \text{for either } I_2 \text{ or } CH_3I \text{ given below; and} \\ PC_I &= \text{user-input partition coefficient.} \end{aligned}$$

The gas phase mass transfer (based on mass density difference) coefficients (m/s) are obtained from

$$k_{gI} = \frac{D_{I,sa}}{D} (2 + 0.6 Re^{1/2} Sc^{1/3}) \quad (6-199)$$

where

$$\begin{aligned} D_{I,sa} &= \text{diffusivity of iodine in a steam-air mixture,} \\ &\quad \text{which is defined below;} \\ D &= \text{drop diameter (m);} \end{aligned}$$

$$\begin{aligned}
\text{Re} &= \frac{v_t D \rho_1}{\mu_a}, \\
v_t &= \text{terminal velocity,} \\
\rho_a &= \text{atmosphere density, and} \\
\mu_a &= \text{atmosphere viscosity; and} \\
\text{Sc} &= \mu_a / (\rho_a D_{I,sa}) .
\end{aligned}$$

The diffusivity of iodine in a steam-air mixture used in Equation (6-199) is

$$D_{I,sa} = \left[\frac{Y_s}{D_{I,s}} + \frac{(1 - Y_s)}{D_{I,a}} \right]^{-1}$$

$$\begin{aligned}
Y_s &= P_{\text{vap}}/P_a, \\
P_{\text{vap}} &= \text{partial pressure of the water vapor} \\
&\quad \text{in the atmosphere, and} \\
P_a &= \text{atmosphere pressure; and} \\
D_{I,s} &= \text{diffusivity in a steam atmosphere at} \\
&\quad \text{temperature } T \text{ and pressure } P \text{ for either } I_2 \\
&\quad \text{(subscript I2 below) or } CH_3I \text{ (subscript MI} \\
&\quad \text{below):}
\end{aligned}$$

$$D_{I2,s} = \frac{3.2801 \cdot 10^{-4} T^{1.5}}{P \left(0.7075 + \frac{454.72}{T} \right)}$$

$$D_{MI,s} = \frac{4.3306 \cdot 10^{-4} T^{1.5}}{P \left(0.7075 + \frac{475.7}{T} \right)}$$

$$D_{I,a} = \text{Diffusivity in air at temperature } T \text{ and pressure } P \text{ for either } I_2 \text{ (subscript I2 below) or } CH_3I \text{ (subscript MI below) are obtained from}$$

$$D_{I2,a} = \frac{2.064 \cdot 10^{-4} T^{1.5}}{P \left(0.7075 + \frac{141.73}{T} \right)}$$

$$D_{MI,a} = \frac{2.6731 \cdot 10^{-4} \cdot T_a^{1.5}}{P_a \left(0.7075 + \frac{148.27}{T_a} \right)}$$

The liquid phase mass transfer (based on mass density difference) coefficients (m/s) are now given.

For iodine,

$$k_{\ell, I_2} = \frac{6.9757 D_{I_2, \ell}}{D} \quad (6-200)$$

where

$$D_{I_2, \ell} = \frac{3.906 \cdot 10^{-11} \cdot T_D}{\mu_{\ell}}$$

T_D = drop temperature, and
 μ_{ℓ} = water viscosity at T_D .

For CHI_3 ,

$$k_{\ell, \text{MI}} = 1.0801 k_{\ell, I_2}$$

7.0 SUMMARY

This report describes the phenomenological equations and the numerical procedures used by the CONTAIN 1.1 code to determine the conditions within nuclear power plant containment during a severe accident. The CONTAIN detailed models provide the capability to mechanistically calculate the containment internal thermal-hydraulic conditions and the amount of radioactive matter that would be released to the environment if there were a leak from the containment. Note that the CONTAIN models can be verified by comparing the code calculations to experimental results. The models described include those to account for the flows of mass and energy between containment compartments, the exchange of energy between the atmosphere and heat structures, the thermodynamic conditions, the distributions of aerosols, the decay and transport of FPs, the deflagration of hydrogen and carbon monoxide, BWR suppression pool behavior, and, ESFs, including a CS, FCs, and an IC. These models are solved with implicit coupling, where appropriate, to obtain a stable and computationally efficient solution.

This manual includes a summary of the validation and assessments performed for CONTAIN. The improvements made to CONTAIN after Version 1.1 are also briefly described. As a result, this reference manual can be used for Versions 1.11 and 1.12, which were released after Version 1.1. All new CONTAIN models will be described in the CONTAIN 1.2 Users Manual.

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APPENDIX A

Description of CONTAIN Models Changed in Versions Beyond CONTAIN 1.1

The CONTAIN code is the product of an ongoing research and code development effort. As a result, new models and correlations are incorporated into the code as they are completed and processed through the CONTAIN quality assurance and testing procedures. These new models are made available to analysts in the form of code revisions. Unfortunately, the time required to create and publish formal documentation, such as this manual, typically exceeds the time required for new code revisions to be completed and released to analysts. Two such releases, CONTAIN 1.11 and CONTAIN 1.12, have occurred since CONTAIN 1.1 was released and the time this document went to print. The purpose of this appendix is to briefly describe the modeling changes that are incorporated into these two new CONTAIN code revisions.

This appendix includes narrative descriptions of modeling improvements, error corrections, and new models for phenomena not previously considered. Unfortunately, inclusion of the governing equations for these new and improved models is beyond the scope of this appendix for reasons of time and resource constraints.

Two CONTAIN revisions have been created between the time CONTAIN 1.1 was released and the time this document went to print. These two revisions, CONTAIN 1.11 and CONTAIN 1.12, were released simultaneously in early 1991 for programmatic reasons. The modeling additions in CONTAIN 1.11 and 1.12 fall into two major categories: model corrections and improvements and new models for previously unconsidered phenomena. The majority of the modeling improvements and bug fixes are in CONTAIN 1.11. CONTAIN 1.12 mostly consists of the addition of the new direct containment heating models.

Model Corrections and Improvements

Material Properties The properties of the standard materials have been heavily revised in CONTAIN 1.11; however, not all of the properties for every material have been revised completely. Also, certain materials will no longer be supported after Version 1.11. Table A-1 indicates the status of materials that have properties that can be completely referenced in 1.11 and are therefore recommended for use.

Moving-Grid Aerosol Growth Model A new moving-grid soluble aerosol condensation model was implemented in CONTAIN 1.11. The new moving-grid technique enhances both the computational and the modeling capabilities of CONTAIN for simulating aerosol particle growth by water vapor condensation. The technique is computationally superior to the fixed-grid method described in Section 4.2 in that numerical diffusion and stiffness are greatly

Table A-1
Materials Recommended for Use in CONTAIN 1.11

aluminum oxide	AL2O3	argon	AR
calcium oxide	CAO	carbon dioxide	CO2
carbon monoxide	CO	concrete	CONC
graphite	GRAPH	helium	HE
hydrogen	H2	ice	H2O
liquid water	H2OL	magnesium oxide	MGO
nitrogen	N2	oxygen	O2
silicon dioxide	SiO2	sodium hydroxide	NAOH
solid iron	FE	solid uranium	U
solid uranium oxide	UO2	stainless steel	SS
titanium dioxide	TiO2	water vapor	H2OV
zirconium	ZR	zirconium oxide	ZRO2

reduced. This improvement, however, does require additional computation time. The new technique improves the modeling capability of CONTAIN by incorporating the solubility and the Kelvin effects on particle growth. These two models are discussed in the Modeling Additions section below.

Heat Conduction The solution algorithm for the heat conduction equation for curvilinear structures (cylinders and spheres) was in error in CONTAIN 1.1. The conduction algorithm was replaced with a completely new heat conduction solver that properly models cylindrical and spherical structures. The new solver also allows for semi-implicit (Crank-Nicholson) time integration as a user option as opposed to the less accurate (but inherently stable) fully implicit method used in CONTAIN 1.1. Unlike the algorithm described in Section 6.4.2.2, the new conduction algorithm supports a variety of new boundary conditions, including constant heat flux, constant temperature, and convective (with user-controlled heat transfer coefficient). Finally, the new conduction solver is intimately integrated with the new concrete outgassing model described later in this appendix.

Heat Conduction Between Cells In a severe accident, both sides of a structure that separates two cells (that is, containment rooms) may be heated, cooled, or exposed to condensing conditions. An inherent limitation of CONTAIN is that condensation and other heat and mass transfer processes are modeled mechanistically only for inner structure surfaces. Therefore, in CONTAIN 1.1 a structure that separates two cells would either have one of its sides not modeled mechanistically or it would be split between the two cells with no path made for thermal communication between the two cells. This limitation is discussed at length in Section 6.3 and 6.4. In CONTAIN 1.11, however, this situation can be handled by connecting together two structures that have their inner surfaces in separate cells. By doing this, heat and mass transfer can be modeled for both sides of the structure mechanistically, and the two cells

involved will still communicate thermally with each other by way of conduction through the coupled structures. This new CONTAIN 1.11 capability was found to have an energy conservation error, which is also in CONTAIN 1.12. This error has been corrected and an update with the correction is available. The new capability should only be used if the error correction is obtained from the CONTAIN code project.

Heat and Mass Transfer The heat and mass transfer models, see Section 6.3, used for condensation/evaporation at structure surfaces, pool surfaces, and in the ice condenser and fan cooler have been improved in CONTAIN 1.11. The main improvement is that a non-zero temperature drop is now modeled across the film. That is, the film to atmosphere interface temperature differs from the surface temperature of the structure. This interface temperature is determined by balancing conduction heat flux through the film against the mass transfer and convection heat transfer fluxes on the atmosphere side of the interface iteratively.

Restart Capabilities CONTAIN 1.11 includes a major enhancement to the restart capability. The restart capabilities have been expanded to allow the user to respecify flow model parameters, engineered safety feature parameters, and hydrogen burn model parameters. The new flow restart features, coupled with the old flow path logic, created a situation where the default initial state (that is, opened or closed) of flow paths was difficult to determine. Consequently, the algorithm for setting the default initial state has also been simplified. For an initial run, with the two exceptions discussed below, it is open. On a restart run, it is always in the same status as at the end of the previous run. Therefore, new input keywords have been added to allow the user to explicitly state whether the flow path is open or closed upon restart.

The first exception occurs when and only when the pressure-dependent flow path opening option (DP) is specified in the flow control block of the initial run. In this instance, the flow path is assumed to be initially closed. This is consistent with CONTAIN's previous treatment of DP (in the FLOW block). The second exception occurs when and only when the flow path opening time (TOPEN) is specified in an initial run. For this case the flow path is also assumed to be initially closed.

Convection Heat Transfer The convection heat transfer model in CONTAIN 1.1 has been improved to incorporate a forced convection correlation based on the velocity corresponding to the intercell flow. As described in Section 6.3.1, the CONTAIN 1.1 model uses a natural convection correlation to determine heat transfer between structures and the atmosphere unless the user specifies the use of a forced convection table for a structure. In the latter case, the larger of the natural or forced convection heat transfer coefficients is used. In CONTAIN 1.11, the heat transfer rate is still computed using the larger of the forced convection heat transfer coefficient and the natural convection coefficient.

However, if user-input tables are not used, the forced convection heat transfer coefficient is determined from the velocities corresponding to the mass flow rates into and out of the cell, utilizing an appropriate averaging scheme. No provisions are included in CONTAIN 1.11 for automatically disabling the forced convection calculation; however, the averaging algorithm is user-controllable. For example, natural convection heat transfer can be imposed by setting the hydraulic area (using the new structure keyword HYDAREA) for each structure to a large value. This will cause the forced convection heat transfer coefficient to always be smaller than the natural convection value.

Lower Cell Improvements The lower cell model has (once again) been extensively revised in CONTAIN 1.11, and a number of problems have been corrected. The two major areas in which improvements have been made are: the treatment of null or transient layers, especially in situations in which a transient pool layer exists only for part of the cell timestep; and the CORCON-MOD2 to CONTAIN interface. A large number of bugs or deficiencies were found for null or transient layers. Most notably, the inability of CONTAIN 1.1 to calculate condensation on cold lower cell layers when a pool is not initially present has been removed in CONTAIN 1.11. Other bugs were found in the proper setting of boundary conditions and heat transfer coefficients for transient pools that do not survive the timestep. A number of problems were found with the CORCON-MOD2 to CONTAIN interface, particularly for transient pools. A potentially serious error in calculating the amount of decay heat in the CORCON-MOD2 layers was corrected. This error occurred in cases in which the CONTAIN DECAY-HT option is invoked along with CORCON-MOD2. The CORCON-MOD2 to CONTAIN interface was also made to be explicitly energy conservative in all situations.

Aerosol Deposition in Pools The aerosol deposition model was modified in CONTAIN 1.11 to include the treatment of gravitational settling into coolant pools. This only includes gravitational forces and does not take coolant fluxes at the atmosphere/pool interface into account.

Improved Aerosol Runge-Kutta Integrator Prior to CONTAIN 1.11, certain situations would cause the Runge-Kutta integrator to attempt to reduce the integration timestep to less than one microsecond when considering conditions of rapid condensation onto aerosols. This resulted in a code abort with an appropriate error message. The abort was intentional to avoid the large CPU time associated with such small timesteps. However, under these circumstances, such small increments are usually only necessary for the first few timesteps. Therefore, the abort is not really necessary. A quick fix for this problem was introduced in the CONTAIN 1.06 Newsletter dated February 28, 1987. In CONTAIN 1.11, the Runge-Kutta integrator allows up to one thousand timesteps smaller than a microsecond. Therefore, with CONTAIN 1.11, the quick fix for the Runge-Kutta code bomb is no longer necessary.

Flexible Shutdown Time for Decay Power Another change introduced in CONTAIN 1.11 is the ability to control the initiation time of the decay models. Provisions have been made to allow for a delay in the activation of the ANSI Makeup Decay Power option and for a time of reactor shutdown other than $t=0$ in the CORCON-MOD2 decay model.

Concrete Ablation Temperatures The default concrete ablation temperatures used by the CORCON-MOD2 code have been modified in CONTAIN 1.11. Formerly, a single value of 1575 K was used for all preset concrete types, even though in some cases this temperature was below the default solidus temperature. The new default temperatures are two-thirds of the way from the default solidus to the liquidus temperatures. The new values are

Concrete Type	T_{solidus}	T_{liquidus}	T_{ablation}
Basalt	1350	1650	1550
CMN Sand/Lime	1420	1620	1590
High Lime	1690	1875	1810
Perlite	1400	1650	1570

Improved Bubble Humidification Model The bubble humidification model described in Section 3.5.2 for the evaporation of coolant into bubbles with noncondensable gas bubbling through pools has been improved in CONTAIN 1.12. The bubble humidification model describes the evaporation of coolant into bubbles of noncondensable gas bubbling through pools. A relatively crude model is used in CONTAIN 1.1 and 1.11 to describe the humidification of gases generated by CORCON-MOD2 and gases vented into the pool through the Safety Relief Valve (SRV) model. (This modeling is already included for suppression vent flow.) The relatively crude model assumes temperature and pressure equilibrium of gas bubbles emerging from the pool top surface in cases in which the vapor content of the bubble is relatively small. The equilibrium temperature is assumed to be the beginning-of-timestep pool temperature. However, for large vapor content, temperature equilibrium is assumed, but the vapor carried in the gas bubble is arbitrarily limited to five times the number of moles of noncondensable gas. A more sophisticated model for gas humidification has been implemented. It assumes temperature equilibration between the bubbles and the pool and 95% vapor saturation of the bubbles at the equilibrium temperature. In contrast to the previous modeling, the equilibrium temperature used is a self-consistent pool temperature that takes into account the evolution of the vapor from the bubble walls. This self-consistency eliminates problems of excessive cooling of shallow pools.

Model Additions

Soluble Aerosol and Kelvin Effect Modeling A new model for aerosol growth by condensation of vapor has been added in CONTAIN 1.11, including the incorporation of solubility and Kelvin effects. The solubility effect lowers the particle water vapor pressure, and

thus enhances particle growth. The Kelvin effect increases the particle water vapor pressure, and thus reduces particle growth. Although these two effects are offsetting, the solubility effect is normally more important than the Kelvin effect for soluble aerosol particles, and the solubility effect does not apply at all to insoluble particles. The Kelvin effect may become significant for particles less than approximately 0.1 μm in diameter.

Direct Containment Heating CONTAIN 1.12 adds direct containment heating (DCH) models to CONTAIN. The foundation of the DCH modeling in CONTAIN 1.12 is a new dispersed debris field that is allowed to have different characteristics and components for each cell. This new field is similar to the gas field in CONTAIN in that for each cell the dispersed debris is treated as a well-mixed repository of material. Masses of the different chemical constituents of the debris present in the containment atmosphere resulting from a high pressure melt ejection (HPME) event are represented in this repository for each cell. One temperature describes the thermodynamic state of the bulk debris field.

A second feature of the DCH models added to CONTAIN is in intercell particle transport. Airborne debris particles are transported along with the gas under a zero slip assumption.

As a third capability, the DCH models in CONTAIN also treat chemical interactions. Chemical reactions can occur in the atmosphere during a DCH event if Zr and/or Fe metal is present and the atmosphere contains oxygen and/or steam.

A fourth element of the 1.12 DCH models in CONTAIN is in the modeling of heat transfer from debris. Three forms of energy exchange are modeled for the dispersed debris: convection to the gas, radiation to the gas, and radiation to structures. Debris radiation to the atmosphere, all structure inner surfaces, the ice condenser, the upper lower cell layer, and the surrounding gas are all modeled.

A fifth feature of the capabilities in CONTAIN 1.12 is debris trapping models. The process of debris removal as a result of interaction with containment structures and/or gravitational fall-out is a process referred to as trapping. This process remains highly uncertain and experiments have shown that particle trapping is subject to scale distortions. A variety of methods for modeling trapping are available in CONTAIN. These models are mostly parametric, although there is some degree of mechanism associated with some of the approaches.

Finally, CONTAIN 1.12 includes a major enhancement of the code's capabilities in modeling cavity phenomena for DCH. The vessel blowdown and debris dispersal modeling code CORDE (Core Debris Ejection Model) has been fully integrated into CONTAIN. In addition, the vessel blowdown and debris entrainment code GASBLOW2 has also been incorporated into CONTAIN. CORDE was developed at Winfrith in the UK, while GASBLOW2 was developed at Sandia National

Laboratories. The addition of these codes gives CONTAIN the ability for mechanistic modeling of vessel blowdown, hole ablation, and debris entrainment/de-entrainment during DCH accident sequences. Recent applications using CONTAIN 1.12, however, have shown that considerable uncertainty remains in our understanding of these processes, even given the availability of these models. Therefore, the ability to perform DCH calculations without using these models has been retained to permit sensitivity studies and the analysis of scaled experiments.

Concrete Outgassing Model A concrete outgassing model was added in CONTAIN 1.11 and later corrected and improved in CONTAIN 1.12. The concrete outgassing model includes the release of evaporable water and bound water and carbon dioxide. The gas release models are not completely mechanistic; however, certain important aspects of the governing physical processes are treated in a relatively rigorous manner.

The evaporable water release model is based on a temperature range for gas release. The outgassing initiation temperature is assumed to be the saturation temperature at the cell pressure. The upper temperature is determined by a user-specified temperature increase from the initiation temperature. The bound gas release is more mechanistic than the evaporable water release model. The bound gas release is described by an Arrhenius rate law. The bound gas release model is limited to the decomposition of only one compound for bound water and another for bound carbon dioxide. For example, the decomposition of $MgCO_3$ and $CaCO_3$, both of which produce carbon dioxide gas, can not be represented by separate Arrhenius rate equations. The user can represent the two reactions with one Arrhenius rate equation by adjusting the rate constant accordingly.

Two significant improvements were made to the outgassing model in CONTAIN 1.12. The first is the addition of an option to specify the destination cell for released gases, which can only occur through the inner surface of the structure. The second change was the implementation of a new algorithm that tracks the outgassing wet/dry interface within the structure as gases are released.

APPENDIX B

CONTAIN Code Validation Summary

The purpose of this appendix is to present the results of the CONTAIN-code validation and assessment reported in Was90. This summary is essentially a copy of the model by model summary presented in Was90.

The CONTAIN code validation and assessment (CV&A) presented in Was90 demonstrated that the CONTAIN code is capable of performing complete containment severe-accident analyses. These analyses can include an accounting for all of the major severe-accident containment phenomena and the interactions between the phenomena. In addition, the capability was validated by the successful prediction with CONTAIN of the time evolution of the experimental data from the following major validation exercises:

- (1) The ABCOVE series, which provided important blind validation of CONTAIN for dry aerosol behavior.
- (2) The German HDR experiments, which were used to validate, in a post-test blind mode, the gas mixing and atmospheric thermal-hydraulic behavior for a large break steam blowdown.
- (3) The LACE experiment series, which recently provided the opportunity to validate both the thermal-hydraulic and the aerosol behavior modeling in CONTAIN.

The discussion below summarizes the overall results of the individual CV&A presented in Section 6.3 of Was90. Note that to make this summary current, the specific information from the individual CV&A were expanded, where appropriate, with information known to represent the current status of CONTAIN. The conclusions regarding the adequacy of CONTAIN for the performance of severe-accident analyses based on the individual CV&A are now presented for each modeling area defined in the Was90 organization.

B.1 Material Properties - This modeling is believed to be adequate, in general, because of the successful use of the properties for the many CV&A calculations performed, the improvements made since the CV&A, and the current capability of CONTAIN that allows the user to add property values.

B.2 Intercell Flow and Atmosphere/Pool Thermal-hydraulics - The area of atmosphere thermodynamics was generally validated by the various calculations performed and the comparisons with other codes. It was observed that the aerosol option should be specified to avoid an unrealistic supersaturated condition. Other specific areas included in this general category are discussed below.

B.2.1 Intercell Flow and Buoyancy - For well-mixed gases, the intercell flow model mass flow rate was found to be acceptable, including the flow resulting from buoyancy created by temperature differences. Specific observations that were made regarding intercell flow were that (a) choked flow through an orifice could be as much as 16% too high, a comparison that could be improved, if desired, by the use of a different flow path density and (b) flow through a long duct may require four or more cells to represent the duct.

The temperature-driven buoyancy calculations were found to be acceptable with the recommendation made that (a) the noding in the vertical direction should be varied to provide assurance that the noding is adequate and (b) the effect of complex geometries on the buoyancy should be investigated. It should be noted that the modeling of buoyancy is very sensitive to details such as (a) the geometry, (b) the noding, and (c) the use of the aerosol and/or the drop-out options, which can affect the existence of liquid drops. The latter specification was found to have dramatic effects in some of the calculation performed and is believed to be the primary potential reason for other unrealistic calculated results.

There remains a need for a better accounting of the separation and stratification of hydrogen. This is needed to identify the possible existence of (a) local areas of high hydrogen concentration, which may lead to detonation and/or (b) high-temperature zones, which may cause the overheating of safety-related instruments.

B.2.2 Coolant Pool Boiling - Only one simple investigation was performed and it verified the code values.

B.2.3 Condensation and Evaporation - The current modeling was found to be generally acceptable. The following recommendations were made: (a) The aerosol option should be used when there is a significant amount of steam so that water drops can form and thereby avoid an unrealistic state of supersaturation. (b) Additional investigation should be made regarding the modeling of the condensation, for example, with regard to the effect of interfacial waves on mass and energy transfers.

B.2.4 Heat Conduction and Concrete Outgassing - The heat conduction and the outgassing models are now considered acceptable based on the CV&A and recent improvements to CONTAIN.

B.2.5 Radiation Heat Transfer - Gas-mixture thermal radiation emissivity modeling was found to be quite acceptable. However, the need was identified to improve the modeling of debris (for DCH scenarios) and aerosol clouds, including the effects of scattering and absorption.

B.2.6 Hydrogen Burning - Only single pulsed burns were investigated and the modeling was found to be generally acceptable. However, the need for improvement was identified with regard to the fraction of hydrogen burned, the burn time and the effect of dilutents.

Also, consideration should be given to the addition of the capability of modeling continuous burning, deflagration to detonation transition, and the potential for detonation. Note that the CONTAIN models are obtained from the HECTR code, where the models are improved as new experimental or analytical information becomes available.

B.3 Aerosol Behavior (including LACE) - This modeling of the overall aerosol behavior was strongly confirmed. Of particular note is validation by the LACE experiments of the newly added modeling to include accounting for the solute effect and surface tension (Kelvin) effect in the condensation on and evaporation from aerosols, and a new numerical method with a moving grid for the solute model.

B.4 Fission Product Behavior - With the exception of the decay process, this modeling is very dependent on user input and, therefore, not amenable to validation. Some basic modeling features were confirmed by hand calculations.

B.5 Corium-Concrete Interaction - There were no CV&A for this modeling accounted for in this report. It is recommended that reference be made to the literature related to the development and validation of the CORCON-MOD2 code.

B.6 Engineered Safety Features (e.g., Ice Condensers) - The general capability to model the effect of sprays on radionuclide was demonstrated with one CV&A. Model validation is needed for the other ESF features, such as, the fan cooler, pumps, and heat exchangers.

Ice-condenser modeling was qualitatively confirmed by comparison with test results. The CONTAIN ice-condenser modeling could be validated more extensively by comparison of CONTAIN calculated results with those from other established codes, such as, the CONTENPT4/Mod6 and the COMPARE codes or experimental data.

B.7 BWR Models - There were no comparisons with test results. An integral calculation was performed. The CONTAIN BWR modeling could be validated more extensively by comparison of CONTAIN calculated results with those from other established codes, such as, the CONTENPT/LT28 code and experimental data.

B.8 Direct Containment Heating - The general debris chemical reaction modeling was found to be acceptable. However, it was recommended that improvements be made in the accounting of (a) the effect of the debris cloud on radiation and oxygen availability and (b) the effect of debris-structure interaction to cause removal of the debris from the flow field. Note that the CONTAIN 1.12 version has improved capability to model cavity entrainment and the determination of debris particle size. However, these modeling features are yet to be validated. A more detailed assessment of the DCH models has recently been performed and is documented in a letter report to the US Nuclear Regulatory Commission [Ost91].

References

- Ost91 R. W. Ostensen, R. O. Griffith, K. E. Washington, and D. C. Williams, "Models and Correlations for Direct Containment Heating," FIN A1198, Task 1.1, Letter Report enclosed in letter to Dr. Allen Notafrancesco (Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission) from Raymond W. Ostensen (Sandia National Laboratories), Albuquerque, NM, March 15, 1991.
- Was90 K. E. Washington and R. G. Gido, "CONTAIN Developmental Assessment," FIN A1198, Task 3, Letter Report enclosed in letter to Dr. Allen Notafrancesco (Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission) from Richard G. Gido (Sandia National Laboratories), Albuquerque, NM, October 22, 1990.

APPENDIX C

Explicit Flow Option

This appendix has two sections. The first section details the use of the explicit flow option for intercell flow calculations. The second part describes the self-consistent pressure and temperature thermodynamic states as related to the explicit flow option.

The explicit flow option in CONTAIN became obsolete because of its lesser computational efficiency in comparison to the implicit flow option (see Section 3 of this manual). In addition, the explicit flow option is only applicable to the regular flow path and cannot make use of the more flexible engineered vent flow paths. Because of these limitations, the user is advised to use the implicit flow option as described in Section 3. This appendix provides information regarding the explicit flow option for user reference.

C.1 Thermal-Hydraulic State

Similar to the implicit flow option, the explicit flow option requires a thermodynamic state iteration to get a correct cell temperature and pressure before flow calculation can start. The flow diagrams in Figures C-1 to C-3 show the necessary thermal-hydraulic calculations as performed in the explicit flow model.

Figure C-1 depicts all upper cell (UC) atmospheric flow models which use the explicit flow option. Thus, this option can be used with the quasi-steady, inertial, and quiescent regimes (see Section 3). Note that the critical flow model is not applicable to the explicit flow option.

The explicit flow model operates by explicitly calculating the time derivatives,

$$\frac{dm}{dt}, \frac{dU}{dt}, \text{ and } \frac{dW}{dt}$$

for the mass, energy, and momentum conservation equations, respectively. These equations are presented in Tables 1-1, 1-2, and 1-3 of this manual. Given these derivatives evaluated at a given point in time, a Runge-Kutta integrator is used to solve for the masses and internal energies at the end of the desired timestep. CONTAIN uses a standard fourth order integrator. This integrator divides the timestep into smaller time increments based on the magnitude of the derivatives. These smaller time increments are referred to as Runge-Kutta timesteps and are not visible to or controllable by the user.

If the quasi-steady flow option is used, dW/dt is taken to be zero and the mass flux W can be solved for directly. Therefore, the number of equations solved by the Runge-Kutta integrator is reduced

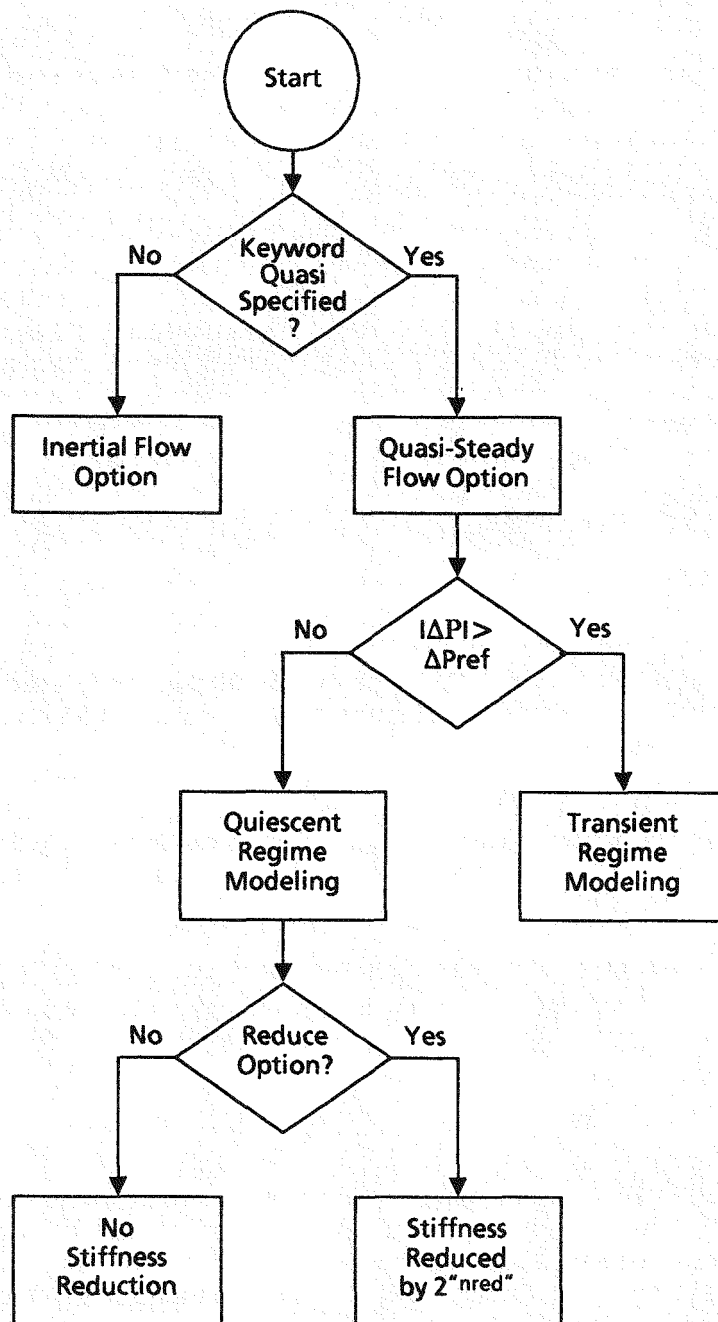


Figure C-1. CONTAIN 1.1 Explicit Flow Options

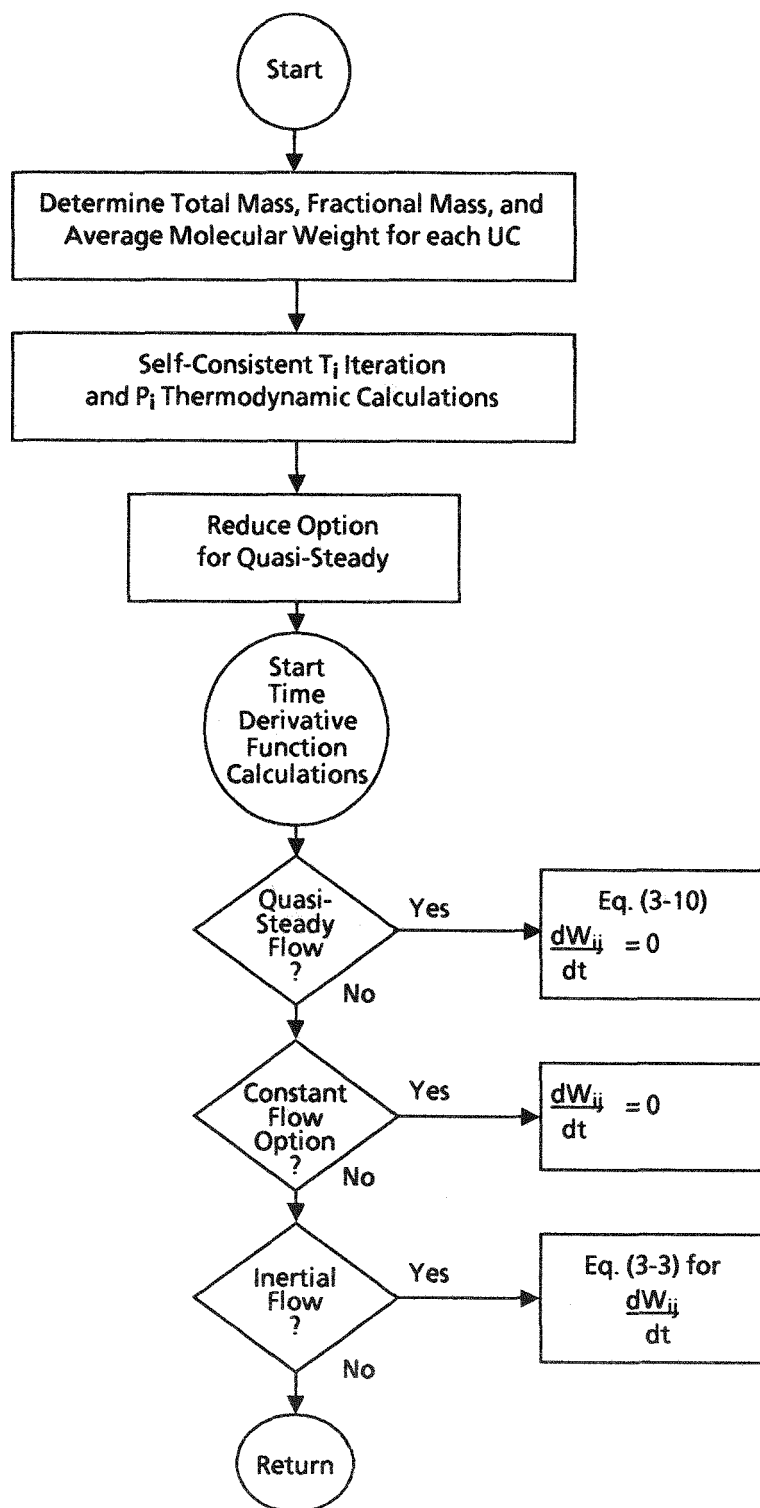
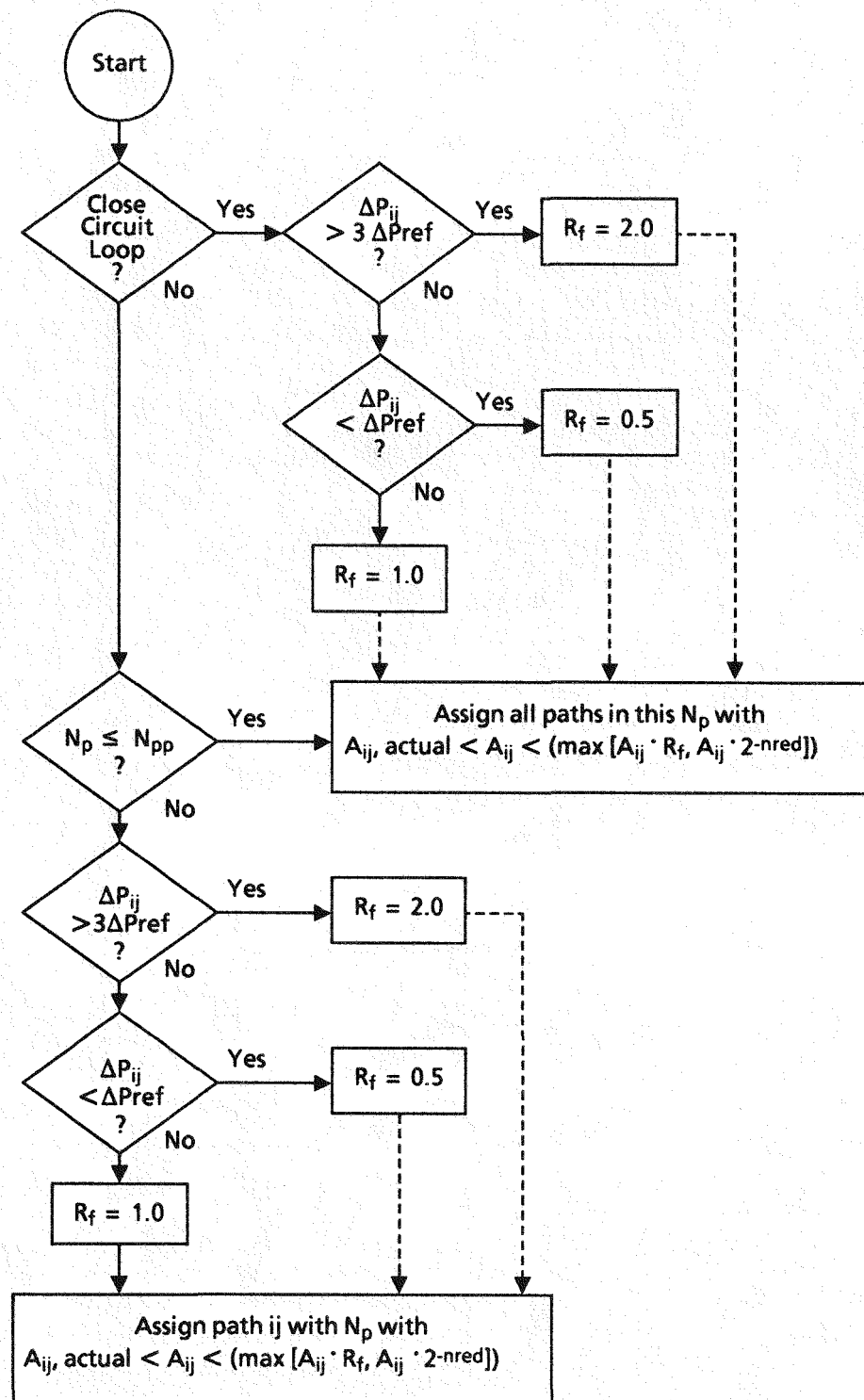


Figure C-2. Time Derivative Calculations for the Runge-Kutta Integration



ΔP_{pref} = User-defined maximum ΔP_{ij} for area reduction calculation (P_d),
 ΔP_{ij} = $P_i - P_j$ (P_d), R_f = area multiplier, N_p = flow path number, and
 N_{pp} = Close circuit flow path number

Figure C-3. Flow Chart for the Reduce Option

to include only dm/dt and dU/dt for the known flow rate W in the quasi-steady case.

The REDUCE option may be used in the explicit flow model to control the stiffness associated with quasi-steady flow where the pressure differential between the flow path ij , ΔP_{ij} is small. Thus the REDUCE option allows the user to artificially adjust the flow area within the bounds to be described later.

Figure C-2 is a flow chart for the time derivative calculations of the Runge-Kutta Integrator. The total mass, fractional masses, and average molecular weights are first determined. Then the self-consistent thermodynamic calculations are made to determine if the temperature iterations converge consistently for each atmospheric UC (see Section C.2).

Upon the completion of such an iteration, the REDUCE option can then be invoked under user control for the quasi-steady flow calculation. If invoked, it will allow the flow areas to be adjusted artificially, so that relatively slow changing flow rates (within a cell timestep) can be changed with respect to the cell and Runge-Kutta timesteps, to ensure accurate and stable Runge-Kutta numerical solutions to the flow differential equations. (This REDUCE process is equivalent, but it uses a reverse method, which generally uses small timesteps for numerically solving differential equations with fast rise and/or fall time outputs.) Additional details on how CONTAIN handles numerical stiffness in the REDUCE user option is given below.

The stiffness calculation of the REDUCE user option is presented in Figure C-3. The network of cells and flow paths is examined in the closed circuit loop test to determine the connectivity in terms of serial and parallel paths. Figure C-4 shows such a network. A path is indicated by a pair of numbers (i,j) . In Figure C-4, $(1,2)$ and $(4,5)$ are serial paths. In addition, two sets of parallel-connected (closed circuit) paths are available: $(2,3)$, $(2,4)$, $(3,4)$ and $(5,6)$, $(5,7)$, $(6,7)$. Recall that the purpose of this option is to overcome stiffness in solving flow equations.

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 ΔP_{ij} , 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 $\Delta P_{ij} < \Delta P_{ref}$, decrease flow area by a factor of 2 ($R_f=0.5$);
- if $\Delta P_{ref} < \Delta P_{ij} < 3 \Delta P_{ref}$, keep the area the same ($R_f=1$); and

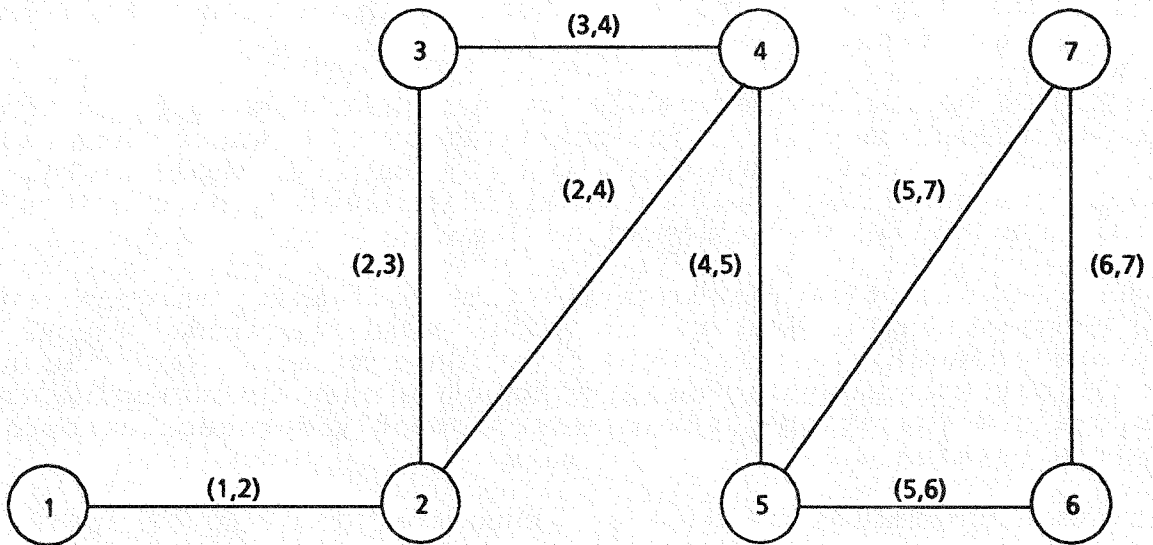


Figure C-4. Network of Cells Connected by Series and Parallel (Closed Circuit) Flow Paths

- if $3 \Delta P_{\text{ref}} < \Delta P_{ij}$, increase flow area by a factor of $2^{(R_f=2)}$.

The areas are reduced at most by a factor of $2^{\text{"nred"}}$ where "nred" is user-specified. The default value for "nred" is zero. The areas are not increased beyond their normal size.

The serial and parallel flow connection branches in Figure C-3 use the above prescriptions for artificially adjusting flow areas to assist in solving stiff flow equations.

The equation for the artificially adjusted flow areas A_{ij} for both series and parallel flow connections in the flow path ij is given by

$$A_{ij} = \max \left[(R_f)(A_{ij}), (A_{ij})(2)^{-\text{nred}} \right] \quad (\text{C-1})$$

where

- max = maximum value of the two area options inside the brackets,
- A_{ij} = the actual flow path area that connects cell i to cell j , and
- nred = a user-defined area reduction number.

Upon completion of the REDUCE user option step for the quasi-steady flow calculations, the mass, energy, and mass flux time derivatives are evaluated. For both the quasi-steady flow model, which uses Equation (3-9), and the user-defined constant flow option, the mass flux time derivatives dW/dt are set to zero. However, the time

derivative calculations for the inertial flow model (Equation 3-3) is used for calculating dW_{ij}/dt . These time derivatives are used by the Runge-Kutta integrator to advance the mass, energy, and flux forward in time.

The quasi-steady flow model is controlled by a linear flow coefficient C_{LFC} , and the flow resistance, as used by the inertial flow model, is controlled by a turbulent flow coefficient C_{FC} . The modeling of the flows in the quasi-steady flow option distinguishes, for practical reasons, between two different flow regimes expected in containment analysis, the transient regime and the quiescent regime. 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 can set the value of C_{LFC} through the ΔP_{ref} , which is the pressure difference at which the flow resistance will cross over from turbulent to laminar. By definition, when $|\Delta P_{ij}|$ is equal to ΔP_{ref} , the two terms in Equation 3-9 are equal. It follows that

$$C_{LFC} = [\Delta P_{ref} C_{FC} / 2 \rho_{ij} A_{ij}]^{1/2} \quad (C-2)$$

where C_{FC} , ρ_{ij} , and A_{ij} are all defined in Section 3.3.2.2.

At much smaller pressure differences the laminar term will dominate, while at much larger pressure differences the turbulent term will dominate. The default value for the crossover point ΔP_{ref} is 1000 Pa.

The artificial laminar flow resistance term means that, in general, the flow resistance will not be modeled accurately for pressure differences less than ΔP_{ref} . Two questions arise here: 1) What is the magnitude of the flow into a given cell? 2) What is 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, ΔP_{ref} . Therefore, ΔP_{ref} should be set to a value that is negligible compared to the pressure within the cells.

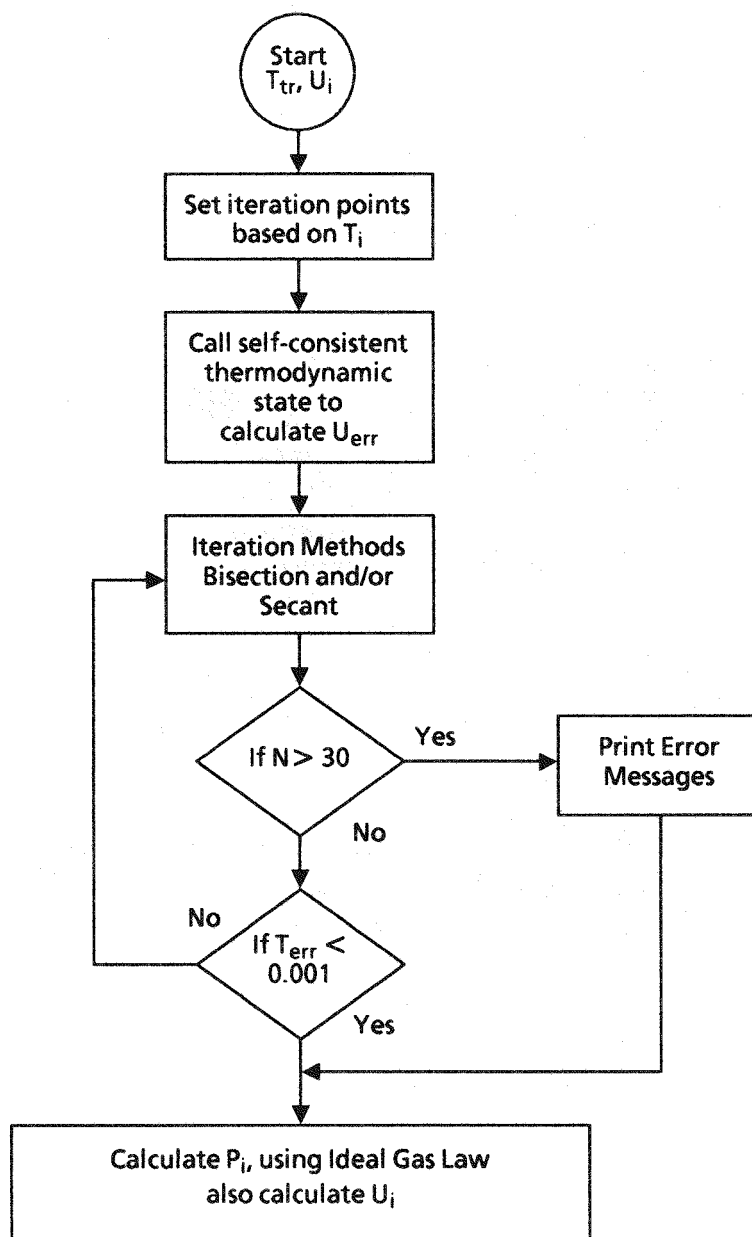
The desired level of accuracy in the pressure calculation is problem-dependent, but consideration should be given to the sensitivity to pressure of pressure-dependent processes within the cell. In particular, ΔP_{ref} should have a negligible effect on the source rate to the atmosphere.

The driving pressure that can be developed by certain sources could be much smaller than the default value of ΔP_{ref} . 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 ΔP_{ref} were reduced to the extent required to handle buoyancy pressures. For this reason, buoyancy effects are not modeled in the explicit flow option.

C.2 Self-Consistent Thermodynamic State

For the explicit flow option, an iteration is used to determine the thermodynamic state of cell temperature. The purpose of this calculation is to determine the atmospheric temperature from atmospheric internal energy and then calculate the cell pressure from the gas atmosphere temperature. Figure C-5 shows how this temperature and its corresponding pressure are calculated. The resulting pressure is then used to calculate the derivatives used in the Runge-Kutta integrator as described earlier. Figure C-5 illustrates the relationship between pressure and temperatures in the explicit flow model.

The iteration begins by selecting two temperature points T_1 and T_2 . The self-consistent thermodynamic state calculation is then performed for ΔU_1 and ΔU_2 using T_1 and T_2 and other atmospheric parameters. Changes in atmospheric internal energy ΔU_1 and ΔU_2 are calculated, respectively, at the temperatures T_1 and T_2 , between consecutive timesteps. Next, the bisection numerical method tries to solve for the saturation temperature point as a function of the internal energy change of the atmospheric UC. The bisection method then iteratively solves for the saturation temperature $T_{\text{sat}} = T_{\text{gas}}$ for an atmospheric UC, by straddling the $\Delta U_i = f(T_{\text{tr}})$ curve with two temperatures T_1 and T_2 determining when $\Delta U_{\text{uc}} = 0$. So, CONTAIN must determine when $\Delta U_i < 0$, that is a change in sign.



T_{tr} = Trial cell temperature (K) for cell i , U_i = Actual total internal energy (J) for cell i ,
 U_{err} = Internal energy error based on T_{tr} and U_i , N - number of iterations,
 T_{err} = Cell temperature error (K), and P_i = Pressure (Pa) for cell i .

Figure C-5. Flow Chart for Self-Consistent Thermodynamic States

The new estimate for T_{tr} is computed using

$$T_{tr} = \frac{T_1 + T_2}{2} \quad (C-3)$$

An error message will be printed if the number of iterations exceeds 30 or if the change in total internal energy for two consecutive passes in the secant solver equals zero.

Finally, the self-consistent pressure and specific enthalpy for each atmospheric UC are determined from the iterated temperature T_{tr} . The pressure for cell i is determined from the ideal gas law and the water vapor partial pressure:

$$P_i(T_{tr}) = \sum_{j=1}^{N_{nc}} \frac{R m_j T_{tr} V_i}{M_j} + P_{wv}(T_{tr}) \quad (C-4)$$

where

m_j = mass (kg) of the noncondensable gas j ,
 R = universal gas constant,
 T_{tr} = iterated temperature (K) for cell i ,
 V_i = volume (m^3) for cell i ,
 M_j = molecular weight (kg/kgmole) of noncondensable gas j ,
 P_{wv} = water vapor pressure (Pa), and
 N_{nc} = total number of noncondensable gases.

P_{wv} in Equation (C-4) is also calculated according to the ideal gas law as

$$P_{wv}(T_{tr}) = \frac{X m_w R T_{tr}}{M_w} V_i \quad (C-5)$$

where

X = water vapor fraction,
 m_w = total water mass in the atmosphere (kg), and
 M_w = molecular weight of water (kg/kgmole).

For cell i , the atmospheric specific enthalpy is given by:

$$h_i = \frac{U_i + P_i V_i}{m_{atm}} \quad (C-6)$$

where

U_i = total internal energy in the cell (J), and
 m_{atm} = total gas mass in the atmosphere (kg).

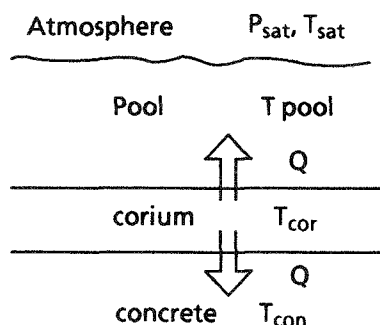
APPENDIX D

Implicit Lower Cell Pool Boiling Model

This appendix briefly describes the implicit lower cell (LC) pool boiling model and its interaction with the implicit flow option described in Section 3.3.2.5. CORCON-MOD2 heat transfer correlations used in the LC pool boiling are also described.

As illustrated in Figure D-1, if the CORCON-MOD2 module is not involved, only heat transfer from the corium to the pool and to the concrete is calculated. A heat conduction solver for the LC, which uses the CORCON-MOD2 heat transfer coefficient and boiling curve, performs a one-dimensional heat conduction calculation. It calculates the amount of energy transferred to allow T_{pool} to reach T_{sat} . Any additional energy transferred is stored until the end of the system timestep. Then, this excess energy is passed to the intercell flow model solver (see Section 3) for the calculation of the amount of pool mass to be boiled (or flashed). (The explicit LC pool boiling is not discussed here because it is not calculated in the intercell flow model.) If CORCON-MOD2 is invoked, the LC heat conduction calculation is ignored and the result from CORCON-MOD2 is given to the implicit flow solver. The important equations from the CORCON-MOD2 code for pool heat transfer calculations are presented below.

General CORCON-MOD2 heat transfer correlations used for the LC pool boiling are described in this appendix. Although CORCON-MOD2 is designed for the situation when a core-concrete interaction occurs, CONTAIN also uses CORCON-MOD2 heat transfer correlations to calculate the amount of boiling in a pool if any, without any core-concrete interaction.



P_{sat} = saturation pressure
 T_{sat} = saturation temperature
 T_{cor} = temperature corium
 T_{con} = temperature concrete
 Q = heat transfer

Figure D-1. Pool Boiling

For the implicit flow option, as described in Section 3.3.2.5, pool boiling in the LC is first calculated using CORCON-MOD2 correlations. The information is then passed to the implicit flow option for the implicit pool boiling calculation. CONTAIN uses the CORCON-MOD2 boiling model with both the CORCON-MOD2 and pool boiling models in the LC. In CORCON-MOD2, the pool is located above the core debris layer, and the concept of boiling off a horizontal flat plate is assumed. The CORCON-MOD2 correlations model all regimes of heat transfer from a pool.

The heat transfer correlations described in this appendix are those equations presented in the CONTAIN code. CONTAIN calculates the heat transfer coefficient and heat flux between the pool and the heating surface for boiling calculations.

CORCON-MOD2 uses a fit for calculating the saturation temperature T_{sat} (K) of pool water as a function of pool pressure (Pa):

$$T_{\text{sat}}(P_p) = 43.15 - \frac{3880.4}{\ln \left[\frac{P_p}{1.292 \cdot 10^{10}} \right]} \quad (\text{D-1})$$

For nonboiling convective limits (temperature of the heating surface $T_s \leq T_{\text{sat}}$), the convective heat transfer coefficient and the pool heat flux are given as:

$$h_{\text{nb}} = \frac{k_l(\bar{T}) Nu_{\text{nb}}}{L} \quad (\text{D-2})$$

where

h_{nb} = nonboiling convective heat transfer coefficient,
 $k_l(\bar{T})$ = thermal conductivity of water at $\bar{T}$ (W/m-K),
 L = characteristic length as user-specified (m),
 Nu_{nb} = Nusselt number of nonboiling, and
 $\bar{T}$ = arithmetic average temperature of T_s and T_p , the pool temperature (K).

Nu_{nb} in Equation D-2 is given by

$$Nu_{\text{nb}} = \max(2.0, Nu_{\text{lam}}, Nu_{\text{turb}}, Nu_{\text{bnl}}) \quad (\text{D-3})$$

where

$\max$ = maximum values of the quantities inside the parentheses,
 Nu_{lam} = Nusselt number for laminar conditions,

Nu_{turb} = Nusselt number for turbulent conditions, and
 Nu_{bnl} = Nusselt number for liquid/liquid heat transfer with bubble agitation.

Nu_{lam} in Equation D-3 is calculated as

$$Nu_{lam} = 0.54 Ra^{1/4} \quad (D-4)$$

where

Ra = Rayleigh number, and given as

$$Ra = (3.9 + 0.06 [\bar{T} - 313]) \cdot 1.0 \cdot 10^{-4} \cdot g L^3 \rho_\ell^2(\bar{T}) c_{p\ell}(\bar{T}) \cdot \left| \frac{T_s - T_p}{\mu_\ell(\bar{T}) - K_\ell(\bar{T})} \right| \quad (D-5)$$

where

g = acceleration of gravity (9.8 m/s^2),
 ρ_ℓ = water density evaluated at $\bar{T}$ (kg/m^3),
 $c_{p\ell}$ = specific heat of water evaluated at $\bar{T}$ (J/kg-K), and
 μ_ℓ = viscosity of water evaluated at $\bar{T}$ (N-s/m^2)

Nu_{turb} in Equation D-3 is calculated as

$$Nu_{turb} = 0.14 Ra^{1/3} \quad (D-6)$$

Nu_{bnl} in Equation D-3 is given by

$$Nu_{bnl} = \frac{L h_{bnl}}{K_\ell(T_p)} \quad (D-7)$$

where

h_{bnl} = heat transfer coefficient for liquid/liquid transfer with gas agitation ($\text{W/m}^2 \cdot \text{K}$), and it is given by

$$h_{bnl} = \frac{5.05 k_\ell(T_p) Re^{0.5} Pr^{0.8}}{d_b} \quad (D-8)$$

where

Re = Reynolds number evaluated at T_p ,
 Pr = Prandtl number evaluated at T_p , and
 d_b = bubble diameter (m).

Re and Pr in Equation D-8 are defined as

$$Re = \frac{\rho_l(T_p) v_s d_b}{\mu_l(T_p)} \quad (D-9)$$

and

$$Pr = \frac{\mu_l(T_p) c_{pl}(T_p)}{K_l(T_p)} \quad (D-10)$$

where v_s is the superficial velocity of the bubble (m/s).

Based on h_{nb} calculated from Equation D-2, the pool heat flux, q_{pool} is calculated as

$$q_{pool} = h_{nb}(T_s - T_p) \quad (D-11)$$

For nucleate boiling and other parts of the boiling regimes, $T_s > T_{sat}$. CONTAIN models two heat fluxes and temperature differences for CORCON-MOD2. By using the Zuber-Rohsenow correlation at the departure to nucleate boiling, q_{DNB} and ΔT_{DNB} are given as

$$q_{DNB}(P_{bar}) = \frac{1.50 \cdot 10^6 P_{bar}^{0.415}}{1 + 5.97 \cdot 10^{-3} P_{bar}^{1.117}} \quad (D-12)$$

and

$$\Delta T_{DNB}(P_{bar}) = C_{sf} \frac{1.17 \times 10^3 P_{bar}^{-0.112}}{1 + 7.02 \times 10^{-8} P_{bar}^{3.181}} \quad (D-13)$$

where

q_{DNB} = heat flux at departure of nucleate boiling,
 P_{bar} = pool pressure in bars (1 bar = $1 \cdot 10^5$ Pa),
 ΔT_{DNB} = temperature difference at departure to nucleate boiling, and
 C_{sf} = surface coefficient, which is equal to 0.01.

For the Leidenfrost point (minimum film boiling) in the boiling regime, the heat flux and temperature difference are given as

$$q_{\text{Leid}}(P_{\text{bar}}) = \frac{1.88 \cdot 10^4 P_{\text{bar}}^{0.894}}{1 + 7.58 \cdot 10^{-3} P_{\text{bar}}^{0.956}} \quad (\text{D-14})$$

and

$$\Delta T_{\text{Leid}}(P_{\text{bar}}) = \frac{8.56 P_{\text{bar}}^{0.848}}{1 + 0.138 P_{\text{bar}}^{0.75}} \quad (\text{D-15})$$

where

q_{Leid} = heat flux at Leidenfrost point, and
 ΔT_{Leid} = temperature difference at Leidenfrost point.

For subcooled nucleate boiling in which $T_p < T_{\text{sat}}$, then

$$q_{\text{pool}} = C_{\text{Ivey}} q_{\text{DNB}} \quad (\text{D-16})$$

and

$$\Delta T_{\text{pool}} = \Delta T_{\text{DNB}} C_{\text{Ivey}}^{1/3.03} \quad (\text{D-17})$$

where

$$\begin{aligned} C_{\text{Ivey}} &= \text{Ivey factor, which is defined as} \\ &= 1.0 + \frac{4.77 \cdot 10^{-2} P_{\text{bar}}^{-0.683}}{1 - 6.29 \cdot 10^{-3} P_{\text{bar}}^{0.862}} \end{aligned} \quad (\text{D-18})$$

For saturation and supersaturation boiling ($T_p \geq T_{\text{sat}}$), both Zuber-Rohsenow and Leidenfrost correlations are used.

For nucleate boiling,

$$\Delta T_{\text{sat}} \leq \Delta T_{\text{DNB}} \quad (\text{D-19})$$

where

ΔT_{sat} = temperature difference between the pool and saturation.

Thus, the heat flux across the surface q and heat transfer coefficient h are based on the following heat fluxes:

$$q_{\text{conv}} = h_{\text{nb}} (T_s - T_p) \quad (\text{D-20})$$

and

$$q_{\text{pool}} = q_{\text{DNB}} (\Delta T_{\text{sat}} / \Delta T_{\text{DNB}})^{3.03} \quad (\text{D-21})$$

where

$$\begin{aligned} q_{\text{conv}} &= \text{convective heat flux calculated using } h_{\text{nb}} \text{ calculated from Equation D-2, and} \\ q_{\text{pool}} &= \text{heat flux being corrected with saturation and departure nucleate boiling for } q_{\text{DNB}} \text{ is calculated in Equation D-12.} \end{aligned}$$

Therefore,

$$\left. \begin{aligned} q &= q_{\text{pool}} \\ h &= 3.03 \cdot q_{\text{pool}} / \Delta T_{\text{sat}} \end{aligned} \right\} \text{for } q_{\text{pool}} > q_{\text{conv}} \quad (\text{D-22})$$

and

$$\left. \begin{aligned} q &= q_{\text{conv}} \\ h &= h_{\text{nb}} \end{aligned} \right\} \text{for } q_{\text{pool}} \leq q_{\text{conv}} \quad (\text{D-23})$$

For film boiling in which $\Delta T_{\text{sat}} \geq \Delta T_{\text{Leid}}$, the following are defined:

$$T_{\text{Leid}} = T_{\text{sat}} + \Delta T_{\text{Leid}} \quad (\text{D-24})$$

and

$$\sigma_{\text{eff}} = \frac{\sigma}{\frac{1}{\epsilon_p} + \frac{1}{\epsilon_s} - 1} \quad (\text{D-25})$$

where

$$\begin{aligned} T_{\text{Leid}} &= \text{Leidenfrost temperature,} \\ \sigma_{\text{eff}} &= \text{effective radiation constant,} \\ \sigma &= \text{Stefan-Boltzman constant (W/m}^2\text{-K}^4\text{),} \\ \epsilon_p &= \text{emissivity of the pool (0.94), and} \\ \epsilon_s &= \text{emissivity of the heating surface.} \end{aligned}$$

The Leidenfrost radiation heat flux q_{rLeid} is given by

$$q_{rLeid} = \sigma_{eff} (T_{Leid}^4 - T_{sat}^4) \quad (D-26)$$

The convective heat flux in the absence of radiation q_c is given by

$$q_c = q_{Leid} \left(\frac{[q_{Leid} - q_{rLeid}] \Delta T_{sat}}{q_{Leid} \Delta T_{Leid}} \right)^{0.75} \quad (D-27)$$

The radiation heat flux q_{rad} is given by

$$q_{rad} = \sigma_{eff} (T_s^4 - T_{sat}^4) \quad (D-28)$$

Thus, the total film boiling heat flux, taking into account the Leidenfrost transfer and radiation, is calculated as

$$q_{tot} = q_c + q_{rad} \quad (D-29)$$

As a result of radiation inclusion, Leidenfrost quantities are no longer constant. To calculate q_{tot} in Equation D-29 correctly, a Newton iteration method is employed to solve

$$q_{tot} = q_c \left(\frac{q_c}{q_{tot}} \right)^{1/3} + q_{rad} \quad (D-30)$$

For regimes between departure to nucleate boiling and critical heat flux point in which $\Delta T_{sat} < \Delta T_{DNB}$, both heat flux q and heat transfer coefficient h are interpolated as

$$q = q_{DNB} \left(\frac{q_{Leid}}{q_{DNB}} \right)^{C_x} \quad (D-31)$$

and

$$h = q \ln \frac{\left(\frac{q_{Leid}}{q_{DNB}} \right)}{\Delta T_{Leid} - \Delta T_{DNB}} \quad (D-32)$$

where

$$C_x = \frac{\Delta T_{\text{sat}} - \Delta T_{\text{DNB}}}{\Delta T_{\text{Leid}} - \Delta T_{\text{DNB}}} \quad (\text{D-33})$$

For more details about any correlations presented in this appendix, the reader is referred to the CORCON-MOD2 user's manual (Reference Col84 in Section 8 of this manual).